



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:15 PM UTC

PDB ID : 4A0K / pdb_00004a0k
Title : STRUCTURE OF DDB1-DDB2-CUL4A-RBX1 BOUND TO A 12 BP ABA-SIC SITE CONTAINING DNA-DUPLEX
Authors : Fischer, E.S.; Scrima, A.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-09
Resolution : 5.93 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

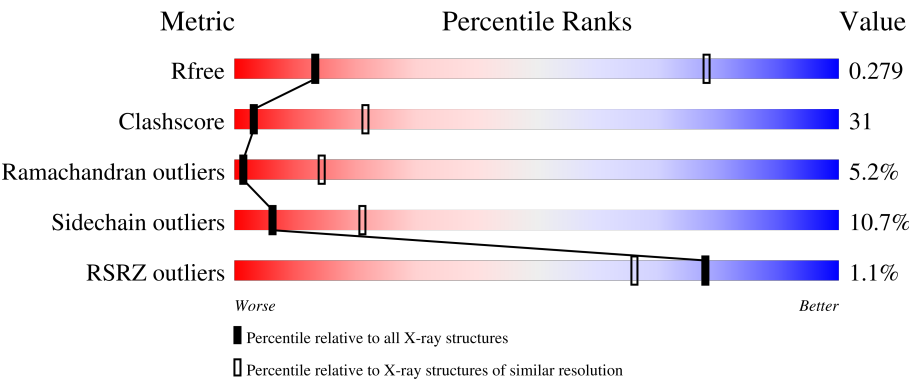
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 5.93 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1137 (7.88-4.00)
Clashscore	190562	1203 (7.88-4.00)
Ramachandran outliers	187476	1028 (7.88-4.00)
Sidechain outliers	187428	1018 (7.88-3.98)
RSRZ outliers	180081	1130 (7.88-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	742	3% 32% 46% 17% • •
2	B	117	8% • 5% • 82%
3	C	1159	62% 25% 8% • 5%
4	D	382	% 74% 15% • • 7%
5	E	12	83% 17%

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Mol	Chain	Length	Quality of chain
6	F	12	58% 42%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17885 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CULLIN-4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	719	5809	3692	1007	1076	34	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP Q13619
A	19	HIS	-	expression tag	UNP Q13619
A	20	HIS	-	expression tag	UNP Q13619
A	21	HIS	-	expression tag	UNP Q13619
A	22	HIS	-	expression tag	UNP Q13619
A	23	HIS	-	expression tag	UNP Q13619
A	24	HIS	-	expression tag	UNP Q13619
A	25	VAL	-	expression tag	UNP Q13619
A	26	ASP	-	expression tag	UNP Q13619
A	27	GLU	-	expression tag	UNP Q13619
A	28	GLU	-	expression tag	UNP Q13619
A	29	ASN	-	expression tag	UNP Q13619
A	30	LEU	-	expression tag	UNP Q13619
A	31	TYR	-	expression tag	UNP Q13619
A	32	PHE	-	expression tag	UNP Q13619
A	33	GLN	-	expression tag	UNP Q13619
A	34	GLY	-	expression tag	UNP Q13619
A	35	GLY	-	expression tag	UNP Q13619
A	36	GLY	-	expression tag	UNP Q13619
A	37	ARG	-	expression tag	UNP Q13619

- Molecule 2 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	21	184	126	32	26	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP P62877
B	-7	HIS	-	expression tag	UNP P62877
B	-6	HIS	-	expression tag	UNP P62877
B	-5	HIS	-	expression tag	UNP P62877
B	-4	HIS	-	expression tag	UNP P62877
B	-3	HIS	-	expression tag	UNP P62877
B	-2	HIS	-	expression tag	UNP P62877
B	-1	VAL	-	expression tag	UNP P62877
B	0	ASP	-	expression tag	UNP P62877
B	1	GLU	-	expression tag	UNP P62877
B	2	GLU	-	expression tag	UNP P62877
B	3	ASN	-	expression tag	UNP P62877
B	4	LEU	-	expression tag	UNP P62877
B	5	TYR	-	expression tag	UNP P62877
B	6	PHE	-	expression tag	UNP P62877
B	7	GLN	-	expression tag	UNP P62877
B	8	GLY	-	expression tag	UNP P62877
B	9	GLY	-	expression tag	UNP P62877
B	10	GLY	-	expression tag	UNP P62877
B	11	ARG	-	expression tag	UNP P62877

- Molecule 3 is a protein called DNA DAMAGE-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	1105	Total	C	N	O	S	0	0	0
			8605	5460	1442	1657	46			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-18	MET	-	expression tag	UNP Q16531
C	-17	HIS	-	expression tag	UNP Q16531
C	-16	HIS	-	expression tag	UNP Q16531
C	-15	HIS	-	expression tag	UNP Q16531
C	-14	HIS	-	expression tag	UNP Q16531
C	-13	HIS	-	expression tag	UNP Q16531
C	-12	HIS	-	expression tag	UNP Q16531
C	-11	VAL	-	expression tag	UNP Q16531
C	-10	ASP	-	expression tag	UNP Q16531
C	-9	GLU	-	expression tag	UNP Q16531
C	-8	ASN	-	expression tag	UNP Q16531

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	LEU	-	expression tag	UNP Q16531
C	-6	TYR	-	expression tag	UNP Q16531
C	-5	PHE	-	expression tag	UNP Q16531
C	-4	GLN	-	expression tag	UNP Q16531
C	-3	GLY	-	expression tag	UNP Q16531
C	-2	GLY	-	expression tag	UNP Q16531
C	-1	GLY	-	expression tag	UNP Q16531
C	0	ARG	-	expression tag	UNP Q16531

- Molecule 4 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	355	Total	C	N	O	S	0	0	0
			2804	1781	491	521	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	76	MET	-	expression tag	UNP Q2YDS1
D	77	HIS	-	expression tag	UNP Q2YDS1
D	78	HIS	-	expression tag	UNP Q2YDS1
D	79	HIS	-	expression tag	UNP Q2YDS1
D	80	HIS	-	expression tag	UNP Q2YDS1
D	81	HIS	-	expression tag	UNP Q2YDS1
D	82	HIS	-	expression tag	UNP Q2YDS1
D	83	ARG	-	expression tag	UNP Q2YDS1
D	84	ARG	-	expression tag	UNP Q2YDS1
D	85	LEU	-	expression tag	UNP Q2YDS1
D	86	VAL	-	expression tag	UNP Q2YDS1
D	87	PRO	-	expression tag	UNP Q2YDS1
D	88	ARG	-	expression tag	UNP Q2YDS1
D	89	GLY	-	expression tag	UNP Q2YDS1
D	90	SER	-	expression tag	UNP Q2YDS1
D	91	GLY	-	expression tag	UNP Q2YDS1
D	92	GLY	-	expression tag	UNP Q2YDS1
D	93	ARG	-	expression tag	UNP Q2YDS1
D	180	GLN	LEU	variant	UNP Q2YDS1
D	214	ARG	TRP	variant	UNP Q2YDS1

- Molecule 5 is a DNA chain called 12 BP THF CONTAINING DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	12	Total 234	C 111	N 41	O 70	P 12	0	0	0

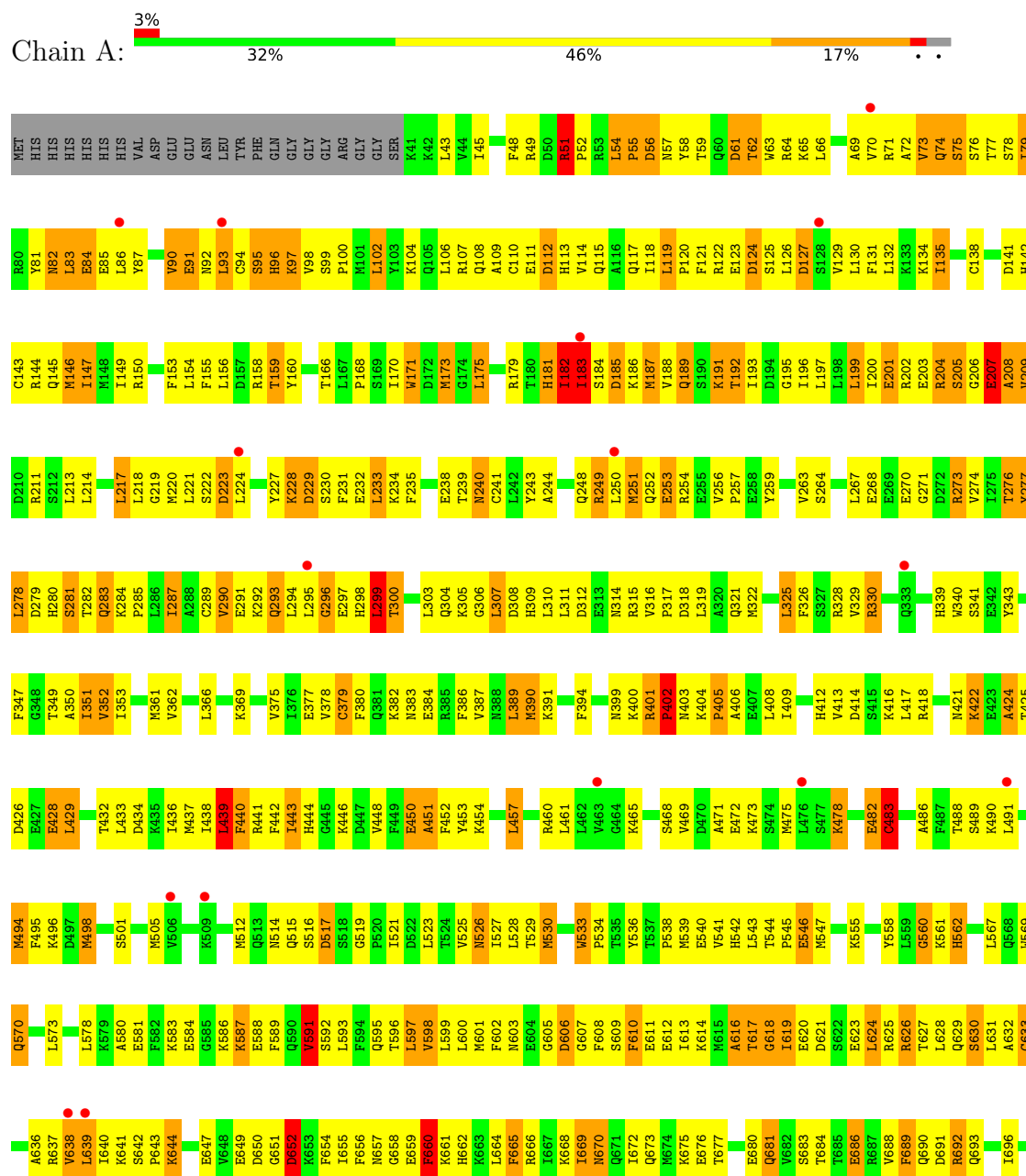
- Molecule 6 is a DNA chain called 12 BP DNA.

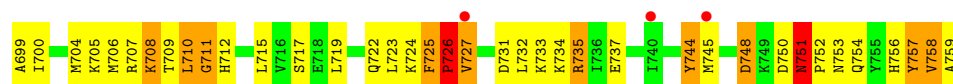
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	12	Total 249	C 118	N 47	O 72	P 12	0	0	0

3 Residue-property plots

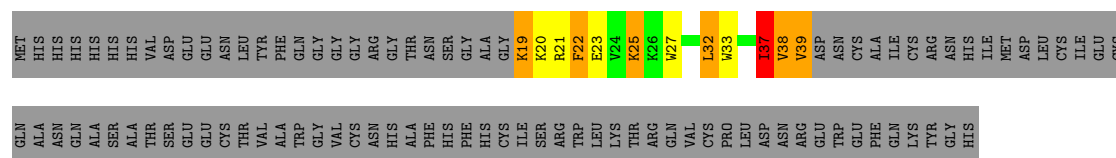
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CULLIN-4A

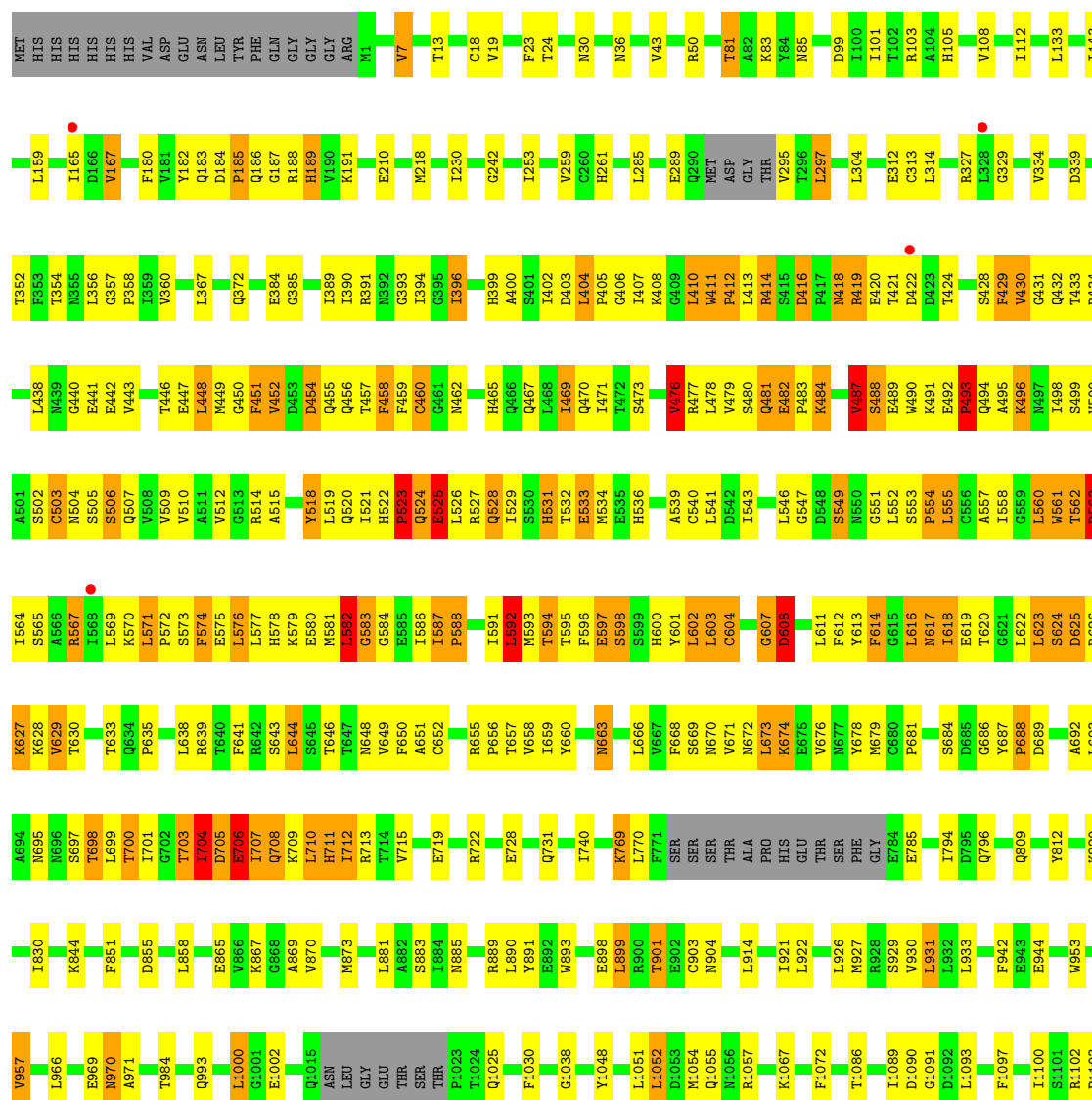


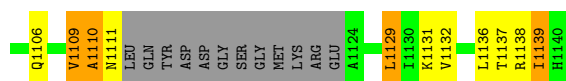


• Molecule 2: E3 UBIQUITIN-PROTEIN LIGASE RBX1

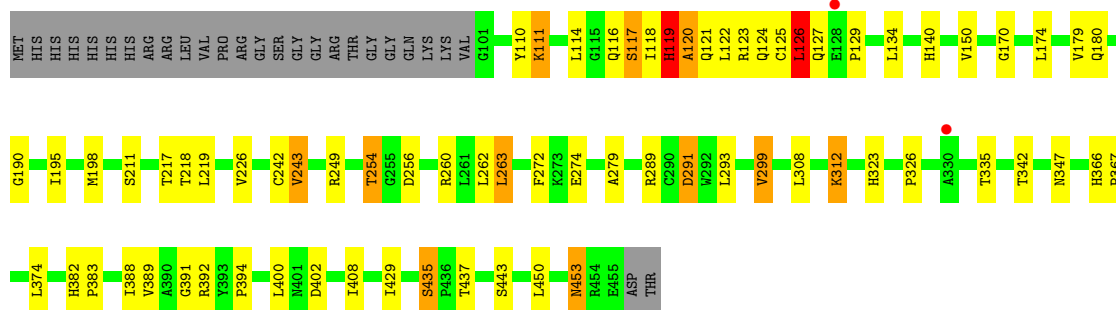
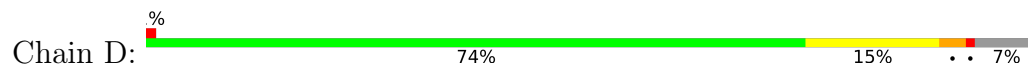


