



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:09 PM UTC

PDB ID : 6R7B / pdb_00006r7b
Title : Crystal structure of Csx1 in complex with cyclic oligoadenylate cOA4 conformation 1
Authors : Molina, R.; Montoya, G.; Sofos, N.; Stella, S.
Deposited on : 2019-03-28
Resolution : 3.12 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
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

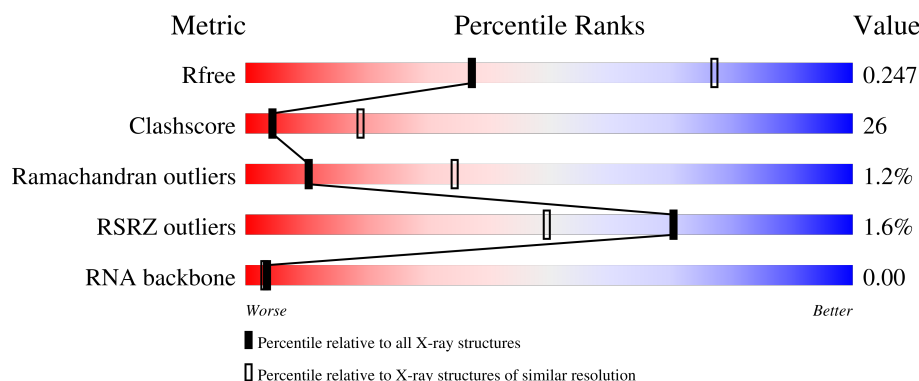
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)
RNA backbone	3983	1017 (3.34-2.90)

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	454	2% 56% 41% .
1	B	454	2% 60% 36% .
1	C	454	% 64% 33% .
2	D	4	25% 75%
2	E	4	25% 25% 50%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11153 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 CRISPR-associated (Cas) DxTHG family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			
1	B	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			
1	C	454	Total	C	N	O	S	0	0	0
			3642	2324	607	693	18			

- Molecule 2 is a RNA chain called RNA (5'-R(P*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			
2	E	2	Total	C	N	O	P	0	0	0
			44	20	10	12	2			

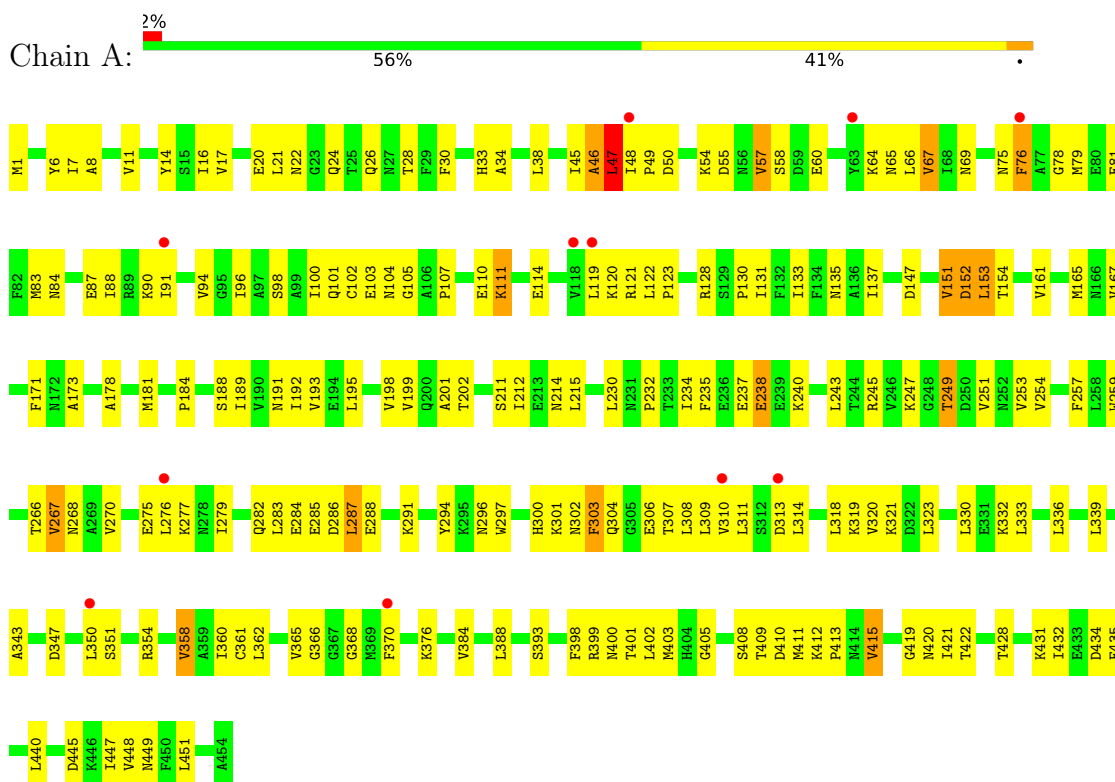
- Molecule 3 is water.

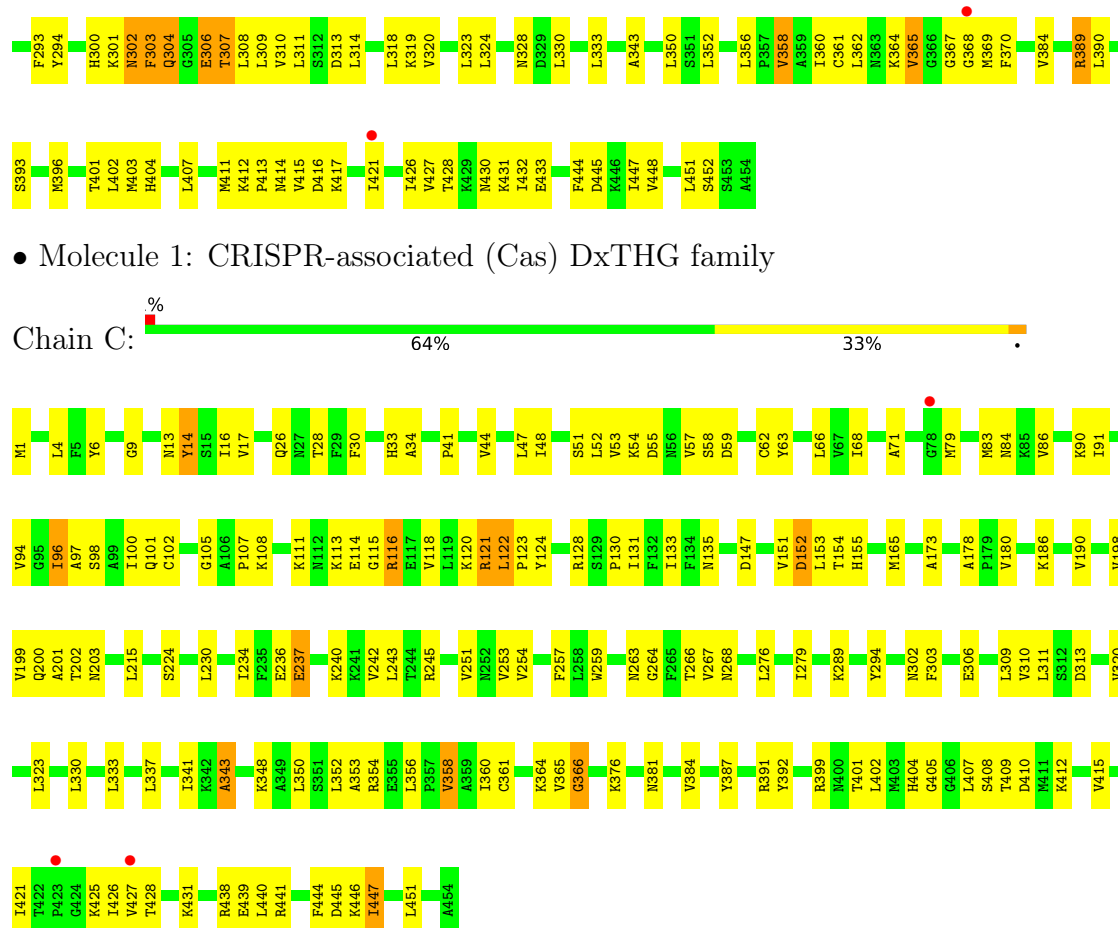
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total	O	0	0
			21	21		
3	B	29	Total	O	0	0
			29	29		
3	C	45	Total	O	0	0
			45	45		

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: CRISPR-associated (Cas) DxTHG family





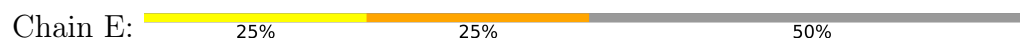
• Molecule 1: CRISPR-associated (Cas) D_xTHG family