• Molecule 3: DNA DAMAGE-BINDING PROTEIN 1

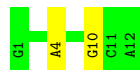
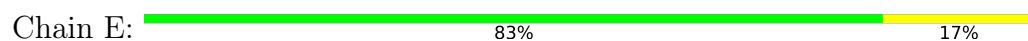




• Molecule 4: DNA DAMAGE-BINDING PROTEIN 2



• Molecule 5: 12 BP THF CONTAINING DNA



• Molecule 6: 12 BP DNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	210.65Å 78.02Å 276.62Å 90.00° 108.50° 90.00°	Depositor
Resolution (Å)	19.98 – 5.93 19.98 – 5.93	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.98-5.93) 96.6 (19.98-5.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 6.15Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.269 , 0.270 0.283 , 0.279	Depositor DCC
R_{free} test set	565 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	261.2	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 261.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17885	wwPDB-VP
Average B, all atoms (Å ²)	326.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3DR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	3/5915 (0.1%)	1.18	63/7954 (0.8%)
2	B	0.45	0/190	0.61	0/257
3	C	0.60	5/8762 (0.1%)	0.94	50/11875 (0.4%)
4	D	0.46	0/2877	0.77	0/3912
5	E	0.37	0/248	0.72	0/377
6	F	0.40	0/279	0.83	0/429
All	All	0.56	8/18271 (0.0%)	1.00	113/24804 (0.5%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	354	THR	C-N	-20.12	1.06	1.33
3	C	13	THR	C-N	11.93	1.49	1.33
3	C	706	GLU	C-N	-9.31	1.21	1.33
3	C	582	LEU	C-N	7.88	1.45	1.33
3	C	1138	ARG	CA-C	6.49	1.62	1.52
1	A	298	HIS	CA-C	-5.92	1.44	1.52
1	A	183	ILE	N-CA	-5.56	1.40	1.46
1	A	181	HIS	CB-CG	5.08	1.57	1.50