• Molecule 2: RNA (5'-R(P*AP*AP*AP*A)-3')



• Molecule 2: RNA (5'-R(P*AP*AP*AP*A)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.08Å 117.68Å 357.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.29 – 3.12 48.29 – 3.12	Depositor EDS
% Data completeness (in resolution range)	60.3 (48.29-3.12) 60.2 (48.29-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.41 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.180 , 0.229 (Not available) , 0.247	Depositor DCC
R_{free} test set	1180 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 111.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11153	wwPDB-VP
Average B, all atoms (Å ²)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

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	0.88	1/3703 (0.0%)	1.54	39/4990 (0.8%)
1	B	0.88	3/3703 (0.1%)	1.52	38/4990 (0.8%)
1	C	0.90	2/3703 (0.1%)	1.54	49/4990 (1.0%)
2	D	0.65	0/99	0.75	0/152
2	E	0.67	0/49	0.86	0/74
All	All	0.88	6/11257 (0.1%)	1.53	126/15196 (0.8%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	VAL	CA-C	6.38	1.61	1.52
1	B	412	LYS	CA-C	6.36	1.57	1.53
1	A	412	LYS	CA-C	6.27	1.57	1.53
1	C	96	ILE	CG1-CD1	6.06	1.75	1.51
1	C	412	LYS	CA-C	5.52	1.57	1.53
1	B	304	GLN	CA-C	5.39	1.59	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	LEU	N-CA-C	-12.21	98.01	111.07
1	B	303	PHE	N-CA-C	-10.23	100.81	113.18
1	C	447	ILE	N-CA-C	-10.21	100.91	110.82
1	B	97	ALA	CA-C-N	-9.12	110.17	122.85
1	B	97	ALA	C-N-CA	-9.12	110.17	122.85
1	B	302	ASN	N-CA-C	-8.92	102.91	113.88
1	B	110	GLU	N-CA-C	8.89	123.40	108.20
1	C	13	ASN	CA-CB-CG	8.79	121.39	112.60
1	A	111	LYS	N-CA-C	8.66	122.63	108.52
1	A	67	VAL	N-CA-CB	8.61	120.62	110.55
1	A	201	ALA	N-CA-C	-8.61	104.81	114.62
1	A	30	PHE	CA-CB-CG	8.32	122.12	113.80
1	A	303	PHE	N-CA-C	-8.31	104.16	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	PHE	CA-CB-CG	8.21	122.01	113.80
1	A	76	PHE	N-CA-C	8.14	121.53	109.24
1	C	201	ALA	N-CA-C	-8.10	105.39	114.62
1	B	389	ARG	N-CA-C	8.05	122.20	112.38
1	C	115	GLY	N-CA-C	7.83	120.94	112.33
1	B	431	LYS	CA-C-N	7.63	130.17	120.56
1	B	431	LYS	C-N-CA	7.63	130.17	120.56
1	C	447	ILE	N-CA-CB	7.58	121.44	110.52
1	C	198	VAL	N-CA-C	7.47	119.13	110.62
1	B	120	LYS	N-CA-C	7.34	121.41	109.59
1	B	307	THR	N-CA-C	-7.31	104.16	113.23
1	A	65	ASN	N-CA-C	7.16	121.84	113.18
1	B	365	VAL	CB-CA-C	-7.14	102.79	111.85
1	C	237	GLU	N-CA-C	7.10	119.02	111.28
1	B	343	ALA	N-CA-C	-7.09	98.48	109.76
1	B	30	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	287	LEU	N-CA-CB	6.69	119.71	110.01
1	A	275	GLU	N-CA-C	-6.68	103.92	111.14
1	B	58	SER	N-CA-C	6.66	120.50	107.98
1	B	84	ASN	CA-CB-CG	6.66	119.25	112.60
1	C	445	ASP	N-CA-C	6.64	119.34	111.71
1	B	235	PHE	CA-CB-CG	6.63	120.43	113.80
1	B	358	VAL	N-CA-C	-6.60	104.32	110.53
1	C	59	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	121	ARG	N-CA-C	-6.56	104.16	111.71
1	C	438	ARG	CA-C-N	6.49	128.98	120.28
1	C	438	ARG	C-N-CA	6.49	128.98	120.28
1	C	303	PHE	CA-CB-CG	6.42	120.22	113.80
1	C	358	VAL	N-CA-C	-6.40	104.52	110.53
1	A	47	LEU	CA-C-N	6.32	133.83	122.13
1	A	47	LEU	C-N-CA	6.32	133.83	122.13
1	A	211	SER	N-CA-C	-6.32	104.31	111.07
1	C	343	ALA	N-CA-C	-6.26	100.31	110.20
1	C	153	LEU	N-CA-C	-6.23	103.83	112.30