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	182	ILE	N-CA-C	25.21	136.18	110.72
1	A	73	VAL	N-CA-C	-18.71	96.75	111.90
1	A	298	HIS	CB-CA-C	-10.80	88.92	110.42
1	A	296	GLY	N-CA-C	-10.79	99.52	111.93
1	A	48	PHE	N-CA-C	-10.48	92.43	108.67
1	A	252	GLN	OE1-CD-NE2	-10.19	112.41	122.60
3	C	524	GLN	OE1-CD-NE2	-9.76	112.84	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	MET	N-CA-C	-9.62	100.67	111.82
1	A	182	ILE	N-CA-CB	-9.01	97.07	110.58
3	C	624	SER	N-CA-C	8.99	129.96	110.80
1	A	637	ARG	N-CA-C	8.81	125.74	114.56
3	C	411	TRP	CA-C-N	8.80	130.84	119.84
3	C	411	TRP	C-N-CA	8.80	130.84	119.84
1	A	146	MET	N-CA-C	-8.60	102.54	113.72
1	A	74	GLN	N-CA-C	-8.54	96.53	109.60
1	A	690	GLN	N-CA-C	-8.22	98.12	109.71
1	A	665	PHE	N-CA-C	-8.22	96.50	109.23
1	A	362	VAL	N-CA-C	8.15	118.08	110.42
3	C	688	PRO	N-CA-C	8.13	129.22	112.47
3	C	689	ASP	N-CA-C	-8.09	93.58	110.80
1	A	253	GLU	N-CA-C	7.87	123.18	113.50
1	A	560	GLY	N-CA-C	-7.75	101.52	112.37
1	A	689	PHE	N-CA-C	-7.62	102.32	111.69
1	A	638	VAL	N-CA-CB	-7.47	105.51	111.64
3	C	451	PHE	N-CA-C	7.21	119.83	110.53
3	C	1137	THR	N-CA-C	7.18	121.31	112.54
3	C	1139	ILE	N-CA-C	-7.14	102.52	113.16
1	A	181	HIS	CB-CA-C	7.14	124.62	110.42
1	A	403	ASN	N-CA-C	7.14	123.11	113.97
3	C	655	ARG	CA-C-N	7.13	128.76	119.84
3	C	655	ARG	C-N-CA	7.13	128.76	119.84
1	A	443	ILE	N-CA-C	7.08	119.21	109.80
1	A	379	CYS	N-CA-C	6.89	120.57	111.75
1	A	465	LYS	N-CA-C	6.88	119.20	110.33
3	C	524	GLN	CG-CD-NE2	6.80	126.60	116.40
1	A	252	GLN	CG-CD-NE2	6.80	126.60	116.40
1	A	277	TYR	N-CA-C	6.75	121.22	113.19
1	A	725	PHE	CA-C-N	6.73	128.25	119.84
1	A	725	PHE	C-N-CA	6.73	128.25	119.84
3	C	1132	VAL	N-CA-C	6.71	116.86	110.42
3	C	698	THR	N-CA-C	6.64	119.41	108.99
1	A	400	LYS	N-CA-C	-6.47	105.35	113.18
1	A	352	VAL	N-CA-C	6.45	118.36	112.43
3	C	458	PHE	N-CA-C	-6.43	106.02	114.31
3	C	354	THR	O-C-N	6.41	131.53	123.01
1	A	192	THR	N-CA-C	-6.34	105.20	113.12
1	A	533	TRP	CA-C-N	6.27	127.67	119.84
1	A	533	TRP	C-N-CA	6.27	127.67	119.84
3	C	688	PRO	CA-N-CD	-6.26	103.24	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	429	PHE	N-CA-C	-6.23	100.33	109.18
3	C	571	LEU	N-CA-C	6.12	123.34	109.81
3	C	525	GLU	N-CA-C	6.01	118.43	108.99
1	A	351	ILE	N-CA-C	-5.99	106.97	112.96
1	A	51	ARG	CB-CA-C	-5.92	98.51	110.17
1	A	401	ARG	CA-C-N	5.88	127.19	119.84
1	A	401	ARG	C-N-CA	5.88	127.19	119.84
1	A	630	SER	N-CA-C	-5.85	100.79	109.86
1	A	51	ARG	N-CA-C	5.83	122.68	109.81
3	C	651	ALA	N-CA-C	5.82	118.64	108.52
1	A	183	ILE	CA-C-O	5.80	124.47	118.96
3	C	574	PHE	N-CA-C	-5.80	106.15	113.23
1	A	591	VAL	N-CA-C	5.80	117.70	108.89
1	A	314	ASN	N-CA-C	5.78	119.67	111.92
1	A	439	LEU	N-CA-C	-5.78	103.79	111.24
3	C	555	LEU	N-CA-C	5.76	119.07	110.14
3	C	624	SER	CB-CA-C	-5.75	98.99	110.42
3	C	528	GLN	N-CA-C	5.69	118.15	109.62
3	C	487	VAL	N-CA-C	5.68	117.66	112.43
1	A	62	THR	N-CA-C	-5.68	106.48	113.41
1	A	669	ILE	N-CA-C	-5.64	104.76	113.16
3	C	523	PRO	CA-N-CD	-5.61	104.14	112.00
3	C	1139	ILE	N-CA-CB	5.60	123.64	111.76
1	A	636	ALA	CA-C-N	-5.60	113.51	122.08
1	A	636	ALA	C-N-CA	-5.60	113.51	122.08
3	C	506	SER	N-CA-C	5.57	120.08	113.12
3	C	582	LEU	O-C-N	5.56	129.99	122.59
3	C	393	GLY	O-C-N	-5.55	118.26	123.87
1	A	744	TYR	N-CA-C	-5.53	107.08	113.88
3	C	523	PRO	N-CA-C	5.51	123.82	112.47
1	A	109	ALA	N-CA-C	-5.49	105.21	111.14
3	C	416	ASP	CA-C-N	5.44	125.11	119.56
3	C	416	ASP	C-N-CA	5.44	125.11	119.56
1	A	751	ASN	CA-C-N	5.44	126.64	119.84
1	A	751	ASN	C-N-CA	5.44	126.64	119.84
1	A	686	GLU	N-CA-C	-5.41	105.46	111.36
1	A	299	LEU	N-CA-C	-5.41	99.28	110.80
1	A	61	ASP	N-CA-C	-5.40	106.69	113.28
3	C	625	ASP	N-CA-C	-5.40	99.30	110.80
3	C	607	GLY	N-CA-C	-5.38	107.27	115.66
3	C	524	GLN	N-CA-C	-5.37	104.15	111.56
1	A	273	ARG	N-CA-C	-5.36	105.55	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1138	ARG	CB-CA-C	-5.33	100.88	110.37
1	A	402	PRO	N-CA-C	5.33	123.45	112.47
3	C	484	LYS	N-CA-C	5.33	117.68	111.02
3	C	1025	GLN	CB-CG-CD	-5.29	103.60	112.60
3	C	554	PRO	N-CA-C	-5.29	106.83	114.18
3	C	604	CYS	N-CA-C	-5.27	102.95	110.59
1	A	183	ILE	N-CA-C	-5.25	107.70	113.43
1	A	183	ILE	N-CA-CB	-5.25	106.44	112.21
3	C	588	PRO	N-CA-C	-5.24	103.22	111.34
1	A	147	ILE	N-CA-C	-5.23	104.97	112.35
3	C	608	ASP	N-CA-C	-5.23	105.48	111.07
3	C	687	TYR	CA-C-N	5.20	126.34	119.84
3	C	687	TYR	C-N-CA	5.20	126.34	119.84
1	A	424	ALA	N-CA-C	5.17	119.46	113.20
1	A	181	HIS	CA-C-N	5.16	127.74	120.42
1	A	181	HIS	C-N-CA	5.16	127.74	120.42
3	C	496	LYS	N-CA-C	-5.14	103.74	110.53
3	C	929	SER	N-CA-C	5.12	116.09	108.31
1	A	183	ILE	O-C-N	5.12	127.42	122.25
3	C	476	VAL	N-CA-C	-5.12	101.04	109.12
3	C	523	PRO	N-CA-CB	-5.12	97.88	103.25
1	A	278	LEU	N-CA-C	5.03	118.21	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5809	0	5796	657	0
2	B	184	0	192	29	0
3	C	8605	0	8543	390	1
4	D	2804	0	2720	47	0
5	E	234	0	132	3	0
6	F	249	0	136	7	0
All	All	17885	0	17519	1097	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1097) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CZ	1:A:188:VAL:HA	1.63	1.33
1:A:696:ILE:CD1	1:A:723:LEU:HG	1.57	1.33
1:A:118:ILE:CD1	1:A:181:HIS:HB3	1.60	1.29
1:A:135:ILE:HD11	1:A:188:VAL:CG1	1.63	1.26
1:A:696:ILE:HD13	1:A:723:LEU:CD1	1.69	1.21
1:A:696:ILE:HD13	1:A:723:LEU:CG	1.71	1.20
1:A:135:ILE:CD1	1:A:188:VAL:CG1	2.21	1.19
1:A:118:ILE:HD11	1:A:181:HIS:CB	1.73	1.16
1:A:131:PHE:CZ	1:A:188:VAL:HG13	1.79	1.15
1:A:118:ILE:HD11	1:A:181:HIS:HB3	1.20	1.15
1:A:699:ALA:HB1	1:A:722:GLN:NE2	1.63	1.13
1:A:692:ARG:CB	1:A:725:PHE:CE2	2.32	1.12
1:A:118:ILE:HD11	1:A:181:HIS:CG	1.84	1.12
1:A:183:ILE:HD11	1:A:220:MET:CE	1.83	1.08
1:A:43:LEU:HD11	3:C:400:ALA:HB1	1.17	1.08
1:A:131:PHE:HZ	1:A:188:VAL:CA	1.67	1.07
1:A:601:MET:HE3	1:A:616:ALA:CB	1.83	1.07
1:A:69:ALA:HA	1:A:79:ILE:HG21	1.33	1.07
2:B:25:LYS:HE3	2:B:25:LYS:HA	1.30	1.07
2:B:37:ILE:HD13	2:B:38:VAL:N	1.69	1.07
2:B:37:ILE:HD13	2:B:37:ILE:C	1.80	1.06
1:A:692:ARG:HB3	1:A:725:PHE:CE2	1.89	1.06
1:A:692:ARG:HB2	1:A:725:PHE:CZ	1.90	1.05
1:A:107:ARG:NH1	1:A:173:MET:HG3	1.70	1.05
1:A:129:VAL:HG13	1:A:130:LEU:N	1.71	1.04
2:B:37:ILE:HG12	2:B:38:VAL:H	1.20	1.04
1:A:700:ILE:HD13	1:A:719:LEU:HD21	1.38	1.04
1:A:129:VAL:CG1	1:A:130:LEU:H	1.72	1.03
1:A:135:ILE:HD11	1:A:188:VAL:HG11	1.04	1.03
3:C:539:ALA:HB2	3:C:561:TRP:CD1	1.94	1.02
2:B:37:ILE:CG1	2:B:38:VAL:H	1.71	1.02
3:C:562:THR:O	3:C:564:ILE:HG13	1.61	1.01
3:C:185:PRO:HD3	4:D:289:ARG:HB3	1.40	1.01
1:A:131:PHE:CZ	1:A:188:VAL:CA	2.44	1.00
1:A:183:ILE:HD11	1:A:220:MET:HE3	1.37	1.00
1:A:122:ARG:HD2	1:A:186:LYS:HZ2	1.26	1.00
1:A:626:ARG:HA	1:A:629:GLN:HB2	1.41	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ARG:HB2	1:A:725:PHE:CE2	1.94	0.99
3:C:539:ALA:HB2	3:C:561:TRP:HD1	1.26	0.99
1:A:705:LYS:HB2	1:A:757:TYR:CE2	1.98	0.99
3:C:185:PRO:CD	4:D:289:ARG:HB3	1.93	0.99
1:A:422:LYS:NZ	1:A:422:LYS:HB3	1.77	0.98
1:A:700:ILE:CD1	1:A:719:LEU:HD21	1.93	0.98
1:A:642:SER:HB2	1:A:643:PRO:HD3	1.46	0.97
1:A:696:ILE:HD13	1:A:723:LEU:HD11	1.44	0.97
1:A:657:ASN:HD21	1:A:659:GLU:HB2	1.28	0.96
1:A:696:ILE:HD13	1:A:723:LEU:HG	1.32	0.96
1:A:74:GLN:HE22	1:A:110:CYS:HA	1.31	0.96
1:A:197:LEU:CD2	1:A:235:PHE:HA	1.96	0.96
1:A:491:LEU:HA	1:A:494:MET:HG3	1.48	0.96
1:A:705:LYS:HA	1:A:757:TYR:CD2	2.01	0.95
1:A:638:VAL:HG12	1:A:639:LEU:HD23	1.48	0.95
3:C:465:HIS:ND1	3:C:523:PRO:HD3	1.82	0.95
3:C:329:GLY:HA3	3:C:384:GLU:HG2	1.45	0.95
2:B:37:ILE:CD1	2:B:38:VAL:N	2.30	0.94
1:A:131:PHE:HZ	1:A:188:VAL:HA	1.13	0.94
1:A:251:MET:HA	1:A:251:MET:HE2	1.50	0.94
1:A:131:PHE:CE1	1:A:191:LYS:HD3	2.04	0.93
1:A:118:ILE:CG1	1:A:181:HIS:HB3	1.98	0.93
1:A:183:ILE:HD11	1:A:220:MET:SD	2.09	0.93
1:A:696:ILE:HD11	1:A:723:LEU:HG	1.51	0.91
1:A:197:LEU:HD22	1:A:235:PHE:HA	1.50	0.91
1:A:131:PHE:HZ	1:A:188:VAL:CB	1.84	0.91
3:C:507:GLN:NE2	3:C:552:LEU:HA	1.85	0.91
2:B:19:LYS:HE3	2:B:19:LYS:HA	1.53	0.91
1:A:82:ASN:OD1	1:A:85:GLU:HG3	1.69	0.90
1:A:51:ARG:O	1:A:51:ARG:HG2	1.72	0.90
1:A:122:ARG:CD	1:A:186:LYS:HZ2	1.84	0.90
1:A:63:TRP:CZ3	1:A:102:LEU:HA	2.07	0.90
1:A:196:ILE:HD13	1:A:218:LEU:HD21	1.53	0.90
1:A:129:VAL:CG1	1:A:130:LEU:N	2.30	0.90
3:C:356:LEU:HD21	3:C:712:ILE:HD13	1.52	0.90
3:C:465:HIS:CE1	3:C:523:PRO:HD3	2.07	0.90
3:C:18:CYS:HB2	3:C:313:CYS:SG	2.12	0.90
1:A:131:PHE:CZ	1:A:188:VAL:CG1	2.54	0.89
1:A:745:MET:HA	1:A:757:TYR:O	1.71	0.89
1:A:43:LEU:CD1	3:C:400:ALA:HB1	2.03	0.89
2:B:37:ILE:CG1	2:B:38:VAL:N	2.30	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:SER:HB2	1:A:100:PRO:HD3	1.53	0.88
1:A:696:ILE:CD1	1:A:723:LEU:CG	2.35	0.88
1:A:106:LEU:HD22	1:A:153:PHE:CE2	2.09	0.87
3:C:578:HIS:CD2	3:C:623:LEU:HD12	2.09	0.87
4:D:323:HIS:NE2	4:D:342:THR:HG21	1.88	0.87
1:A:538:PRO:HA	1:A:570:GLN:HE22	1.40	0.87
1:A:70:VAL:HG21	1:A:106:LEU:CD1	2.05	0.87
3:C:649:VAL:HG12	3:C:650:PHE:H	1.39	0.86
1:A:196:ILE:HD13	1:A:218:LEU:CD2	2.06	0.86
1:A:274:VAL:HA	1:A:278:LEU:HB2	1.57	0.86
1:A:605:GLY:O	1:A:606:ASP:HB2	1.75	0.86
3:C:482:GLU:CD	3:C:483:PRO:HD3	2.00	0.86
1:A:131:PHE:CD1	1:A:191:LYS:HD3	2.11	0.86
1:A:144:ARG:HA	1:A:147:ILE:HD12	1.58	0.86
1:A:63:TRP:CH2	1:A:102:LEU:HA	2.11	0.85
3:C:711:HIS:CG	3:C:712:ILE:N	2.43	0.85
3:C:23:PHE:H	3:C:30:ASN:HD22	1.21	0.85
1:A:199:LEU:HD12	1:A:214:LEU:HD11	1.59	0.85
3:C:165:ILE:HD11	3:C:188:ARG:NH2	1.92	0.85
1:A:213:LEU:O	1:A:217:LEU:HD12	1.76	0.85
3:C:81:THR:HG21	3:C:85:ASN:HD22	1.41	0.84
1:A:422:LYS:HB3	1:A:422:LYS:HZ2	1.38	0.84
1:A:704:MET:C	1:A:757:TYR:HD2	1.86	0.84
1:A:704:MET:HG3	1:A:745:MET:HE2	1.59	0.83
1:A:115:GLN:HG2	1:A:181:HIS:CE1	2.14	0.83
1:A:696:ILE:HA	1:A:723:LEU:HD11	1.60	0.83
1:A:119:LEU:HB2	1:A:120:PRO:HD3	1.60	0.83
3:C:446:THR:HG22	3:C:447:GLU:H	1.43	0.83
1:A:204:ARG:HH21	1:A:270:GLU:CD	1.86	0.83
3:C:520:GLN:HG3	3:C:529:ILE:HG13	1.60	0.82
3:C:707:ILE:HG23	3:C:708:GLN:N	1.92	0.82
3:C:218:MET:HE3	3:C:261:HIS:HD2	1.41	0.82
1:A:135:ILE:CD1	1:A:188:VAL:HG13	2.06	0.82
1:A:581:GLU:HB2	2:B:21:ARG:HA	1.62	0.82
1:A:93:LEU:HD22	1:A:93:LEU:O	1.79	0.81
1:A:705:LYS:HB2	1:A:757:TYR:HE2	1.45	0.81
3:C:602:LEU:C	3:C:603:LEU:HD23	2.04	0.81
1:A:699:ALA:CB	1:A:722:GLN:NE2	2.43	0.81
2:B:38:VAL:HG12	2:B:38:VAL:O	1.80	0.81
3:C:413:LEU:HB2	3:C:424:THR:HB	1.62	0.81
3:C:507:GLN:HE22	3:C:553:SER:H	1.25	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:CD1	1:A:220:MET:HE3	2.11	0.81
3:C:534:MET:HE1	3:C:569:LEU:HD21	1.63	0.81
1:A:757:TYR:HE1	1:A:759:ALA:HA	1.47	0.80
3:C:708:GLN:HA	3:C:708:GLN:NE2	1.94	0.80
1:A:284:LYS:HB3	1:A:285:PRO:HD3	1.61	0.80
1:A:131:PHE:HZ	1:A:188:VAL:CG1	1.93	0.80
1:A:366:LEU:HD23	1:A:439:LEU:HD12	1.62	0.80
1:A:131:PHE:CE2	1:A:188:VAL:HG13	2.16	0.80
1:A:680:GLU:O	1:A:684:THR:HG22	1.81	0.80
1:A:296:GLY:O	1:A:297:GLU:HB2	1.82	0.79
3:C:509:VAL:HG23	3:C:543:ILE:HD13	1.62	0.79
1:A:705:LYS:CA	1:A:757:TYR:CD2	2.65	0.79
1:A:93:LEU:O	1:A:93:LEU:CD2	2.30	0.79
1:A:122:ARG:NE	1:A:186:LYS:NZ	2.30	0.79
1:A:599:LEU:HD21	1:A:631:LEU:HD12	1.64	0.79
1:A:211:ARG:HD2	1:A:276:THR:HG21	1.64	0.79
3:C:182:TYR:O	3:C:188:ARG:CB	2.30	0.79
1:A:696:ILE:HD11	1:A:725:PHE:CZ	2.18	0.78
3:C:412:PRO:HB2	3:C:422:ASP:OD2	1.83	0.78
3:C:185:PRO:CG	4:D:289:ARG:CB	2.62	0.78
1:A:692:ARG:O	1:A:696:ILE:HG12	1.84	0.78
1:A:138:CYS:SG	1:A:182:ILE:CD1	2.71	0.77
1:A:175:LEU:HD12	1:A:223:ASP:O	1.85	0.77
3:C:649:VAL:HG12	3:C:650:PHE:N	2.00	0.77
1:A:527:ILE:HD11	1:A:567:LEU:HD22	1.65	0.77
1:A:239:THR:C	1:A:241:CYS:H	1.91	0.77
1:A:274:VAL:HG11	1:A:283:GLN:HE21	1.49	0.77
3:C:185:PRO:HG3	4:D:289:ARG:HB2	1.65	0.77
1:A:129:VAL:HG13	1:A:130:LEU:H	1.32	0.77
3:C:578:HIS:NE2	3:C:623:LEU:HD12	1.99	0.77
1:A:186:LYS:HB3	1:A:188:VAL:HG23	1.67	0.76
1:A:603:ASN:OD1	2:B:22:PHE:HB2	1.86	0.76
3:C:23:PHE:H	3:C:30:ASN:ND2	1.83	0.76
3:C:452:VAL:HG12	3:C:454:ASP:OD1	1.86	0.75
1:A:329:VAL:HG12	1:A:330:ARG:H	1.49	0.75
1:A:601:MET:HE1	1:A:613:ILE:HA	1.69	0.75
1:A:597:LEU:HB3	1:A:617:THR:HG21	1.68	0.75
1:A:276:THR:HG22	1:A:277:TYR:N	2.02	0.75
1:A:578:LEU:HD11	1:A:596:THR:HG23	1.67	0.75
3:C:450:GLY:HA3	3:C:479:VAL:CG2	2.17	0.75
3:C:448:LEU:HB3	3:C:451:PHE:HD2	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:469:ILE:HD11	3:C:476:VAL:HG23	1.69	0.74
3:C:507:GLN:HE22	3:C:552:LEU:HA	1.49	0.74
3:C:389:ILE:HD13	3:C:713:ARG:HG2	1.68	0.74
1:A:279:ASP:OD1	1:A:281:SER:HB3	1.87	0.74
1:A:705:LYS:O	1:A:708:LYS:NZ	2.21	0.74
3:C:185:PRO:CG	4:D:289:ARG:HB2	2.17	0.74
1:A:595:GLN:HE22	1:A:669:ILE:HG22	1.53	0.74
1:A:316:VAL:HB	1:A:317:PRO:HD3	1.70	0.74
1:A:601:MET:HE3	1:A:616:ALA:HB3	1.70	0.74
1:A:688:VAL:O	1:A:692:ARG:HG3	1.88	0.73
1:A:696:ILE:O	1:A:700:ILE:HG12	1.88	0.73
1:A:106:LEU:HD22	1:A:153:PHE:CZ	2.22	0.73
1:A:122:ARG:CD	1:A:186:LYS:NZ	2.51	0.73
3:C:451:PHE:CD1	3:C:470:GLN:HB2	2.24	0.73
1:A:294:LEU:O	1:A:295:LEU:HD23	1.86	0.73
1:A:630:SER:HB3	1:A:672:ILE:HD11	1.70	0.73
3:C:578:HIS:CD2	3:C:623:LEU:H	2.06	0.73
1:A:609:SER:O	1:A:612:GLU:HG2	1.87	0.73
1:A:77:THR:HG22	1:A:78:SER:H	1.53	0.73
3:C:1055:GLN:HE22	3:C:1090:ASP:H	1.37	0.73
1:A:118:ILE:HG12	1:A:181:HIS:HB3	1.71	0.73
1:A:122:ARG:NE	1:A:186:LYS:HZ3	1.85	0.73
1:A:601:MET:HE3	1:A:616:ALA:HB2	1.69	0.73
3:C:465:HIS:O	3:C:467:GLN:HG3	1.89	0.72
1:A:138:CYS:SG	1:A:182:ILE:HD13	2.29	0.72
1:A:135:ILE:HD12	1:A:188:VAL:HG13	1.70	0.72
3:C:184:ASP:HB2	3:C:185:PRO:HD2	1.70	0.72
1:A:529:THR:HA	2:B:33:TRP:NE1	2.03	0.72
3:C:657:THR:HG22	3:C:658:VAL:H	1.54	0.72
1:A:240:ASN:OD1	1:A:289:CYS:HB3	1.90	0.72
1:A:340:TRP:CH2	1:A:390:MET:HB2	2.25	0.72
1:A:49:ARG:HD2	1:A:51:ARG:NH2	2.05	0.72
1:A:208:ALA:O	1:A:209:VAL:CB	2.38	0.72
3:C:465:HIS:HB2	3:C:467:GLN:HE21	1.55	0.72
3:C:469:ILE:HD13	3:C:470:GLN:N	2.05	0.72
3:C:579:LYS:HG2	3:C:581:MET:HE3	1.72	0.71
1:A:82:ASN:O	1:A:83:LEU:C	2.33	0.71
3:C:182:TYR:O	3:C:188:ARG:HB2	1.89	0.71
4:D:263:LEU:HB2	4:D:272:PHE:HB3	1.73	0.71
1:A:660:PHE:O	1:A:662:HIS:N	2.23	0.71
3:C:329:GLY:HA3	3:C:384:GLU:CG	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:889:ARG:HD3	3:C:901:THR:HB	1.73	0.71
1:A:118:ILE:HD11	1:A:181:HIS:ND1	2.06	0.71
1:A:432:THR:O	1:A:436:ILE:HG13	1.91	0.71
3:C:185:PRO:CG	4:D:289:ARG:HB3	2.21	0.71
1:A:602:PHE:HD2	1:A:656:PHE:HB2	1.54	0.70
3:C:561:TRP:O	3:C:587:ILE:CG2	2.40	0.70
1:A:643:PRO:CD	1:A:652:ASP:HA	2.21	0.70
1:A:83:LEU:O	1:A:84:GLU:C	2.35	0.70
3:C:396:ILE:HA	3:C:704:ILE:O	1.90	0.70
3:C:451:PHE:CE1	3:C:470:GLN:HB2	2.25	0.70
3:C:592:LEU:HD23	3:C:593:MET:O	1.92	0.70
1:A:204:ARG:NH2	1:A:270:GLU:OE1	2.23	0.70
1:A:578:LEU:HD13	1:A:591:VAL:CG2	2.21	0.70
1:A:129:VAL:HG12	1:A:130:LEU:H	1.55	0.70
1:A:601:MET:CE	1:A:616:ALA:CB	2.68	0.70
1:A:705:LYS:CB	1:A:757:TYR:CE2	2.73	0.70
1:A:587:LYS:H	1:A:587:LYS:HD2	1.57	0.69
3:C:399:HIS:NE2	3:C:703:THR:HG22	2.07	0.69
1:A:734:LYS:HA	1:A:737:GLU:CD	2.18	0.69
1:A:692:ARG:O	1:A:725:PHE:HZ	1.76	0.69
3:C:188:ARG:C	3:C:189:HIS:CG	2.71	0.69
3:C:218:MET:HE3	3:C:261:HIS:CD2	2.25	0.69
3:C:652:CYS:HB3	3:C:676:VAL:O	1.91	0.69
3:C:706:GLU:HA	3:C:706:GLU:OE1	1.90	0.69
3:C:704:ILE:O	3:C:705:ASP:HB2	1.91	0.69
1:A:329:VAL:HG12	1:A:330:ARG:N	2.08	0.69
3:C:188:ARG:C	3:C:189:HIS:CD2	2.71	0.69
3:C:480:SER:O	3:C:484:LYS:HA	1.92	0.69
3:C:532:THR:HG22	3:C:533:GLU:N	2.06	0.69
1:A:619:ILE:HG22	1:A:620:GLU:H	1.56	0.69
1:A:630:SER:C	1:A:632:ALA:H	2.01	0.69
3:C:618:ILE:HG13	3:C:619:GLU:N	2.08	0.68
3:C:452:VAL:HG23	3:C:470:GLN:OE1	1.93	0.68
4:D:119:HIS:O	4:D:120:ALA:C	2.36	0.68
1:A:560:GLY:O	1:A:561:LYS:HB2	1.93	0.68
1:A:751:ASN:O	1:A:753:ASN:N	2.27	0.68
3:C:536:HIS:CD2	3:C:563:ASP:HB3	2.29	0.68
3:C:722:ARG:NH2	3:C:812:TYR:OH	2.26	0.68
1:A:204:ARG:CZ	1:A:243:TYR:HE2	2.07	0.68
3:C:450:GLY:HA3	3:C:479:VAL:HG21	1.74	0.68
3:C:440:GLY:O	3:C:686:GLY:HA3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1051:LEU:HB2	3:C:1089:ILE:HD13	1.76	0.68
1:A:122:ARG:HD2	1:A:186:LYS:NZ	2.06	0.67
1:A:555:LYS:HD2	1:A:569:TRP:HZ3	1.58	0.67
1:A:70:VAL:HG21	1:A:106:LEU:HD11	1.77	0.67
1:A:630:SER:CB	1:A:672:ILE:HD11	2.24	0.67
3:C:596:PHE:HE1	3:C:648:ASN:HA	1.58	0.67
1:A:249:ARG:O	1:A:253:GLU:HB2	1.95	0.67
3:C:711:HIS:CG	3:C:712:ILE:H	2.08	0.67
1:A:630:SER:O	1:A:631:LEU:HB2	1.94	0.67
1:A:63:TRP:CH2	1:A:102:LEU:CA	2.77	0.67
3:C:165:ILE:CD1	3:C:188:ARG:NH2	2.58	0.67
1:A:609:SER:H	1:A:612:GLU:CD	2.03	0.66
2:B:37:ILE:C	2:B:37:ILE:CD1	2.54	0.66
1:A:63:TRP:NE1	1:A:93:LEU:HD11	2.10	0.66
1:A:274:VAL:HG11	1:A:283:GLN:HB2	1.76	0.66
1:A:593:LEU:HD21	2:B:27:TRP:HE1	1.60	0.66
3:C:460:CYS:HA	3:C:469:ILE:O	1.95	0.66
1:A:49:ARG:HD2	1:A:51:ARG:HH21	1.60	0.66
1:A:126:LEU:O	1:A:127:ASP:CG	2.38	0.66
1:A:183:ILE:CD1	1:A:220:MET:SD	2.84	0.66
1:A:409:ILE:HG13	1:A:443:ILE:CD1	2.26	0.66
1:A:538:PRO:CA	1:A:570:GLN:HE22	2.08	0.66
1:A:705:LYS:N	1:A:757:TYR:HD2	1.94	0.66
1:A:79:ILE:HD12	1:A:79:ILE:H	1.59	0.66
1:A:203:GLU:C	1:A:205:SER:H	2.03	0.66
3:C:189:HIS:HB3	3:C:210:GLU:O	1.95	0.66
1:A:696:ILE:HD11	1:A:725:PHE:CE1	2.31	0.66
3:C:582:LEU:O	3:C:583:GLY:O	2.14	0.66
1:A:118:ILE:CG2	1:A:186:LYS:HE3	2.25	0.66
1:A:512:MET:HE2	1:A:512:MET:HA	1.77	0.66
3:C:711:HIS:O	3:C:712:ILE:HG13	1.95	0.66
3:C:507:GLN:HE22	3:C:553:SER:N	1.94	0.66
1:A:366:LEU:CD2	1:A:439:LEU:HD12	2.25	0.65
4:D:443:SER:HB2	4:D:450:LEU:HB2	1.77	0.65
1:A:74:GLN:HE22	1:A:110:CYS:CA	2.07	0.65
1:A:709:THR:O	1:A:710:LEU:HB2	1.95	0.65
1:A:539:MET:HE1	1:A:619:ILE:HG23	1.79	0.65
1:A:688:VAL:O	1:A:692:ARG:CG	2.45	0.65
3:C:520:GLN:HG3	3:C:529:ILE:CG1	2.27	0.65
3:C:184:ASP:O	3:C:187:GLY:N	2.30	0.65
1:A:96:HIS:O	1:A:97:LYS:CB	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ALA:O	1:A:73:VAL:HG23	1.97	0.65
3:C:562:THR:O	3:C:564:ILE:N	2.30	0.65
1:A:84:GLU:O	1:A:87:TYR:N	2.29	0.64
1:A:54:LEU:CB	1:A:55:PRO:HD3	2.27	0.64
1:A:312:ASP:HB3	1:A:343:TYR:OH	1.97	0.64
3:C:601:TYR:CE2	3:C:666:LEU:HD21	2.32	0.64
4:D:119:HIS:O	4:D:122:LEU:N	2.30	0.64
1:A:233:LEU:O	1:A:234:LYS:C	2.39	0.64
1:A:707:ARG:O	1:A:708:LYS:C	2.40	0.64
1:A:183:ILE:HG21	1:A:221:LEU:HD23	1.78	0.64
1:A:249:ARG:HB3	1:A:249:ARG:HH11	1.62	0.64
1:A:437:MET:HE1	1:A:475:MET:CE	2.28	0.64
1:A:461:LEU:HB3	1:A:498:MET:HE2	1.79	0.64
3:C:507:GLN:NE2	3:C:553:SER:H	1.94	0.64
1:A:642:SER:CB	1:A:643:PRO:HD3	2.24	0.64
2:B:25:LYS:HA	2:B:25:LYS:CE	2.15	0.64
1:A:94:CYS:SG	1:A:156:LEU:HD13	2.37	0.64
3:C:926:LEU:CD2	4:D:129:PRO:HG3	2.28	0.64
4:D:125:CYS:O	4:D:127:GLN:N	2.30	0.64
1:A:707:ARG:CD	1:A:710:LEU:HD22	2.28	0.64
3:C:184:ASP:O	3:C:186:GLN:N	2.31	0.63
3:C:692:ALA:C	3:C:693:LEU:HD23	2.23	0.63
4:D:124:GLN:O	4:D:124:GLN:CG	2.45	0.63
1:A:197:LEU:HD21	1:A:235:PHE:HA	1.78	0.63
1:A:422:LYS:HB3	1:A:422:LYS:HZ3	1.63	0.63
1:A:705:LYS:CA	1:A:757:TYR:CE2	2.82	0.63
1:A:705:LYS:N	1:A:757:TYR:CD2	2.67	0.63
1:A:292:LYS:HD2	1:A:292:LYS:O	1.99	0.63
1:A:183:ILE:HG21	1:A:221:LEU:CD2	2.28	0.63
1:A:404:LYS:N	1:A:405:PRO:HD2	2.14	0.63
3:C:414:ARG:CB	3:C:462:ASN:HD21	2.12	0.63
4:D:249:ARG:HE	4:D:291:ASP:HB3	1.64	0.63
1:A:108:GLN:HA	1:A:111:GLU:HB3	1.81	0.63
1:A:122:ARG:CZ	1:A:186:LYS:NZ	2.61	0.63
1:A:118:ILE:HG23	1:A:186:LYS:HE3	1.80	0.62
1:A:437:MET:HE1	1:A:475:MET:HE3	1.81	0.62
1:A:523:LEU:HD11	1:A:525:VAL:HG22	1.81	0.62
1:A:700:ILE:HD13	1:A:719:LEU:CD2	2.23	0.62
3:C:482:GLU:OE1	3:C:483:PRO:HD3	2.00	0.62
3:C:518:TYR:HD1	3:C:519:LEU:N	1.95	0.62
1:A:77:THR:HG22	1:A:78:SER:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:O	1:A:96:HIS:C	2.42	0.62
1:A:757:TYR:O	1:A:758:VAL:HB	1.99	0.62
3:C:446:THR:CG2	3:C:447:GLU:H	2.06	0.62
3:C:591:ILE:O	3:C:592:LEU:HB2	2.00	0.62
1:A:540:GLU:CD	1:A:540:GLU:H	2.08	0.62
3:C:657:THR:HG21	3:C:668:PHE:HB3	1.82	0.62
3:C:669:SER:O	3:C:670:ASN:C	2.43	0.62
1:A:726:PRO:O	1:A:727:VAL:HB	2.00	0.62
3:C:399:HIS:CE1	3:C:703:THR:HG22	2.34	0.62
3:C:476:VAL:HG13	3:C:490:TRP:HB3	1.81	0.61
1:A:66:LEU:HD23	1:A:86:LEU:HD22	1.81	0.61
1:A:692:ARG:O	1:A:725:PHE:CZ	2.52	0.61
1:A:57:ASN:O	1:A:59:THR:N	2.27	0.61
1:A:310:LEU:HD22	1:A:315:ARG:HB2	1.81	0.61
5:E:10:DG:N2	6:F:4:DG:C2	2.69	0.61
1:A:228:LYS:HD3	1:A:232:GLU:HG2	1.81	0.61
3:C:562:THR:HG22	3:C:563:ASP:N	2.16	0.61
1:A:132:LEU:HD21	1:A:192:THR:HA	1.83	0.61
1:A:409:ILE:O	1:A:413:VAL:HG23	2.00	0.61
3:C:7:VAL:HG13	3:C:1091:GLY:HA3	1.81	0.61
1:A:183:ILE:HD13	1:A:221:LEU:HD23	1.81	0.61
1:A:570:GLN:HG2	2:B:32:LEU:HD11	1.81	0.61
1:A:624:LEU:CD2	1:A:628:LEU:HG	2.30	0.61
1:A:696:ILE:CD1	1:A:723:LEU:CD1	2.63	0.61
3:C:562:THR:C	3:C:564:ILE:H	2.08	0.61
3:C:582:LEU:HD13	3:C:583:GLY:H	1.65	0.61
3:C:617:ASN:HD21	3:C:619:GLU:HB2	1.64	0.61
1:A:131:PHE:CD1	1:A:191:LYS:CD	2.84	0.61
1:A:461:LEU:HD22	1:A:498:MET:HE2	1.83	0.61
1:A:689:PHE:O	1:A:693:GLN:NE2	2.33	0.61
1:A:640:ILE:O	1:A:654:PHE:HA	2.01	0.61
3:C:492:GLU:HG3	3:C:496:LYS:HB2	1.83	0.61
3:C:927:MET:SD	4:D:129:PRO:HB2	2.41	0.61
1:A:83:LEU:O	1:A:86:LEU:N	2.30	0.60
1:A:276:THR:HG22	1:A:277:TYR:H	1.67	0.60
1:A:340:TRP:HH2	1:A:390:MET:HB2	1.65	0.60
1:A:724:LYS:HE2	1:A:724:LYS:HA	1.82	0.60
1:A:486:ALA:HA	1:A:489:SER:HB2	1.83	0.60
1:A:751:ASN:C	1:A:753:ASN:H	2.10	0.60
3:C:446:THR:HG22	3:C:447:GLU:N	2.16	0.60
1:A:73:VAL:HG12	1:A:145:GLN:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PRO:HA	1:A:570:GLN:NE2	2.12	0.60
1:A:707:ARG:HD2	1:A:710:LEU:HD22	1.84	0.60
3:C:889:ARG:HG3	3:C:904:ASN:ND2	2.16	0.60
3:C:167:VAL:HG13	3:C:180:PHE:HB3	1.84	0.60
1:A:251:MET:HA	1:A:251:MET:CE	2.27	0.60
4:D:127:GLN:O	4:D:127:GLN:HG2	2.00	0.60
1:A:527:ILE:HD11	1:A:567:LEU:CD2	2.31	0.60
1:A:587:LYS:H	1:A:587:LYS:CD	2.15	0.60
3:C:396:ILE:HD13	3:C:396:ILE:H	1.66	0.60
1:A:183:ILE:CG2	1:A:221:LEU:CD2	2.79	0.60
1:A:602:PHE:CD2	1:A:656:PHE:HB2	2.35	0.60
3:C:573:SER:OG	3:C:575:GLU:HB2	2.01	0.60
1:A:51:ARG:H	1:A:52:PRO:HD2	1.67	0.60
1:A:589:PHE:CD1	1:A:669:ILE:HD11	2.37	0.60
1:A:700:ILE:CD1	1:A:719:LEU:CD2	2.74	0.60
3:C:407:ILE:HG21	3:C:410:LEU:HD23	1.84	0.59
3:C:889:ARG:HG3	3:C:904:ASN:HD21	1.67	0.59
1:A:751:ASN:N	1:A:751:ASN:HD22	2.00	0.59
3:C:498:ILE:HD12	3:C:498:ILE:N	2.17	0.59
1:A:138:CYS:SG	1:A:182:ILE:HD11	2.42	0.59
1:A:725:PHE:HB2	1:A:726:PRO:HD2	1.84	0.59
3:C:562:THR:C	3:C:564:ILE:N	2.60	0.59
1:A:192:THR:O	1:A:196:ILE:HG13	2.02	0.59
1:A:417:LEU:HD23	1:A:460:ARG:HH12	1.66	0.59
1:A:521:ILE:HD12	1:A:521:ILE:N	2.18	0.59
3:C:922:LEU:HD23	3:C:957:VAL:HG13	1.85	0.59
4:D:110:TYR:CZ	4:D:114:LEU:HD11	2.37	0.59
1:A:118:ILE:CD1	1:A:181:HIS:CB	2.44	0.59
1:A:454:LYS:HD2	1:A:534:PRO:HG3	1.83	0.59
3:C:414:ARG:HB3	3:C:462:ASN:HD21	1.68	0.59
3:C:673:LEU:HD23	3:C:674:LYS:H	1.68	0.59
1:A:282:THR:O	1:A:285:PRO:HD2	2.01	0.59
1:A:405:PRO:O	1:A:409:ILE:HG12	2.02	0.59
1:A:597:LEU:O	1:A:598:VAL:C	2.45	0.59
1:A:699:ALA:HB1	1:A:722:GLN:HE22	1.64	0.59
1:A:296:GLY:O	1:A:297:GLU:CB	2.50	0.59
1:A:305:LYS:HG3	1:A:305:LYS:O	2.02	0.58
1:A:621:ASP:O	1:A:625:ARG:HG2	2.03	0.58
3:C:518:TYR:C	3:C:518:TYR:CD1	2.79	0.58
3:C:705:ASP:O	3:C:706:GLU:CB	2.51	0.58
3:C:851:PHE:HB3	3:C:858:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LYS:HA	1:A:232:GLU:HB2	1.84	0.58
1:A:665:PHE:O	1:A:666:ARG:HB2	2.03	0.58
1:A:692:ARG:HB3	1:A:725:PHE:CD2	2.38	0.58
3:C:588:PRO:HB3	3:C:604:CYS:SG	2.43	0.58
1:A:228:LYS:CE	1:A:232:GLU:HG2	2.34	0.58
3:C:695:ASN:OD1	3:C:697:SER:N	2.30	0.58
1:A:601:MET:HB3	1:A:608:PHE:HE2	1.69	0.58
1:A:643:PRO:HD2	1:A:652:ASP:HA	1.86	0.58
1:A:239:THR:O	1:A:241:CYS:N	2.36	0.58
1:A:705:LYS:O	1:A:708:LYS:CE	2.51	0.58
3:C:553:SER:O	3:C:571:LEU:HD12	2.03	0.58
6:F:5:DT:H73	6:F:6:DA:C6	2.39	0.58
1:A:244:ALA:HA	1:A:293:GLN:OE1	2.03	0.58
3:C:903:CYS:HB3	3:C:942:PHE:CE2	2.39	0.58
1:A:43:LEU:HD12	3:C:402:ILE:HD13	1.85	0.58
1:A:369:LYS:HE2	1:A:390:MET:CE	2.33	0.58
1:A:708:LYS:HD3	1:A:708:LYS:N	2.19	0.58
3:C:441:GLU:HG2	3:C:441:GLU:O	2.02	0.58
3:C:704:ILE:HD12	3:C:704:ILE:H	1.68	0.58
1:A:228:LYS:HE2	1:A:232:GLU:OE2	2.03	0.58
3:C:429:PHE:O	3:C:430:VAL:O	2.22	0.58
1:A:82:ASN:HD21	1:A:85:GLU:CD	2.12	0.57
1:A:240:ASN:ND2	1:A:289:CYS:SG	2.77	0.57
1:A:249:ARG:HH11	1:A:249:ARG:CB	2.16	0.57
3:C:712:ILE:O	3:C:712:ILE:HG22	2.03	0.57
1:A:429:LEU:O	1:A:433:LEU:HB2	2.03	0.57
1:A:528:LEU:HD22	1:A:533:TRP:CZ2	2.40	0.57
1:A:657:ASN:HD21	1:A:659:GLU:CB	2.10	0.57
3:C:432:GLN:HA	3:C:455:GLN:O	2.04	0.57
1:A:468:SER:HB3	1:A:471:ALA:HB2	1.86	0.57
3:C:188:ARG:O	3:C:189:HIS:CG	2.58	0.57
3:C:414:ARG:HH11	3:C:414:ARG:HG2	1.69	0.57
3:C:600:HIS:HB2	3:C:616:LEU:O	2.04	0.57
1:A:159:THR:HG22	1:A:160:TYR:N	2.19	0.57
4:D:242:CYS:O	4:D:254:THR:HG23	2.05	0.57
1:A:732:LEU:O	1:A:733:LYS:C	2.45	0.57
3:C:536:HIS:HB2	3:C:560:LEU:HD13	1.87	0.57
3:C:622:LEU:HD12	3:C:622:LEU:C	2.29	0.57
1:A:541:VAL:HG12	1:A:618:GLY:O	2.05	0.57
1:A:642:SER:C	1:A:644:LYS:H	2.11	0.57
3:C:493:PRO:HB2	3:C:494:GLN:HE22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:711:HIS:NE2	3:C:713:ARG:N	2.53	0.57
1:A:227:TYR:CD1	1:A:227:TYR:C	2.83	0.57
3:C:890:LEU:HB3	3:C:903:CYS:HB2	1.84	0.57
1:A:197:LEU:HB3	1:A:238:GLU:OE1	2.04	0.57
3:C:477:ARG:HG2	3:C:489:GLU:HG3	1.86	0.56
3:C:578:HIS:CE1	3:C:623:LEU:HD12	2.39	0.56
1:A:660:PHE:C	1:A:662:HIS:H	2.14	0.56
3:C:185:PRO:HG3	4:D:289:ARG:CB	2.30	0.56
1:A:199:LEU:HD13	1:A:209:VAL:CB	2.35	0.56
1:A:390:MET:O	1:A:394:PHE:HB2	2.06	0.56
1:A:422:LYS:NZ	1:A:422:LYS:CB	2.59	0.56
3:C:454:ASP:OD1	3:C:454:ASP:N	2.28	0.56
1:A:84:GLU:HG2	3:C:499:SER:HB3	1.87	0.56
3:C:433:THR:HG22	3:C:434:ARG:H	1.68	0.56
1:A:49:ARG:CD	1:A:51:ARG:HH21	2.18	0.56
3:C:165:ILE:CD1	3:C:188:ARG:HH22	2.19	0.56
3:C:389:ILE:HB	3:C:713:ARG:HB3	1.87	0.56
3:C:502:SER:O	3:C:503:CYS:HB2	2.04	0.56
1:A:129:VAL:CG1	1:A:130:LEU:HG	2.35	0.56
3:C:503:CYS:SG	3:C:504:ASN:N	2.78	0.56
3:C:534:MET:HE2	3:C:558:ILE:HD13	1.87	0.56
3:C:430:VAL:HG12	3:C:431:GLY:N	2.19	0.56
3:C:490:TRP:CG	3:C:491:LYS:H	2.24	0.56
1:A:404:LYS:O	1:A:405:PRO:C	2.49	0.56
1:A:676:GLU:HA	1:A:680:GLU:OE1	2.06	0.56
3:C:403:ASP:HA	3:C:698:THR:HG22	1.88	0.56
1:A:166:THR:O	1:A:168:PRO:HD3	2.06	0.56
1:A:601:MET:CE	1:A:616:ALA:HB2	2.34	0.56
3:C:557:ALA:HB2	3:C:593:MET:HE2	1.88	0.56
3:C:644:LEU:HD12	3:C:706:GLU:OE2	2.06	0.56
3:C:711:HIS:CE1	3:C:712:ILE:C	2.84	0.55
4:D:140:HIS:HB2	4:D:453:ASN:HB2	1.88	0.55
1:A:155:PHE:O	1:A:159:THR:HB	2.06	0.55
1:A:183:ILE:HG23	1:A:221:LEU:HD21	1.88	0.55
1:A:439:LEU:O	1:A:440:PHE:C	2.49	0.55
1:A:643:PRO:HG2	1:A:652:ASP:HA	1.88	0.55
1:A:93:LEU:O	1:A:93:LEU:HD23	2.05	0.55
3:C:522:HIS:HB3	3:C:523:PRO:HD2	1.88	0.55
3:C:525:GLU:OE2	3:C:527:ARG:NH2	2.39	0.55
3:C:433:THR:HG22	3:C:434:ARG:N	2.22	0.55
1:A:197:LEU:HD21	1:A:235:PHE:CA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:184:ASP:C	3:C:184:ASP:OD1	2.48	0.55