1	A	198	VAL	N-CA-C	6.16	117.64	110.62
1	A	343	ALA	N-CA-C	-6.08	100.60	110.20
1	C	14	TYR	N-CA-C	6.07	119.28	110.42
1	B	428	THR	CA-C-N	5.93	128.55	120.54
1	B	428	THR	C-N-CA	5.93	128.55	120.54
1	C	425	LYS	N-CA-C	-5.93	100.76	109.18
1	C	13	ASN	CA-C-N	5.89	130.75	121.56
1	C	13	ASN	C-N-CA	5.89	130.75	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	ILE	N-CA-C	5.82	121.44	109.34
1	A	152	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	82	PHE	CA-CB-CG	5.75	119.55	113.80
1	C	116	ARG	CA-C-N	5.75	129.43	120.75
1	C	116	ARG	C-N-CA	5.75	129.43	120.75
1	A	67	VAL	N-CA-C	-5.73	104.92	110.42
1	B	99	ALA	N-CA-C	5.73	117.29	110.19
1	B	330	LEU	CA-C-N	5.70	128.49	120.28
1	B	330	LEU	C-N-CA	5.70	128.49	120.28
1	C	200	GLN	CB-CG-CD	5.70	122.28	112.60
1	C	330	LEU	CA-C-N	5.69	128.47	120.28
1	C	330	LEU	C-N-CA	5.69	128.47	120.28
1	B	65	ASN	CA-C-N	5.67	128.65	120.38
1	B	65	ASN	C-N-CA	5.67	128.65	120.38
1	C	55	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	393	SER	CA-C-N	5.58	126.14	120.00
1	A	393	SER	C-N-CA	5.58	126.14	120.00
1	A	171	PHE	N-CA-C	-5.57	106.33	113.02
1	B	431	LYS	N-CA-C	-5.56	104.11	111.96
1	A	121	ARG	N-CA-C	-5.55	104.86	111.69
1	A	249	THR	N-CA-C	-5.55	101.43	109.59
1	A	30	PHE	CA-C-N	5.53	129.98	121.19
1	A	30	PHE	C-N-CA	5.53	129.98	121.19
1	C	245	ARG	CA-C-N	5.50	127.49	120.56
1	C	245	ARG	C-N-CA	5.50	127.49	120.56
1	C	439	GLU	N-CA-C	5.49	117.26	111.28
1	A	151	VAL	N-CA-C	5.48	116.17	108.17
1	A	153	LEU	N-CA-C	-5.46	104.29	112.54
1	A	434	ASP	N-CA-C	5.46	117.23	111.28
1	A	422	THR	CB-CA-C	5.43	116.75	109.42
1	B	27	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	135	ASN	CA-CB-CG	5.41	118.01	112.60
1	B	245	ARG	CA-C-N	5.41	127.37	120.56
1	B	245	ARG	C-N-CA	5.41	127.37	120.56
1	C	152	ASP	CA-CB-CG	5.39	117.99	112.60
1	B	59	ASP	CA-C-N	5.38	127.49	120.28
1	B	59	ASP	C-N-CA	5.38	127.49	120.28
1	A	245	ARG	CA-C-N	5.35	127.30	120.56
1	A	245	ARG	C-N-CA	5.35	127.30	120.56
1	C	84	ASN	N-CA-C	-5.35	106.89	113.41
1	A	277	LYS	N-CA-C	-5.32	105.48	111.28
1	C	426	ILE	CB-CA-C	-5.31	102.59	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	SER	CA-C-N	5.29	125.82	120.00
1	B	393	SER	C-N-CA	5.29	125.82	120.00
1	B	135	ASN	CA-CB-CG	5.27	117.87	112.60
1	A	358	VAL	N-CA-C	-5.26	105.58	110.53
1	A	296	ASN	CA-CB-CG	5.24	117.84	112.60
1	C	135	ASN	CA-CB-CG	5.23	117.83	112.60
1	A	432	ILE	N-CA-C	-5.22	105.99	110.74
1	B	151	VAL	N-CA-C	5.21	115.00	106.72
1	C	366	GLY	N-CA-C	5.21	125.53	113.18
1	C	59	ASP	CA-C-N	5.17	127.16	120.44
1	C	59	ASP	C-N-CA	5.17	127.16	120.44
1	B	219	TYR	N-CA-CB	5.16	118.08	110.33
1	C	200	GLN	CA-C-N	5.16	131.49	121.63
1	C	200	GLN	C-N-CA	5.16	131.49	121.63
1	A	238	GLU	N-CA-C	-5.16	105.35	110.97
1	A	7	ILE	N-CA-C	-5.16	101.21	108.12
1	C	431	LYS	CA-C-N	5.15	127.16	120.88
1	C	431	LYS	C-N-CA	5.15	127.16	120.88
1	C	428	THR	CA-C-N	5.13	128.51	120.82
1	C	428	THR	C-N-CA	5.13	128.51	120.82
1	C	306	GLU	CB-CG-CD	5.11	121.29	112.60
1	B	59	ASP	N-CA-C	-5.09	105.73	111.28
1	C	120	LYS	CA-C-N	5.07	127.58	120.28
1	C	120	LYS	C-N-CA	5.07	127.58	120.28
1	A	195	LEU	CA-C-N	5.04	127.28	120.38
1	A	195	LEU	C-N-CA	5.04	127.28	120.38
1	B	365	VAL	CA-C-O	5.03	124.89	119.91
1	C	66	LEU	CA-C-N	5.03	126.85	120.72
1	C	66	LEU	C-N-CA	5.03	126.85	120.72