3:C:493:PRO:HB2	3:C:494:GLN:NE2	2.21	0.55
1:A:72:ALA:HB3	1:A:79:ILE:HG23	1.88	0.55
1:A:129:VAL:HG13	1:A:130:LEU:HG	1.89	0.55
1:A:227:TYR:HD1	1:A:228:LYS:N	2.04	0.55
1:A:292:LYS:HG3	1:A:330:ARG:NH2	2.22	0.55
1:A:421:ASN:O	1:A:424:ALA:HB2	2.07	0.55
1:A:570:GLN:CG	2:B:32:LEU:HD11	2.37	0.55
3:C:502:SER:OG	3:C:543:ILE:HG12	2.07	0.55
1:A:267:LEU:HD23	1:A:290:VAL:HG11	1.87	0.55
1:A:437:MET:HE3	1:A:478:LYS:HB3	1.89	0.55
3:C:582:LEU:CD1	3:C:583:GLY:H	2.19	0.55
3:C:659:ILE:HG22	3:C:660:TYR:N	2.22	0.55
1:A:448:VAL:O	1:A:452:PHE:HD1	1.90	0.55
3:C:1000:LEU:HD13	3:C:1002:GLU:HB2	1.88	0.55
1:A:472:GLU:HG2	1:A:495:PHE:HZ	1.72	0.54
3:C:431:GLY:O	3:C:432:GLN:HB3	2.07	0.54
3:C:479:VAL:HG12	3:C:480:SER:N	2.22	0.54
3:C:644:LEU:CD1	3:C:706:GLU:OE2	2.55	0.54
3:C:649:VAL:CG1	3:C:650:PHE:H	2.17	0.54
3:C:671:VAL:O	3:C:673:LEU:N	2.38	0.54
1:A:171:TRP:CZ3	1:A:175:LEU:HD11	2.42	0.54
1:A:74:GLN:O	1:A:75:SER:C	2.49	0.54
1:A:699:ALA:CB	1:A:722:GLN:HE21	2.17	0.54
1:A:733:LYS:O	1:A:737:GLU:HG3	2.07	0.54
3:C:448:LEU:HD23	3:C:451:PHE:CE2	2.42	0.54
3:C:532:THR:OG1	3:C:574:PHE:HD2	1.91	0.54
1:A:107:ARG:HH12	1:A:173:MET:HG3	1.63	0.54
1:A:141:ASP:C	1:A:143:CYS:N	2.64	0.54
1:A:81:TYR:O	1:A:82:ASN:ND2	2.41	0.54
1:A:382:LYS:O	1:A:383:ASN:C	2.50	0.54
3:C:83:LYS:HB3	3:C:1072:PHE:CE2	2.42	0.54
3:C:285:LEU:HB3	3:C:297:LEU:HD11	1.89	0.54
3:C:596:PHE:CZ	3:C:649:VAL:HG23	2.43	0.54
1:A:708:LYS:HD3	1:A:708:LYS:H	1.72	0.54
3:C:602:LEU:O	3:C:603:LEU:HD23	2.07	0.54
1:A:630:SER:OG	1:A:672:ILE:HD11	2.07	0.54
3:C:532:THR:CG2	3:C:533:GLU:N	2.69	0.54
1:A:655:ILE:HD12	1:A:655:ILE:N	2.23	0.54
3:C:518:TYR:CD1	3:C:519:LEU:N	2.75	0.54
3:C:931:LEU:HD21	3:C:944:GLU:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HD2	1:A:81:TYR:CD2	2.43	0.53
1:A:84:GLU:O	1:A:87:TYR:HB3	2.08	0.53
1:A:287:ILE:O	1:A:291:GLU:HG3	2.07	0.53
1:A:628:LEU:O	1:A:630:SER:O	2.26	0.53
4:D:124:GLN:O	4:D:124:GLN:HG3	2.08	0.53
1:A:316:VAL:CB	1:A:317:PRO:HD3	2.38	0.53
1:A:57:ASN:C	1:A:59:THR:H	2.14	0.53
1:A:182:ILE:HG22	1:A:183:ILE:HG13	1.89	0.53
3:C:184:ASP:HB2	3:C:185:PRO:CD	2.38	0.53
1:A:347:PHE:CE1	1:A:351:ILE:HD11	2.43	0.53
3:C:571:LEU:O	3:C:572:PRO:C	2.50	0.53
1:A:267:LEU:HD13	1:A:328:ARG:NH1	2.22	0.53
3:C:614:PHE:N	3:C:614:PHE:CD1	2.75	0.53
1:A:206:GLY:O	1:A:207:GLU:C	2.51	0.53
1:A:390:MET:O	1:A:390:MET:HE2	2.09	0.53
3:C:602:LEU:C	3:C:602:LEU:HD13	2.33	0.53
4:D:299:VAL:HA	4:D:326:PRO:HB3	1.89	0.53
6:F:5:DT:H73	6:F:6:DA:N6	2.24	0.53
1:A:406:ALA:HB2	1:A:443:ILE:HG21	1.91	0.53
1:A:468:SER:HB3	1:A:471:ALA:CB	2.39	0.53
1:A:100:PRO:O	1:A:104:LYS:HG3	2.09	0.53
1:A:228:LYS:NZ	1:A:232:GLU:HG2	2.24	0.53
1:A:731:ASP:O	1:A:734:LYS:HB3	2.09	0.53
1:A:676:GLU:O	1:A:676:GLU:HG3	2.09	0.52
1:A:227:TYR:O	1:A:229:ASP:N	2.37	0.52
3:C:289:GLU:HA	3:C:295:VAL:HA	1.89	0.52
1:A:43:LEU:HD11	3:C:400:ALA:CB	2.12	0.52
1:A:204:ARG:CZ	1:A:243:TYR:CE2	2.91	0.52
1:A:544:THR:O	1:A:547:MET:HB2	2.08	0.52
3:C:184:ASP:O	3:C:185:PRO:C	2.50	0.52
1:A:248:GLN:O	1:A:249:ARG:C	2.52	0.52
1:A:390:MET:HE2	1:A:390:MET:C	2.35	0.52
2:B:37:ILE:HG12	2:B:38:VAL:N	2.00	0.52
3:C:525:GLU:OE2	3:C:527:ARG:NE	2.41	0.52
1:A:587:LYS:HE3	1:A:664:LEU:O	2.10	0.52
1:A:709:THR:HG22	1:A:710:LEU:N	2.25	0.52
1:A:735:ARG:NE	1:A:735:ARG:HA	2.24	0.52
3:C:649:VAL:CG1	3:C:650:PHE:N	2.71	0.52
3:C:658:VAL:O	3:C:658:VAL:HG12	2.09	0.52
4:D:119:HIS:O	4:D:121:GLN:N	2.43	0.52
1:A:352:VAL:HG12	1:A:361:MET:SD	2.50	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:SER:HB2	1:A:100:PRO:CD	2.35	0.52
1:A:120:PRO:O	1:A:123:GLU:HG3	2.10	0.52
1:A:625:ARG:O	1:A:629:GLN:N	2.43	0.52
3:C:450:GLY:HA3	3:C:479:VAL:HG22	1.91	0.52
3:C:487:VAL:O	3:C:488:SER:HB2	2.09	0.52
3:C:659:ILE:H	3:C:659:ILE:HD12	1.75	0.52
3:C:679:MET:SD	3:C:679:MET:C	2.93	0.52
1:A:643:PRO:CG	1:A:652:ASP:HA	2.39	0.52
3:C:402:ILE:O	3:C:698:THR:HB	2.10	0.52
1:A:43:LEU:CD1	3:C:402:ILE:HD13	2.40	0.52
1:A:657:ASN:ND2	1:A:659:GLU:HB2	2.11	0.52
1:A:699:ALA:HB1	1:A:722:GLN:HE21	1.61	0.52
1:A:257:PRO:HB3	1:A:318:ASP:OD1	2.10	0.51
1:A:299:LEU:HD23	1:A:326:PHE:CE2	2.45	0.51
3:C:448:LEU:HD23	3:C:451:PHE:HE2	1.75	0.51
3:C:573:SER:O	3:C:574:PHE:HB2	2.10	0.51
1:A:73:VAL:C	1:A:74:GLN:O	2.45	0.51
1:A:609:SER:H	1:A:612:GLU:CG	2.24	0.51
1:A:660:PHE:C	1:A:662:HIS:N	2.67	0.51
3:C:578:HIS:CE1	3:C:623:LEU:CD1	2.94	0.51
4:D:217:THR:OG1	4:D:254:THR:HG21	2.09	0.51
1:A:82:ASN:O	1:A:82:ASN:CG	2.53	0.51
1:A:202:ARG:HH21	1:A:207:GLU:CD	2.19	0.51
1:A:516:SER:O	1:A:517:ASP:O	2.29	0.51
3:C:408:LYS:HA	3:C:678:TYR:CE1	2.46	0.51
1:A:251:MET:HE3	1:A:259:TYR:CZ	2.46	0.51
1:A:390:MET:HE2	1:A:391:LYS:HA	1.92	0.51
3:C:594:THR:CG2	3:C:595:THR:N	2.73	0.51
1:A:55:PRO:O	1:A:56:ASP:HB2	2.11	0.51
1:A:158:ARG:NH1	3:C:633:THR:O	2.44	0.51
1:A:583:LYS:O	1:A:584:GLU:HB2	2.10	0.51
3:C:416:ASP:OD1	3:C:418:ASN:HB2	2.11	0.51
3:C:490:TRP:CG	3:C:491:LYS:N	2.79	0.51
1:A:93:LEU:CD2	1:A:93:LEU:C	2.82	0.51
1:A:107:ARG:HH11	1:A:173:MET:HG3	1.72	0.51
1:A:748:ASP:C	1:A:750:ASP:H	2.17	0.51
1:A:757:TYR:HD1	1:A:758:VAL:N	2.09	0.51
3:C:471:ILE:HA	3:C:476:VAL:HA	1.92	0.51
1:A:183:ILE:HD13	1:A:221:LEU:CD2	2.41	0.51
1:A:501:SER:O	1:A:505:MET:HB2	2.11	0.51
3:C:105:HIS:CD2	3:C:1067:LYS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:459:PHE:CD2	3:C:460:CYS:N	2.79	0.51
1:A:630:SER:C	1:A:632:ALA:N	2.67	0.50
1:A:705:LYS:HD3	1:A:705:LYS:C	2.35	0.50
3:C:561:TRP:HA	3:C:587:ILE:HG21	1.92	0.50
1:A:119:LEU:HB2	1:A:120:PRO:CD	2.37	0.50
1:A:122:ARG:CZ	1:A:186:LYS:HZ3	2.23	0.50
1:A:228:LYS:CD	1:A:232:GLU:HG2	2.41	0.50
1:A:417:LEU:HD23	1:A:460:ARG:NH1	2.26	0.50
1:A:130:LEU:O	1:A:131:PHE:C	2.54	0.50
1:A:131:PHE:CD1	1:A:191:LYS:CE	2.95	0.50
1:A:369:LYS:HE2	1:A:390:MET:HE1	1.94	0.50
1:A:602:PHE:N	1:A:602:PHE:CD1	2.79	0.50
1:A:632:ALA:O	1:A:633:CYS:C	2.55	0.50
3:C:512:VAL:HB	3:C:515:ALA:HB3	1.94	0.50
1:A:45:ILE:HD11	3:C:404:LEU:HD21	1.92	0.50
1:A:186:LYS:CB	1:A:188:VAL:HG23	2.40	0.50
3:C:570:LYS:O	3:C:574:PHE:N	2.41	0.50
3:C:613:TYR:CE1	3:C:627:LYS:HB2	2.47	0.50
1:A:96:HIS:O	1:A:97:LYS:HB2	2.11	0.50
1:A:207:GLU:O	1:A:208:ALA:O	2.30	0.50
1:A:380:PHE:CD2	1:A:386:PHE:CD2	3.00	0.50
3:C:183:GLN:HA	3:C:188:ARG:HA	1.94	0.50
3:C:663:ASN:HD21	3:C:1131:LYS:HB3	1.76	0.50
4:D:122:LEU:O	4:D:123:ARG:C	2.54	0.50
1:A:203:GLU:C	1:A:205:SER:N	2.70	0.50
1:A:705:LYS:HA	1:A:757:TYR:CE2	2.43	0.50
2:B:38:VAL:O	2:B:39:VAL:C	2.55	0.50
1:A:135:ILE:CD1	1:A:188:VAL:HG12	2.30	0.50
1:A:182:ILE:O	1:A:188:VAL:HG11	2.12	0.50
1:A:587:LYS:HD2	1:A:587:LYS:N	2.25	0.50
3:C:451:PHE:HD1	3:C:470:GLN:HB2	1.74	0.50
1:A:173:MET:O	1:A:173:MET:HG2	2.11	0.49
1:A:271:GLY:C	1:A:273:ARG:H	2.20	0.49
3:C:492:GLU:CG	3:C:496:LYS:HB2	2.42	0.49
1:A:92:ASN:ND2	3:C:408:LYS:HZ1	2.11	0.49
1:A:206:GLY:O	1:A:207:GLU:O	2.30	0.49
1:A:757:TYR:CE1	1:A:759:ALA:HA	2.37	0.49
3:C:893:TRP:HE3	3:C:899:LEU:HD13	1.77	0.49
1:A:707:ARG:O	1:A:709:THR:O	2.30	0.49
1:A:710:LEU:O	1:A:711:GLY:O	2.30	0.49
3:C:514:ARG:HG3	3:C:514:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:612:PHE:CE2	3:C:628:LYS:HD2	2.47	0.49
3:C:668:PHE:CD1	3:C:668:PHE:N	2.80	0.49
3:C:715:VAL:HG12	3:C:715:VAL:O	2.12	0.49
3:C:1054:MET:SD	3:C:1129:LEU:HD11	2.52	0.49
4:D:211:SER:HB3	4:D:243:VAL:HG13	1.94	0.49
1:A:82:ASN:OD1	1:A:82:ASN:O	2.30	0.49
1:A:330:ARG:H	1:A:330:ARG:CD	2.26	0.49
1:A:412:HIS:HE1	1:A:416:LYS:HE3	1.77	0.49
1:A:710:LEU:O	1:A:711:GLY:C	2.55	0.49
3:C:704:ILE:O	3:C:705:ASP:CB	2.57	0.49
1:A:347:PHE:O	1:A:351:ILE:HG13	2.12	0.49
3:C:596:PHE:CE2	3:C:659:ILE:HG22	2.48	0.49
3:C:709:LYS:O	3:C:710:LEU:O	2.30	0.49
4:D:256:ASP:OD2	4:D:260:ARG:HB2	2.13	0.49
1:A:457:LEU:HD22	1:A:461:LEU:HD12	1.94	0.49
1:A:505:MET:HE3	1:A:525:VAL:O	2.13	0.49
3:C:594:THR:HG23	3:C:595:THR:N	2.28	0.49
3:C:596:PHE:HZ	3:C:649:VAL:HG23	1.78	0.49
4:D:111:LYS:HE2	4:D:118:ILE:CB	2.43	0.49
1:A:193:ILE:C	1:A:195:GLY:N	2.68	0.49
1:A:203:GLU:O	1:A:205:SER:N	2.45	0.49
1:A:256:VAL:O	1:A:257:PRO:C	2.56	0.49
1:A:349:THR:C	1:A:351:ILE:H	2.21	0.49
1:A:469:VAL:HG12	1:A:473:LYS:HE3	1.94	0.49
1:A:696:ILE:CD1	1:A:725:PHE:CZ	2.93	0.49
3:C:490:TRP:CD2	3:C:491:LYS:N	2.81	0.49
1:A:197:LEU:CD2	1:A:235:PHE:CA	2.80	0.49
1:A:440:PHE:CE2	1:A:446:LYS:HD3	2.47	0.49
2:B:21:ARG:O	2:B:22:PHE:CD1	2.66	0.49
3:C:578:HIS:HD2	3:C:623:LEU:H	1.55	0.49
1:A:49:ARG:CD	1:A:51:ARG:NH2	2.75	0.49
1:A:124:ASP:OD1	1:A:124:ASP:N	2.46	0.49
1:A:726:PRO:O	1:A:727:VAL:CB	2.60	0.49
1:A:453:TYR:CD1	1:A:453:TYR:C	2.91	0.48
1:A:649:GLU:HB2	1:A:652:ASP:OD2	2.13	0.48
3:C:731:GLN:HA	3:C:796:GLN:HE21	1.78	0.48
1:A:300:THR:O	1:A:304:GLN:HB2	2.13	0.48
1:A:751:ASN:O	1:A:751:ASN:ND2	2.46	0.48
3:C:587:ILE:HD12	3:C:587:ILE:H	1.78	0.48
3:C:770:LEU:HD13	3:C:865:GLU:HB2	1.96	0.48
4:D:272:PHE:HE2	4:D:312:LYS:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:TRP:HH2	1:A:102:LEU:CA	2.25	0.48
1:A:92:ASN:ND2	3:C:408:LYS:NZ	2.61	0.48
3:C:182:TYR:O	3:C:188:ARG:CA	2.61	0.48
3:C:641:PHE:CE2	3:C:650:PHE:HB2	2.48	0.48
1:A:82:ASN:O	1:A:83:LEU:O	2.31	0.48
1:A:131:PHE:CE2	1:A:188:VAL:CG1	2.91	0.48
1:A:197:LEU:HD11	1:A:234:LYS:HB3	1.94	0.48
1:A:457:LEU:O	1:A:460:ARG:N	2.47	0.48
2:B:38:VAL:O	2:B:39:VAL:O	2.30	0.48
1:A:251:MET:HE3	1:A:259:TYR:CE1	2.48	0.48
1:A:307:LEU:O	1:A:308:ASP:C	2.56	0.48
3:C:565:SER:OG	3:C:567:ARG:NH1	2.46	0.48
3:C:641:PHE:HB2	3:C:681:PRO:HG3	1.94	0.48
3:C:659:ILE:O	3:C:660:TYR:HB3	2.14	0.48
3:C:1136:LEU:O	3:C:1139:ILE:HG12	2.13	0.48
1:A:515:GLN:O	1:A:515:GLN:HG2	2.14	0.48
1:A:541:VAL:HG23	1:A:543:LEU:CD2	2.43	0.48
3:C:443:VAL:O	3:C:443:VAL:HG12	2.13	0.48
1:A:315:ARG:O	1:A:319:LEU:HG	2.14	0.48
3:C:1109:VAL:O	3:C:1111:ASN:N	2.42	0.48
1:A:624:LEU:HD22	1:A:628:LEU:CD1	2.44	0.48
1:A:712:HIS:C	1:A:712:HIS:CD2	2.90	0.48
1:A:149:ILE:O	1:A:150:ARG:C	2.56	0.48
1:A:193:ILE:C	1:A:195:GLY:H	2.22	0.48
1:A:545:PRO:O	1:A:546:GLU:C	2.56	0.48
3:C:184:ASP:C	3:C:186:GLN:N	2.72	0.48
3:C:457:THR:HG22	3:C:458:PHE:N	2.29	0.48
1:A:401:ARG:NH2	1:A:404:LYS:HG3	2.29	0.48
1:A:448:VAL:O	1:A:451:ALA:HB3	2.14	0.48
1:A:692:ARG:HB3	1:A:725:PHE:HE2	1.69	0.48
1:A:719:LEU:HD22	1:A:723:LEU:HD21	1.96	0.48
1:A:106:LEU:HD22	1:A:153:PHE:CD2	2.49	0.47
1:A:529:THR:HA	2:B:33:TRP:CD1	2.49	0.47
1:A:629:GLN:O	1:A:633:CYS:HB2	2.14	0.47
1:A:450:GLU:OE2	1:A:454:LYS:HE3	2.14	0.47
1:A:544:THR:HG23	1:A:545:PRO:HD2	1.96	0.47
3:C:459:PHE:O	3:C:460:CYS:HB3	2.13	0.47
3:C:479:VAL:CG1	3:C:480:SER:N	2.77	0.47
4:D:394:PRO:HB3	4:D:402:ASP:HB3	1.96	0.47
1:A:70:VAL:HG21	1:A:106:LEU:HD13	1.95	0.47
1:A:84:GLU:O	1:A:85:GLU:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:459:PHE:CG	3:C:460:CYS:N	2.82	0.47
1:A:417:LEU:CD2	1:A:460:ARG:HH12	2.27	0.47
3:C:587:ILE:HD12	3:C:587:ILE:N	2.29	0.47
1:A:341:SER:HB3	1:A:389:LEU:HD12	1.97	0.47
1:A:588:GLU:O	1:A:666:ARG:HA	2.15	0.47
1:A:609:SER:O	1:A:610:PHE:C	2.57	0.47
3:C:450:GLY:O	3:C:477:ARG:NH2	2.46	0.47
3:C:1048:TYR:O	3:C:1052:LEU:HB2	2.15	0.47
1:A:74:GLN:HA	1:A:145:GLN:NE2	2.30	0.47
1:A:170:ILE:O	1:A:173:MET:HB3	2.14	0.47
1:A:196:ILE:HG21	1:A:231:PHE:CE1	2.50	0.47
1:A:241:CYS:O	1:A:244:ALA:HB3	2.15	0.47
1:A:308:ASP:OD1	1:A:343:TYR:HD2	1.97	0.47
1:A:627:THR:O	1:A:631:LEU:HD23	2.14	0.47
1:A:641:LYS:HE2	1:A:647:GLU:O	2.14	0.47
1:A:751:ASN:N	1:A:751:ASN:ND2	2.61	0.47
3:C:189:HIS:CD2	3:C:189:HIS:N	2.83	0.47
3:C:433:THR:O	3:C:434:ARG:HG3	2.14	0.47
3:C:611:LEU:C	3:C:611:LEU:HD23	2.40	0.47
3:C:657:THR:HG22	3:C:658:VAL:N	2.25	0.47
3:C:663:ASN:HD21	3:C:1131:LYS:CB	2.27	0.47
1:A:110:CYS:O	1:A:111:GLU:C	2.58	0.47
1:A:707:ARG:HD3	1:A:710:LEU:HD13	1.96	0.47
1:A:95:SER:O	1:A:96:HIS:O	2.33	0.47
1:A:135:ILE:HG23	1:A:220:MET:HE1	1.97	0.47
1:A:638:VAL:HG12	1:A:639:LEU:CD2	2.31	0.47
3:C:385:GLY:HA3	3:C:719:GLU:O	2.14	0.47
3:C:579:LYS:HE3	3:C:581:MET:CE	2.45	0.47
1:A:200:ILE:O	1:A:201:GLU:C	2.58	0.47
1:A:204:ARG:NH2	1:A:270:GLU:CD	2.66	0.47
1:A:757:TYR:CD1	1:A:758:VAL:N	2.82	0.47
3:C:43:VAL:HG21	3:C:50:ARG:CZ	2.45	0.47
3:C:403:ASP:O	3:C:405:PRO:HD3	2.15	0.47
1:A:263:VAL:HG11	1:A:295:LEU:HD21	1.97	0.46
3:C:438:LEU:CD1	3:C:684:SER:HB2	2.46	0.46
3:C:638:LEU:O	3:C:639:ARG:HG2	2.15	0.46
1:A:592:SER:HB2	1:A:673:GLN:NE2	2.29	0.46
1:A:696:ILE:CG1	1:A:725:PHE:HZ	2.28	0.46
1:A:732:LEU:O	1:A:735:ARG:N	2.45	0.46
3:C:407:ILE:CD1	3:C:699:LEU:HB2	2.44	0.46
3:C:531:HIS:ND1	3:C:532:THR:N	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:704:ILE:HD12	3:C:704:ILE:N	2.30	0.46
3:C:1055:GLN:NE2	3:C:1090:ASP:H	2.09	0.46
1:A:196:ILE:HD13	1:A:218:LEU:HD23	1.93	0.46
1:A:204:ARG:NE	1:A:243:TYR:OH	2.48	0.46
1:A:482:GLU:O	1:A:483:CYS:HB2	2.14	0.46
3:C:396:ILE:HD13	3:C:396:ILE:O	2.15	0.46
1:A:189:GLN:CD	1:A:230:SER:HB3	2.41	0.46
3:C:596:PHE:CZ	3:C:659:ILE:HG22	2.50	0.46
1:A:321:GLN:O	1:A:325:LEU:HD12	2.16	0.46
1:A:601:MET:CE	1:A:616:ALA:HB3	2.40	0.46
3:C:402:ILE:HG22	3:C:403:ASP:H	1.80	0.46
3:C:656:PRO:HG2	3:C:676:VAL:HG23	1.97	0.46
1:A:83:LEU:O	1:A:85:GLU:N	2.49	0.46
1:A:651:GLY:O	1:A:652:ASP:C	2.57	0.46
3:C:576:LEU:C	3:C:577:LEU:HD23	2.41	0.46
1:A:200:ILE:O	1:A:203:GLU:N	2.25	0.46
1:A:303:LEU:HD23	1:A:322:MET:CE	2.46	0.46
1:A:440:PHE:CZ	1:A:446:LYS:HD3	2.51	0.46