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	3642	0	3675	260	0
1	B	3642	0	3675	214	0
1	C	3642	0	3675	143	0
2	D	88	0	44	6	0
2	E	44	0	23	6	0
3	A	21	0	0	0	0
3	B	29	0	0	0	0
3	C	45	0	0	1	0
All	All	11153	0	11092	586	0

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 26.

All (586) 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:C:96:ILE:CD1	1:C:96:ILE:CG1	1.75	1.58
1:A:33:HIS:CE1	1:A:79:MET:HE1	1.57	1.39
1:A:181:MET:HG3	2:D:1:A:C2	1.64	1.33
1:A:33:HIS:CE1	1:A:79:MET:CE	2.26	1.17
1:A:266:THR:HG22	1:A:336:LEU:CD2	1.74	1.16
1:A:17:VAL:HG12	1:A:188:SER:HB3	1.30	1.12
1:A:266:THR:HG22	1:A:336:LEU:HD21	1.28	1.09
1:A:47:LEU:HD12	1:A:48:ILE:HG13	1.17	1.08
1:B:57:VAL:HG23	1:B:58:SER:H	1.09	1.07
1:C:387:TYR:CE1	1:C:391:ARG:HG2	1.90	1.07
1:A:310:VAL:CG1	1:A:313:ASP:HB2	1.86	1.04
1:B:267:VAL:HG23	1:B:268:ASN:HD22	1.22	1.04
1:C:356:LEU:HD23	1:C:444:PHE:HZ	1.22	1.04
1:A:287:LEU:HD13	1:A:318:LEU:HD11	1.39	1.04
1:C:356:LEU:HD23	1:C:444:PHE:CZ	1.94	1.01
1:A:232:PRO:HG2	1:A:235:PHE:CD2	1.95	1.00
1:A:103:GLU:HG2	1:A:104:ASN:H	1.22	1.00
1:B:73:GLU:O	1:B:74:LEU:HG	1.63	0.99
1:A:47:LEU:CD1	1:A:48:ILE:HG13	1.93	0.98
1:A:235:PHE:CE1	1:A:240:LYS:HG3	1.99	0.96
1:A:16:ILE:HD12	1:A:76:PHE:HZ	1.28	0.96
1:B:356:LEU:HD23	1:B:444:PHE:HZ	1.31	0.95
1:B:21:LEU:HB2	1:B:192:ILE:HG13	1.44	0.95
1:C:259:TRP:CE2	1:C:263:ASN:ND2	2.34	0.95
1:B:356:LEU:HD23	1:B:444:PHE:CZ	2.03	0.94
1:B:180:VAL:HG13	1:B:190:VAL:HG21	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLU:HB2	1:A:119:LEU:HB2	1.52	0.91
1:A:310:VAL:HG11	1:A:313:ASP:CG	1.95	0.90
1:A:57:VAL:HG12	1:A:58:SER:H	1.35	0.90
1:A:276:LEU:HD23	1:A:279:ILE:HD12	1.53	0.89
1:B:426:ILE:HG13	1:B:427:VAL:H	1.37	0.89
1:A:365:VAL:HG12	1:A:376:LYS:HD3	1.53	0.88
1:A:235:PHE:HE1	1:A:240:LYS:HG3	1.34	0.88
1:B:57:VAL:HG23	1:B:58:SER:N	1.87	0.88
1:C:111:LYS:HG2	1:C:116:ARG:HA	1.55	0.88
1:A:33:HIS:HE1	1:A:79:MET:CE	1.74	0.88
1:B:358:VAL:HG22	1:B:384:VAL:HG21	1.53	0.88
1:B:267:VAL:HG23	1:B:268:ASN:ND2	1.89	0.88