3:C:312:GLU:HG3	3:C:327:ARG:HD2	1.98	0.46
3:C:414:ARG:HB3	3:C:462:ASN:ND2	2.29	0.46
3:C:695:ASN:OD1	3:C:698:THR:N	2.41	0.46
3:C:641:PHE:CD1	3:C:641:PHE:C	2.93	0.46
1:A:113:HIS:O	1:A:117:GLN:HG2	2.16	0.46
1:A:184:SER:O	1:A:185:ASP:C	2.58	0.46
1:A:219:GLY:O	1:A:220:MET:C	2.57	0.46
1:A:534:PRO:HB2	1:A:536:TYR:CE1	2.51	0.46
3:C:23:PHE:N	3:C:30:ASN:ND2	2.59	0.46
3:C:953:TRP:HB2	3:C:970:ASN:HB2	1.98	0.46
1:A:131:PHE:CZ	1:A:188:VAL:HG22	2.51	0.46
1:A:375:VAL:HG13	1:A:379:CYS:HB2	1.98	0.46
1:A:587:LYS:HD3	1:A:660:PHE:CE2	2.51	0.46
3:C:407:ILE:HD11	3:C:699:LEU:HB2	1.98	0.46
3:C:442:GLU:HG3	3:C:443:VAL:H	1.81	0.46
3:C:512:VAL:O	3:C:515:ALA:HB3	2.15	0.46
3:C:889:ARG:HD2	3:C:891:TYR:CZ	2.51	0.46
1:A:491:LEU:HA	1:A:494:MET:CG	2.33	0.45
6:F:5:DT:C7	6:F:6:DA:C6	2.99	0.45
1:A:267:LEU:CD2	1:A:290:VAL:HG11	2.46	0.45
1:A:587:LYS:HB2	1:A:660:PHE:CE2	2.51	0.45
3:C:490:TRP:O	3:C:491:LYS:HB2	2.15	0.45
3:C:705:ASP:O	3:C:706:GLU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:869:ALA:H	3:C:885:ASN:ND2	2.14	0.45
1:A:141:ASP:O	1:A:142:HIS:C	2.58	0.45
1:A:179:ARG:O	1:A:184:SER:HB3	2.16	0.45
1:A:341:SER:CB	1:A:389:LEU:HD12	2.46	0.45
1:A:433:LEU:HD23	1:A:478:LYS:HE3	1.97	0.45
3:C:396:ILE:N	3:C:396:ILE:CD1	2.79	0.45
3:C:411:TRP:HB2	3:C:460:CYS:SG	2.56	0.45
1:A:55:PRO:O	1:A:56:ASP:CB	2.64	0.45
1:A:98:VAL:O	1:A:99:SER:C	2.59	0.45
1:A:303:LEU:HD13	1:A:339:HIS:CD2	2.52	0.45
1:A:512:MET:HE2	1:A:512:MET:CA	2.44	0.45
1:A:527:ILE:O	1:A:527:ILE:CG2	2.65	0.45
2:B:20:LYS:HE3	2:B:20:LYS:HB2	1.72	0.45
3:C:641:PHE:HB3	3:C:679:MET:HE1	1.98	0.45
1:A:100:PRO:HG3	1:A:160:TYR:CZ	2.51	0.45
3:C:830:ILE:HG22	3:C:873:MET:HE1	1.99	0.45
1:A:196:ILE:HG21	1:A:218:LEU:HD21	1.99	0.45
1:A:227:TYR:C	1:A:229:ASP:H	2.24	0.45
1:A:294:LEU:C	1:A:295:LEU:HD23	2.41	0.45
3:C:312:GLU:HG3	3:C:327:ARG:CD	2.47	0.45
3:C:643:SER:O	3:C:644:LEU:C	2.59	0.45
1:A:292:LYS:O	1:A:293:GLN:HG2	2.17	0.45
1:A:295:LEU:HD11	1:A:325:LEU:HD22	1.99	0.45
2:B:37:ILE:HD12	2:B:37:ILE:H	1.82	0.45
3:C:921:ILE:HB	3:C:933:LEU:HB2	1.99	0.45
4:D:123:ARG:HA	4:D:126:LEU:HD12	1.97	0.45
3:C:534:MET:CE	3:C:569:LEU:HD11	2.47	0.45
3:C:663:ASN:HD21	3:C:1131:LYS:HG2	1.81	0.45
1:A:114:VAL:O	1:A:117:GLN:N	2.50	0.45
1:A:141:ASP:OD2	1:A:144:ARG:NH2	2.46	0.45
1:A:200:ILE:O	1:A:202:ARG:N	2.50	0.45
1:A:460:ARG:NH1	1:A:472:GLU:OE2	2.49	0.45
1:A:580:ALA:HB2	2:B:22:PHE:HE1	1.82	0.45
3:C:478:LEU:HB3	3:C:488:SER:HB3	1.99	0.45
3:C:926:LEU:HD21	4:D:129:PRO:HG3	1.99	0.45
1:A:90:VAL:O	1:A:91:GLU:C	2.58	0.45
1:A:93:LEU:HD22	1:A:93:LEU:C	2.42	0.45
1:A:264:SER:O	1:A:268:GLU:HG2	2.17	0.45
1:A:329:VAL:CG1	1:A:330:ARG:H	2.23	0.45
2:B:19:LYS:HA	2:B:19:LYS:CE	2.35	0.45
3:C:390:ILE:HG22	3:C:391:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:557:ALA:N	3:C:593:MET:HE2	2.32	0.45
3:C:597:GLU:O	3:C:598:SER:HB3	2.16	0.45
3:C:607:GLY:HA2	3:C:635:PRO:HB3	1.99	0.45
3:C:705:ASP:OD1	3:C:705:ASP:C	2.60	0.45
1:A:61:ASP:O	1:A:65:LYS:HG3	2.17	0.44
1:A:434:ASP:O	1:A:438:ILE:HG13	2.18	0.44
1:A:601:MET:HB3	1:A:608:PHE:CE2	2.49	0.44
1:A:668:LYS:NZ	1:A:670:ASN:HB3	2.32	0.44
4:D:388:ILE:O	4:D:408:ILE:HA	2.17	0.44
1:A:70:VAL:O	1:A:72:ALA:N	2.50	0.44
1:A:526:ASN:HD22	1:A:526:ASN:HA	1.61	0.44
1:A:610:PHE:C	1:A:610:PHE:CD1	2.94	0.44
1:A:757:TYR:CD1	1:A:757:TYR:C	2.95	0.44
3:C:707:ILE:HG23	3:C:708:GLN:H	1.80	0.44
1:A:135:ILE:CG2	1:A:220:MET:HE1	2.46	0.44
1:A:274:VAL:CG1	1:A:283:GLN:HE21	2.23	0.44
3:C:476:VAL:HG22	3:C:526:LEU:CD1	2.47	0.44
3:C:580:GLU:OE2	3:C:626:ARG:HD2	2.17	0.44
3:C:740:ILE:HG23	3:C:785:GLU:HG3	1.99	0.44
3:C:1057:ARG:HH12	3:C:1110:ALA:HB3	1.83	0.44
1:A:610:PHE:CE1	1:A:614:LYS:HE3	2.52	0.44
3:C:451:PHE:HE1	3:C:470:GLN:HB2	1.79	0.44
3:C:528:GLN:O	3:C:528:GLN:HG2	2.16	0.44
3:C:546:LEU:O	3:C:549:SER:HB3	2.17	0.44
4:D:117:SER:O	4:D:118:ILE:C	2.60	0.44
1:A:234:LYS:O	1:A:235:PHE:C	2.59	0.44
1:A:696:ILE:HG12	1:A:725:PHE:HZ	1.81	0.44
3:C:629:VAL:HG23	3:C:630:THR:N	2.31	0.44
3:C:165:ILE:HG13	3:C:188:ARG:NH1	2.33	0.44
3:C:447:GLU:O	3:C:448:LEU:HD12	2.18	0.44
3:C:586:ILE:HG22	3:C:607:GLY:H	1.83	0.44
3:C:692:ALA:O	3:C:693:LEU:HD23	2.18	0.44
3:C:81:THR:HG21	3:C:85:ASN:ND2	2.22	0.44
1:A:90:VAL:O	1:A:92:ASN:N	2.51	0.44
1:A:184:SER:O	1:A:186:LYS:N	2.50	0.44
1:A:623:GLU:O	1:A:624:LEU:C	2.61	0.44
1:A:758:VAL:HG12	1:A:758:VAL:O	2.17	0.44
1:A:143:CYS:O	1:A:147:ILE:HG13	2.17	0.44
1:A:222:SER:O	1:A:224:LEU:N	2.51	0.44
1:A:227:TYR:CD1	1:A:228:LYS:N	2.83	0.44
1:A:657:ASN:CG	1:A:658:GLY:N	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:396:ILE:HD13	3:C:396:ILE:N	2.29	0.44
1:A:65:LYS:HD2	1:A:81:TYR:HD2	1.82	0.43
1:A:70:VAL:CG2	1:A:106:LEU:HD11	2.47	0.43
1:A:127:ASP:C	1:A:129:VAL:H	2.25	0.43
1:A:146:MET:HE2	1:A:149:ILE:HD12	1.99	0.43
4:D:382:HIS:CG	4:D:383:PRO:HD2	2.53	0.43
3:C:659:ILE:CG2	3:C:660:TYR:N	2.80	0.43
1:A:412:HIS:CE1	1:A:416:LYS:HE3	2.53	0.43
1:A:693:GLN:O	1:A:696:ILE:HB	2.18	0.43
3:C:430:VAL:O	3:C:456:GLN:HB2	2.18	0.43
3:C:532:THR:CG2	3:C:533:GLU:H	2.31	0.43
1:A:90:VAL:O	1:A:94:CYS:N	2.42	0.43
1:A:725:PHE:HB2	1:A:726:PRO:CD	2.47	0.43
3:C:419:ARG:HD3	3:C:421:THR:O	2.18	0.43
3:C:429:PHE:O	3:C:456:GLN:HG3	2.18	0.43
3:C:582:LEU:CD1	3:C:583:GLY:N	2.81	0.43
3:C:663:ASN:HD21	3:C:1131:LYS:CG	2.30	0.43
3:C:893:TRP:CE3	3:C:899:LEU:HD13	2.54	0.43
1:A:704:MET:O	1:A:757:TYR:HB2	2.18	0.43
3:C:185:PRO:HB2	3:C:186:GLN:NE2	2.33	0.43
1:A:183:ILE:CG2	1:A:221:LEU:HD21	2.48	0.43
1:A:240:ASN:CG	1:A:289:CYS:HB3	2.42	0.43
1:A:428:GLU:O	1:A:432:THR:HG23	2.18	0.43
3:C:428:SER:OG	3:C:456:GLN:HG2	2.18	0.43
3:C:586:ILE:HG21	3:C:608:ASP:N	2.34	0.43
5:E:10:DG:C2	6:F:4:DG:C2	3.06	0.43
1:A:63:TRP:CH2	1:A:102:LEU:HG	2.53	0.43
1:A:523:LEU:HD11	1:A:525:VAL:CG2	2.49	0.43
1:A:681:GLN:C	1:A:681:GLN:HE21	2.27	0.43
3:C:532:THR:HG22	3:C:533:GLU:H	1.80	0.43
4:D:279:ALA:HB1	4:D:299:VAL:HG22	2.01	0.43
1:A:118:ILE:O	1:A:119:LEU:C	2.62	0.43
1:A:121:PHE:C	1:A:123:GLU:H	2.27	0.43
1:A:440:PHE:O	1:A:442:PHE:N	2.51	0.43
1:A:450:GLU:HG3	1:A:451:ALA:N	2.34	0.43
4:D:383:PRO:HG3	4:D:435:SER:O	2.18	0.43
1:A:279:ASP:O	1:A:281:SER:N	2.52	0.43
1:A:311:LEU:HD11	1:A:340:TRP:HD1	1.84	0.43
1:A:600:LEU:O	1:A:601:MET:C	2.61	0.43
3:C:889:ARG:CD	3:C:901:THR:HB	2.45	0.43
3:C:1097:PHE:O	3:C:1100:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ILE:C	1:A:202:ARG:N	2.74	0.42
1:A:544:THR:O	1:A:545:PRO:C	2.60	0.42
1:A:555:LYS:HD2	1:A:569:TRP:CZ3	2.47	0.42
1:A:583:LYS:O	1:A:584:GLU:CB	2.66	0.42
1:A:643:PRO:O	1:A:644:LYS:C	2.62	0.42
3:C:407:ILE:HD13	3:C:699:LEU:HD23	2.01	0.42
1:A:131:PHE:CZ	1:A:188:VAL:CB	2.75	0.42
3:C:494:GLN:O	3:C:495:ALA:HB3	2.19	0.42
3:C:505:SER:OG	3:C:506:SER:N	2.51	0.42
3:C:657:THR:CG2	3:C:668:PHE:HB3	2.48	0.42
3:C:697:SER:C	3:C:698:THR:HG23	2.43	0.42
4:D:367:PRO:HG2	4:D:392:ARG:HG3	2.01	0.42
1:A:437:MET:O	1:A:440:PHE:HB3	2.19	0.42
1:A:542:HIS:HB2	1:A:617:THR:HA	2.00	0.42
1:A:592:SER:OG	1:A:595:GLN:HG3	2.19	0.42
1:A:696:ILE:CG1	1:A:725:PHE:CZ	3.01	0.42
3:C:500:VAL:HG12	3:C:541:LEU:HD12	2.01	0.42
3:C:603:LEU:HD23	3:C:603:LEU:N	2.33	0.42
3:C:703:THR:O	3:C:704:ILE:C	2.62	0.42
1:A:141:ASP:O	1:A:145:GLN:HG2	2.19	0.42
1:A:399:ASN:ND2	1:A:444:HIS:CE1	2.87	0.42
1:A:541:VAL:HG23	1:A:543:LEU:HD21	2.02	0.42
1:A:617:THR:OG1	1:A:618:GLY:N	2.50	0.42
3:C:357:GLY:HA2	3:C:358:PRO:C	2.44	0.42
4:D:323:HIS:CD2	4:D:342:THR:HG21	2.53	0.42
4:D:391:GLY:HA3	4:D:429:ILE:O	2.19	0.42
1:A:496:LYS:HD3	1:A:496:LYS:HA	1.84	0.42
1:A:686:GLU:C	1:A:688:VAL:H	2.27	0.42
3:C:579:LYS:CG	3:C:581:MET:HE3	2.46	0.42
3:C:1030:PHE:CZ	3:C:1038:GLY:HA3	2.55	0.42
5:E:4:DA:C2	6:F:10:DA:C2	3.07	0.42
1:A:59:THR:O	1:A:63:TRP:HD1	2.02	0.42
1:A:425:THR:HG22	1:A:426:ASP:N	2.35	0.42
1:A:530:MET:HB2	2:B:33:TRP:O	2.19	0.42
1:A:555:LYS:HB2	1:A:569:TRP:HH2	1.84	0.42
1:A:578:LEU:HD13	1:A:591:VAL:HG21	1.99	0.42
3:C:356:LEU:CD2	3:C:712:ILE:HG21	2.49	0.42
3:C:492:GLU:CD	3:C:496:LYS:HB2	2.44	0.42
3:C:1102:ARG:N	3:C:1103:PRO:HD2	2.35	0.42
1:A:72:ALA:HB1	1:A:77:THR:HB	2.01	0.42
1:A:118:ILE:CG1	1:A:181:HIS:CB	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:CG2	1:A:183:ILE:HG13	2.50	0.42
3:C:230:ILE:HD11	3:C:285:LEU:HD21	2.02	0.42
1:A:75:SER:O	1:A:77:THR:N	2.53	0.42
1:A:218:LEU:HD12	1:A:277:TYR:HB2	2.00	0.42
3:C:557:ALA:H	3:C:593:MET:HE2	1.85	0.42
3:C:643:SER:OG	3:C:644:LEU:N	2.47	0.42
3:C:969:GLU:CD	3:C:971:ALA:H	2.26	0.42
1:A:488:THR:O	1:A:489:SER:C	2.63	0.42
1:A:707:ARG:HD3	1:A:710:LEU:HD22	2.02	0.42
3:C:218:MET:CE	3:C:261:HIS:HD2	2.22	0.42
3:C:404:LEU:HD12	3:C:429:PHE:CZ	2.55	0.42
3:C:578:HIS:CG	3:C:623:LEU:HD12	2.54	0.42
4:D:289:ARG:NH2	4:D:335:THR:O	2.53	0.42
1:A:640:ILE:O	1:A:655:ILE:HD12	2.20	0.42
3:C:563:ASP:OD2	3:C:565:SER:HB3	2.20	0.42
1:A:536:TYR:CD2	1:A:573:LEU:HD11	2.54	0.41
1:A:539:MET:HE3	1:A:619:ILE:HA	2.02	0.41
3:C:185:PRO:HD3	4:D:289:ARG:CB	2.28	0.41
3:C:592:LEU:HD23	3:C:592:LEU:C	2.45	0.41
3:C:1109:VAL:C	3:C:1111:ASN:H	2.25	0.41
1:A:70:VAL:C	1:A:72:ALA:N	2.77	0.41
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.91	0.41
1:A:597:LEU:HA	1:A:600:LEU:HD12	2.01	0.41
3:C:404:LEU:HD13	3:C:404:LEU:HA	1.89	0.41
3:C:571:LEU:HD23	3:C:571:LEU:HA	1.87	0.41
3:C:708:GLN:HB3	3:C:709:LYS:H	1.60	0.41
1:A:267:LEU:HD21	1:A:290:VAL:HG12	2.03	0.41
1:A:461:LEU:HB3	1:A:498:MET:CE	2.48	0.41
3:C:24:THR:H	3:C:30:ASN:ND2	2.18	0.41
3:C:184:ASP:CB	3:C:185:PRO:CD	2.97	0.41
3:C:185:PRO:CD	4:D:289:ARG:CB	2.78	0.41
3:C:523:PRO:HB3	3:C:524:GLN:NE2	2.35	0.41
3:C:534:MET:HE2	3:C:569:LEU:HD11	2.00	0.41
1:A:49:ARG:HA	1:A:49:ARG:NE	2.35	0.41
1:A:74:GLN:NE2	1:A:110:CYS:HA	2.15	0.41
1:A:110:CYS:C	1:A:112:ASP:N	2.76	0.41
1:A:232:GLU:O	1:A:235:PHE:HB3	2.20	0.41
1:A:450:GLU:O	1:A:451:ALA:C	2.63	0.41
1:A:744:TYR:O	1:A:757:TYR:O	2.38	0.41
3:C:416:ASP:OD1	3:C:416:ASP:C	2.63	0.41
3:C:429:PHE:O	3:C:430:VAL:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:469:ILE:HD13	3:C:469:ILE:C	2.45	0.41
3:C:602:LEU:HD22	3:C:603:LEU:N	2.34	0.41
3:C:673:LEU:HD23	3:C:674:LYS:N	2.33	0.41
4:D:347:ASN:HA	4:D:366:HIS:O	2.21	0.41
1:A:79:ILE:H	1:A:79:ILE:CD1	2.23	0.41
1:A:123:GLU:HB3	1:A:124:ASP:H	1.61	0.41
1:A:131:PHE:O	1:A:134:LYS:HB2	2.21	0.41
1:A:232:GLU:O	1:A:233:LEU:C	2.64	0.41
1:A:250:LEU:HD22	1:A:254:ARG:HD3	2.01	0.41
1:A:408:LEU:O	1:A:409:ILE:C	2.63	0.41
3:C:567:ARG:HB3	3:C:579:LYS:HA	2.01	0.41
3:C:580:GLU:C	3:C:581:MET:HE2	2.45	0.41
3:C:711:HIS:CE1	3:C:713:ARG:N	2.88	0.41
1:A:63:TRP:HZ3	1:A:102:LEU:HA	1.75	0.41
3:C:182:TYR:O	3:C:188:ARG:HA	2.20	0.41
4:D:170:GLY:C	4:D:195:ILE:HD11	2.45	0.41
1:A:141:ASP:CG	1:A:144:ARG:HH12	2.28	0.41
1:A:543:LEU:N	1:A:543:LEU:HD22	2.36	0.41
1:A:581:GLU:HB2	2:B:21:ARG:CA	2.43	0.41
1:A:734:LYS:HD3	1:A:737:GLU:OE1	2.21	0.41
1:A:751:ASN:HD21	1:A:754:GLN:HB2	1.86	0.41
1:A:757:TYR:O	1:A:758:VAL:CB	2.65	0.41
3:C:699:LEU:HD13	3:C:700:THR:N	2.35	0.41
6:F:6:DA:C2	6:F:7:DA:N6	2.88	0.41
1:A:74:GLN:HB3	1:A:113:HIS:CE1	2.55	0.41
1:A:578:LEU:HD13	1:A:591:VAL:HG23	1.99	0.41
1:A:650:ASP:OD1	1:A:650:ASP:N	2.53	0.41
1:A:715:LEU:C	1:A:717:SER:N	2.77	0.41
3:C:389:ILE:HD13	3:C:713:ARG:CG	2.45	0.41
1:A:51:ARG:N	1:A:52:PRO:HD2	2.33	0.41
1:A:57:ASN:C	1:A:59:THR:N	2.74	0.41
1:A:309:HIS:C	1:A:309:HIS:CD2	2.97	0.41
1:A:414:ASP:O	1:A:418:ARG:HG3	2.21	0.41
1:A:428:GLU:H	1:A:428:GLU:HG3	1.63	0.41
1:A:454:LYS:HE2	1:A:490:LYS:HD2	2.02	0.41
1:A:578:LEU:HA	2:B:23:GLU:O	2.20	0.41
1:A:587:LYS:HB2	1:A:660:PHE:CZ	2.55	0.41
1:A:598:VAL:O	1:A:599:LEU:C	2.64	0.41
1:A:734:LYS:HA	1:A:737:GLU:OE2	2.20	0.41
1:A:735:ARG:HA	1:A:735:ARG:HE	1.84	0.41
3:C:413:LEU:HB3	3:C:414:ARG:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:457:THR:CG2	3:C:459:PHE:O	2.69	0.41
3:C:502:SER:O	3:C:503:CYS:CB	2.68	0.41
1:A:131:PHE:HZ	1:A:188:VAL:CG2	2.31	0.41
1:A:558:TYR:O	1:A:562:HIS:HB2	2.21	0.41
1:A:602:PHE:N	1:A:602:PHE:HD1	2.19	0.41
3:C:394:ILE:HD13	3:C:708:GLN:HE22	1.85	0.41
3:C:498:ILE:N	3:C:498:ILE:CD1	2.84	0.41
3:C:553:SER:HA	3:C:554:PRO:HD3	1.80	0.41
3:C:870:VAL:HA	3:C:883:SER:O	2.21	0.41
1:A:187:MET:O	1:A:191:LYS:HB2	2.22	0.40
1:A:533:TRP:HB3	1:A:534:PRO:HD2	2.03	0.40
1:A:748:ASP:HB3	1:A:756:HIS:CE1	2.56	0.40
3:C:451:PHE:HD1	3:C:470:GLN:CB	2.34	0.40
3:C:641:PHE:CD2	3:C:679:MET:HE1	2.56	0.40
1:A:409:ILE:HG13	1:A:443:ILE:HD11	1.99	0.40
1:A:704:MET:O	1:A:757:TYR:HD2	2.00	0.40
3:C:108:VAL:HG11	3:C:143:ILE:HD11	2.03	0.40
3:C:184:ASP:CB	3:C:185:PRO:HD2	2.43	0.40
1:A:153:PHE:O	1:A:154:LEU:C	2.64	0.40
1:A:282:THR:O	1:A:283:GLN:C	2.63	0.40
1:A:384:GLU:HA	1:A:387:VAL:HG23	2.04	0.40
1:A:390:MET:CE	1:A:391:LYS:HA	2.51	0.40
1:A:390:MET:HE3	1:A:394:PHE:CD1	2.57	0.40
1:A:457:LEU:CD2	1:A:461:LEU:HG	2.52	0.40
1:A:625:ARG:HD3	1:A:625:ARG:HA	1.91	0.40
3:C:184:ASP:N	3:C:187:GLY:O	2.55	0.40
3:C:402:ILE:HG22	3:C:403:ASP:N	2.37	0.40
1:A:329:VAL:O	1:A:330:ARG:O	2.39	0.40
3:C:561:TRP:O	3:C:587:ILE:HG21	2.19	0.40
3:C:699:LEU:HD13	3:C:699:LEU:C	2.46	0.40
4:D:218:THR:CG2	4:D:226:VAL:HG13	2.52	0.40
1:A:141:ASP:O	1:A:143:CYS:N	2.55	0.40
1:A:274:VAL:HG21	1:A:283:GLN:HB2	2.04	0.40
1:A:675:LYS:HA	1:A:675:LYS:HD3	1.93	0.40
3:C:412:PRO:HG2	3:C:412:PRO:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:ARG:NH1	3:C:769:LYS:NZ[1_565]	2.04	0.16