1:A:33:HIS:HE1	1:A:79:MET:HE1	0.98	0.87
1:A:75:ASN:O	1:A:76:PHE:CD1	2.27	0.87
1:C:276:LEU:HD23	1:C:279:ILE:HD12	1.53	0.87
1:C:71:ALA:HB2	1:C:79:MET:HG3	1.54	0.87
1:A:310:VAL:HG12	1:A:313:ASP:HB2	1.56	0.86
1:A:398:PHE:HD2	1:A:435:PHE:CD2	1.94	0.86
1:A:266:THR:HG22	1:A:336:LEU:HD23	1.56	0.85
1:C:111:LYS:HE2	1:C:116:ARG:HB2	1.57	0.85
1:A:16:ILE:HD12	1:A:76:PHE:CZ	2.12	0.85
1:A:287:LEU:CD2	1:A:291:LYS:HE2	2.07	0.85
1:A:21:LEU:O	1:A:22:ASN:OD1	1.96	0.84
1:C:354:ARG:HH22	1:C:381:ASN:HD21	1.24	0.84
1:B:21:LEU:HD12	1:B:38:LEU:HD11	1.57	0.84
1:A:301:LYS:O	1:A:304:GLN:HB2	1.77	0.84
1:A:310:VAL:HG11	1:A:313:ASP:HB2	1.58	0.84
1:B:364:LYS:HE3	1:B:452:SER:HA	1.60	0.83
1:C:52:LEU:HD12	1:C:52:LEU:O	1.75	0.83
1:B:180:VAL:CG1	1:B:190:VAL:HG21	2.08	0.83
1:A:310:VAL:HG11	1:A:313:ASP:CB	2.09	0.83
1:A:232:PRO:HG2	1:A:235:PHE:CE2	2.14	0.82
1:A:103:GLU:HG2	1:A:104:ASN:N	1.95	0.81
1:A:57:VAL:HG12	1:A:58:SER:N	1.96	0.81
1:A:181:MET:HG3	2:D:1:A:N1	1.95	0.81
1:B:21:LEU:HB2	1:B:192:ILE:CG1	2.09	0.81
1:A:24:GLN:H	1:A:24:GLN:NE2	1.78	0.80
1:A:235:PHE:HE1	1:A:240:LYS:CG	1.94	0.80
1:C:387:TYR:O	1:C:391:ARG:HB2	1.82	0.80
1:B:390:LEU:HD12	1:B:390:LEU:O	1.80	0.80
1:A:165:MET:HE1	1:B:166:ASN:HD21	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:HG12	1:B:313:ASP:HB2	1.64	0.79
1:A:75:ASN:O	1:A:75:ASN:OD1	2.00	0.79
1:A:33:HIS:CE1	1:A:79:MET:SD	2.76	0.79
1:A:307:THR:HA	1:B:131:ILE:HG12	1.64	0.78
1:B:55:ASP:HB3	1:B:102:CYS:HB2	1.65	0.77
1:B:253:VAL:HG12	1:B:276:LEU:HD11	1.66	0.76
1:C:407:LEU:N	1:C:407:LEU:HD23	2.00	0.76
1:A:33:HIS:ND1	1:A:79:MET:SD	2.59	0.76
1:A:249:THR:OG1	1:A:283:LEU:HD11	1.85	0.76
1:A:287:LEU:HD23	1:A:291:LYS:HE2	1.68	0.76
1:A:361:CYS:HB2	1:A:451:LEU:HD21	1.68	0.76
1:C:259:TRP:CZ2	1:C:263:ASN:ND2	2.54	0.75
1:A:47:LEU:HD12	1:A:48:ILE:CG1	2.09	0.75
1:B:111:LYS:HB2	1:B:116:ARG:HG2	1.68	0.75
1:B:174:LYS:HA	1:B:196:THR:HG22	1.67	0.75
1:A:287:LEU:HD13	1:A:318:LEU:CD1	2.16	0.75
1:B:356:LEU:HG	1:B:360:ILE:CD1	2.16	0.75
1:A:45:ILE:N	1:A:45:ILE:HD12	2.02	0.75
1:B:217:GLU:OE1	1:B:262:ARG:HB3	1.87	0.74
1:A:66:LEU:HD12	1:A:67:VAL:N	2.02	0.74
1:C:121:ARG:C	1:C:123:PRO:HD3	2.12	0.74
1:A:96:ILE:HG13	1:B:180:VAL:HG12	1.68	0.74
1:C:354:ARG:HG2	1:C:399:ARG:CZ	2.18	0.74
1:B:69:ASN:ND2	1:B:107:PRO:HD2	2.03	0.73
1:A:310:VAL:CG1	1:A:313:ASP:CB	2.63	0.73
1:B:426:ILE:HG13	1:B:427:VAL:N	2.03	0.72
1:C:165:MET:HE3	1:C:199:VAL:HG22	1.71	0.72
1:B:57:VAL:CG2	1:B:58:SER:H	1.90	0.72
1:A:64:LYS:HE2	1:A:84:ASN:HA	1.72	0.72
1:A:235:PHE:HE1	1:A:240:LYS:CB	2.03	0.72
1:B:154:THR:OG1	1:B:177:SER:HA	1.90	0.72
1:B:28:THR:HG22	1:B:76:PHE:CZ	2.25	0.71
1:A:282:GLN:O	1:A:285:GLU:HG3	1.91	0.71
1:C:415:VAL:HG22	1:C:421:ILE:HD13	1.72	0.71
1:A:64:LYS:CE	1:A:84:ASN:HA	2.21	0.70
1:B:21:LEU:HD13	1:B:21:LEU:O	1.90	0.70
1:C:350:LEU:HD23	1:C:440:LEU:HD13	1.72	0.70
1:A:267:VAL:HG23	1:A:268:ASN:H	1.56	0.70
1:A:154:THR:CG2	1:A:178:ALA:HB3	2.22	0.69
1:B:17:VAL:HG23	1:B:188:SER:HB2	1.74	0.69
1:C:51:SER:HB2	1:C:124:TYR:CD2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:VAL:HG22	1:C:421:ILE:HG23	1.74	0.69
1:A:388:LEU:HD11	1:A:447:ILE:HD13	1.74	0.69
1:A:287:LEU:CD2	1:A:291:LYS:CE	2.71	0.69
1:A:350:LEU:HD12	1:A:402:LEU:HD12	1.73	0.69
1:A:360:ILE:HD13	1:A:448:VAL:HG22	1.73	0.69
1:A:330:LEU:HD13	1:B:421:ILE:HD11	1.74	0.68
1:A:398:PHE:CD2	1:A:435:PHE:CD2	2.80	0.68
1:C:51:SER:HB2	1:C:124:TYR:CG	2.29	0.68
1:B:51:SER:HB3	1:B:124:TYR:CE1	2.29	0.68
1:A:154:THR:HG21	1:A:178:ALA:HB3	1.75	0.68
1:A:287:LEU:HD23	1:A:291:LYS:CE	2.23	0.68
1:A:360:ILE:HD13	1:A:448:VAL:CG2	2.22	0.68
1:B:110:GLU:HB2	1:B:119:LEU:HD22	1.73	0.68
1:A:235:PHE:CE1	1:A:240:LYS:CG	2.74	0.68
1:B:390:LEU:HD12	1:B:390:LEU:C	2.18	0.68
1:B:266:THR:HB	1:B:333:LEU:CD2	2.23	0.68
1:A:266:THR:CG2	1:A:336:LEU:HD23	2.23	0.68
1:B:310:VAL:CG1	1:B:313:ASP:H	2.06	0.68
1:C:52:LEU:O	1:C:100:ILE:HD12	1.93	0.68
1:A:419:GLY:O	1:B:328:ASN:HB2	1.93	0.68
1:C:230:LEU:O	1:C:230:LEU:HD23	1.94	0.68
1:A:75:ASN:O	1:A:76:PHE:HD1	1.72	0.68
1:B:415:VAL:HG23	1:B:421:ILE:HD12	1.76	0.68
1:A:368:GLY:O	1:B:415:VAL:HG12	1.93	0.67