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	717/742 (97%)	512 (71%)	132 (18%)	73 (10%)	0	6
2	B	19/117 (16%)	14 (74%)	4 (21%)	1 (5%)	1	14
3	C	1095/1159 (94%)	963 (88%)	97 (9%)	35 (3%)	3	21
4	D	353/382 (92%)	326 (92%)	22 (6%)	5 (1%)	9	40
All	All	2184/2400 (91%)	1815 (83%)	255 (12%)	114 (5%)	1	14

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	ASP
1	A	58	TYR
1	A	76	SER
1	A	83	LEU
1	A	84	GLU
1	A	127	ASP
1	A	185	ASP
1	A	191	LYS
1	A	207	GLU
1	A	208	ALA
1	A	209	VAL
1	A	276	THR
1	A	330	ARG
1	A	483	CYS
1	A	517	ASP
1	A	587	LYS
1	A	606	ASP
1	A	616	ALA
1	A	633	CYS
1	A	644	LYS
1	A	660	PHE
1	A	661	LYS

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Mol	Chain	Res	Type
1	A	710	LEU
1	A	752	PRO
3	C	367	LEU
3	C	430	VAL
3	C	583	GLY
3	C	598	SER
3	C	672	ASN
3	C	674	LYS
3	C	704	ILE
3	C	705	ASP
3	C	710	LEU
4	D	126	LEU
1	A	96	HIS
1	A	97	LYS
1	A	204	ARG
1	A	229	ASP
1	A	240	ASN
1	A	280	HIS
1	A	441	ARG
1	A	598	VAL
1	A	607	GLY
1	A	652	ASP
1	A	670	ASN
1	A	691	ASP
1	A	711	GLY
3	C	549	SER
3	C	563	ASP
3	C	584	GLY
3	C	855	ASP
3	C	1110	ALA
4	D	120	ALA
1	A	55	PRO
1	A	71	ARG
1	A	75	SER
1	A	82	ASN
1	A	119	LEU
1	A	223	ASP
1	A	350	ALA
1	A	402	PRO
1	A	451	ALA
1	A	586	LYS
1	A	708	LYS

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Mol	Chain	Res	Type
1	A	727	VAL
1	A	757	TYR
1	A	758	VAL
3	C	185	PRO
3	C	418	ASN
3	C	449	MET
3	C	481	GLN
3	C	547	GLY
3	C	562	THR
3	C	624	SER
3	C	644	LEU
3	C	706	GLU
3	C	1109	VAL
1	A	54	LEU
1	A	91	GLU
1	A	189	GLN
1	A	228	LYS
1	A	293	GLN
1	A	325	LEU
1	A	377	GLU
1	A	514	ASN
1	A	610	PHE
1	A	617	THR
1	A	726	PRO
2	B	37	ILE
3	C	36	ASN
3	C	372	GLN
3	C	488	SER
3	C	503	CYS
4	D	119	HIS
4	D	190	GLY
1	A	51	ARG
1	A	201	GLU
1	A	233	LEU
1	A	378	VAL
1	A	440	PHE
1	A	597	LEU
3	C	242	GLY
3	C	592	LEU
3	C	460	CYS
4	D	291	ASP
3	C	493	PRO

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Mol	Chain	Res	Type
3	C	551	GLY
1	A	306	GLY
1	A	618	GLY
1	A	619	ILE
3	C	406	GLY
3	C	712	ILE
1	A	519	GLY
1	A	405	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	631/674 (94%)	565 (90%)	66 (10%)	6	21
2	B	18/99 (18%)	11 (61%)	7 (39%)	0	1
3	C	957/1015 (94%)	852 (89%)	105 (11%)	6	20
4	D	304/335 (91%)	277 (91%)	27 (9%)	9	28
All	All	1910/2123 (90%)	1705 (89%)	205 (11%)	6	21

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	THR
1	A	64	ARG
1	A	79	ILE
1	A	90	VAL
1	A	93	LEU
1	A	95	SER
1	A	102	LEU
1	A	112	ASP
1	A	124	ASP
1	A	125	SER
1	A	135	ILE
1	A	159	THR
1	A	171	TRP

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Mol	Chain	Res	Type
1	A	173	MET
1	A	175	LEU
1	A	182	ILE
1	A	183	ILE
1	A	199	LEU
1	A	205	SER
1	A	207	GLU
1	A	217	LEU
1	A	249	ARG
1	A	251	MET
1	A	281	SER
1	A	283	GLN
1	A	287	ILE
1	A	290	VAL
1	A	299	LEU
1	A	300	THR
1	A	307	LEU
1	A	353	ILE
1	A	389	LEU
1	A	390	MET
1	A	402	PRO
1	A	422	LYS
1	A	428	GLU
1	A	429	LEU
1	A	439	LEU
1	A	450	GLU
1	A	457	LEU
1	A	478	LYS
1	A	482	GLU
1	A	483	CYS
1	A	494	MET
1	A	498	MET
1	A	526	ASN
1	A	530	MET
1	A	546	GLU
1	A	562	HIS
1	A	570	GLN
1	A	591	VAL
1	A	611	GLU
1	A	624	LEU
1	A	626	ARG
1	A	639	LEU

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Mol	Chain	Res	Type
1	A	652	ASP
1	A	660	PHE
1	A	677	THR
1	A	681	GLN
1	A	683	SER
1	A	692	ARG
1	A	706	MET
1	A	726	PRO
1	A	735	ARG
1	A	748	ASP
1	A	751	ASN
2	B	19	LYS
2	B	22	PHE
2	B	25	LYS
2	B	32	LEU
2	B	37	ILE
2	B	38	VAL
2	B	39	VAL
3	C	7	VAL
3	C	19	VAL
3	C	81	THR
3	C	99	ASP
3	C	101	ILE
3	C	112	ILE
3	C	133	LEU
3	C	159	LEU
3	C	167	VAL
3	C	189	HIS
3	C	191	LYS
3	C	253	ILE
3	C	259	VAL
3	C	297	LEU
3	C	304	LEU
3	C	314	LEU
3	C	334	VAL
3	C	339	ASP
3	C	352	THR
3	C	360	VAL
3	C	396	ILE
3	C	404	LEU
3	C	410	LEU
3	C	412	PRO

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Mol	Chain	Res	Type
3	C	414	ARG
3	C	419	ARG
3	C	420	GLU
3	C	448	LEU
3	C	452	VAL
3	C	454	ASP
3	C	469	ILE
3	C	473	SER
3	C	476	VAL
3	C	481	GLN
3	C	482	GLU
3	C	487	VAL
3	C	493	PRO
3	C	510	VAL
3	C	518	TYR
3	C	521	ILE
3	C	523	PRO
3	C	525	GLU
3	C	531	HIS
3	C	533	GLU
3	C	540	CYS
3	C	555	LEU
3	C	560	LEU
3	C	561	TRP
3	C	563	ASP
3	C	567	ARG
3	C	576	LEU
3	C	582	LEU
3	C	587	ILE
3	C	592	LEU
3	C	594	THR
3	C	597	GLU
3	C	602	LEU
3	C	603	LEU
3	C	608	ASP
3	C	614	PHE
3	C	616	LEU
3	C	617	ASN
3	C	618	ILE
3	C	620	THR
3	C	623	LEU
3	C	625	ASP

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Mol	Chain	Res	Type
3	C	627	LYS
3	C	629	VAL
3	C	646	THR
3	C	663	ASN
3	C	673	LEU
3	C	688	PRO
3	C	700	THR
3	C	701	ILE
3	C	703	THR
3	C	704	ILE
3	C	706	GLU
3	C	707	ILE
3	C	708	GLN
3	C	711	HIS
3	C	728	GLU
3	C	769	LYS
3	C	794	ILE
3	C	809	GLN
3	C	820	LYS
3	C	844	LYS
3	C	867	LYS
3	C	881	LEU
3	C	898	GLU
3	C	899	LEU
3	C	901	THR
3	C	914	LEU
3	C	930	VAL
3	C	931	LEU
3	C	957	VAL
3	C	966	LEU
3	C	970	ASN
3	C	984	THR
3	C	993	GLN
3	C	1000	LEU
3	C	1052	LEU
3	C	1086	THR
3	C	1093	LEU
3	C	1106	GLN
3	C	1129	LEU
4	D	111	LYS
4	D	116	GLN
4	D	117	SER

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Mol	Chain	Res	Type
4	D	119	HIS
4	D	126	LEU
4	D	134	LEU
4	D	150	VAL
4	D	174	LEU
4	D	179	VAL
4	D	180	GLN
4	D	198	MET
4	D	219	LEU
4	D	243	VAL
4	D	254	THR
4	D	262	LEU
4	D	263	LEU
4	D	274	GLU
4	D	293	LEU
4	D	299	VAL
4	D	308	LEU
4	D	312	LYS
4	D	374	LEU
4	D	389	VAL
4	D	400	LEU
4	D	435	SER
4	D	437	THR
4	D	453	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	92	ASN
1	A	115	GLN
1	A	145	GLN
1	A	164	ASN
1	A	189	GLN
1	A	283	GLN
1	A	309	HIS
1	A	333	GLN
1	A	338	GLN
1	A	339	HIS
1	A	399	ASN
1	A	412	HIS
1	A	511	HIS

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Mol	Chain	Res	Type
1	A	514	ASN
1	A	526	ASN
1	A	551	GLN
1	A	570	GLN
1	A	575	HIS
1	A	595	GLN
1	A	629	GLN
1	A	657	ASN
1	A	670	ASN
1	A	681	GLN
1	A	712	HIS
1	A	722	GLN
1	A	751	ASN
1	A	754	GLN
2	B	28	ASN
3	C	4	ASN
3	C	30	ASN
3	C	85	ASN
3	C	105	HIS
3	C	156	ASN
3	C	186	GLN
3	C	241	ASN
3	C	261	HIS
3	C	319	ASN
3	C	374	GLN
3	C	432	GLN
3	C	455	GLN
3	C	462	ASN
3	C	467	GLN
3	C	481	GLN
3	C	494	GLN
3	C	507	GLN
3	C	524	GLN
3	C	536	HIS
3	C	550	ASN
3	C	578	HIS
3	C	634	GLN
3	C	663	ASN
3	C	677	ASN
3	C	708	GLN
3	C	731	GLN
3	C	796	GLN

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Mol	Chain	Res	Type
3	C	877	ASN
3	C	885	ASN
3	C	904	ASN
3	C	907	ASN
3	C	993	GLN
3	C	1034	ASN
3	C	1055	GLN
4	D	269	HIS
4	D	397	GLN
4	D	419	GLN
4	D	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	3DR	E	7	5	8,11,12	0.36	0	7,14,17	1.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3DR	E	7	5	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	7	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	354:THR	C	355:ASN	N	1.07

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	719/742 (96%)	0.03	19 (2%) 57 48	288, 322, 371, 414	0
2	B	21/117 (17%)	-0.17	0 100 100	312, 322, 356, 365	0
3	C	1105/1159 (95%)	-0.31	4 (0%) 88 79	185, 326, 367, 403	0
4	D	355/382 (92%)	-0.26	2 (0%) 85 75	275, 310, 352, 367	0
5	E	11/12 (91%)	0.04	0 100 100	342, 359, 437, 441	0
6	F	12/12 (100%)	0.17	0 100 100	363, 379, 420, 442	0
All	All	2223/2424 (91%)	-0.19	25 (1%) 78 66	185, 322, 367, 442	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ILE	4.4
1	A	463	VAL	3.0
1	A	295	LEU	2.7
3	C	165	ILE	2.6
1	A	86	LEU	2.6
4	D	128	GLU	2.5
3	C	328	LEU	2.5
1	A	509	LYS	2.5
1	A	506	VAL	2.4
4	D	330	ALA	2.4
1	A	727	VAL	2.4
1	A	491	LEU	2.4
1	A	70	VAL	2.4
1	A	476	LEU	2.4
1	A	333	GLN	2.3
1	A	224	LEU	2.2
3	C	422	ASP	2.2
1	A	740	ILE	2.1
1	A	128	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	250	LEU	2.1
1	A	639	LEU	2.1
1	A	638	VAL	2.1
1	A	745	MET	2.1
1	A	93	LEU	2.0
3	C	568	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	3DR	E	7	11/12	0.67	0.11	357,362,366,367	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.