1:B:69:ASN:HD21	1:B:107:PRO:HD2	1.57	0.67
1:C:259:TRP:CD2	1:C:263:ASN:ND2	2.61	0.67
1:C:113:LYS:HG2	1:C:114:GLU:HG3	1.75	0.67
1:A:249:THR:CG2	1:A:283:LEU:HD11	2.24	0.67
1:B:310:VAL:HG12	1:B:313:ASP:CB	2.23	0.67
1:C:111:LYS:HG2	1:C:116:ARG:CA	2.25	0.67
1:B:174:LYS:HA	1:B:196:THR:CG2	2.24	0.67
1:B:310:VAL:HG11	1:B:313:ASP:CG	2.20	0.67
1:C:52:LEU:HD12	1:C:52:LEU:C	2.18	0.67
1:A:234:ILE:HD12	1:A:234:ILE:O	1.94	0.66
1:C:356:LEU:HG	1:C:360:ILE:CD1	2.26	0.66
1:A:120:LYS:HA	1:A:122:LEU:HD13	1.76	0.66
1:B:293:PHE:HB3	1:B:300:HIS:CD2	2.30	0.66
1:C:387:TYR:CE1	1:C:391:ARG:CG	2.76	0.66
1:B:21:LEU:HD13	1:B:21:LEU:C	2.20	0.65
1:A:102:CYS:HA	1:A:107:PRO:HA	1.78	0.65
1:C:71:ALA:CB	1:C:79:MET:HG3	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:PHE:HA	1:A:306:GLU:CG	2.27	0.65
1:B:356:LEU:HG	1:B:360:ILE:HD12	1.79	0.65
1:B:53:VAL:CG2	1:B:102:CYS:SG	2.85	0.65
1:A:235:PHE:CE1	1:A:240:LYS:HA	2.31	0.64
1:B:55:ASP:N	1:B:59:ASP:OD1	2.25	0.64
1:B:217:GLU:CD	1:B:262:ARG:NE	2.55	0.64
1:A:28:THR:HG21	1:A:33:HIS:ND1	2.12	0.64
1:C:408:SER:OG	1:C:410:ASP:HB2	1.98	0.64
1:B:51:SER:HB3	1:B:124:TYR:CZ	2.33	0.64
1:A:137:ILE:HG22	1:A:167:VAL:HG11	1.78	0.64
1:B:310:VAL:HG12	1:B:313:ASP:H	1.62	0.64
1:A:306:GLU:O	1:B:131:ILE:HD11	1.98	0.64
1:A:365:VAL:HG11	1:A:376:LYS:HG2	1.80	0.64
1:A:276:LEU:HD23	1:A:279:ILE:CD1	2.26	0.63
1:C:266:THR:HG21	1:C:352:LEU:HD13	1.80	0.63
1:A:131:ILE:HD13	1:B:307:THR:HA	1.80	0.63
1:B:69:ASN:ND2	1:B:107:PRO:CD	2.61	0.63
1:A:111:LYS:O	1:A:111:LYS:HG3	1.98	0.63
1:A:285:GLU:O	1:A:288:GLU:N	2.31	0.63
1:A:310:VAL:HG11	1:A:313:ASP:OD2	1.98	0.63
1:A:358:VAL:HG22	1:A:384:VAL:HG21	1.81	0.63
1:C:267:VAL:HG13	1:C:268:ASN:H	1.64	0.63
1:B:303:PHE:HA	1:B:306:GLU:HG2	1.79	0.63
1:C:350:LEU:HD12	1:C:402:LEU:HD12	1.79	0.63
1:A:98:SER:CA	1:A:122:LEU:HB3	2.30	0.62
1:C:154:THR:CG2	1:C:178:ALA:HB3	2.29	0.62
1:B:356:LEU:HG	1:B:360:ILE:HD11	1.80	0.62
1:C:415:VAL:CG2	1:C:421:ILE:HG23	2.30	0.62
1:C:68:ILE:HD13	1:C:79:MET:HB3	1.82	0.62
1:A:14:TYR:HA	2:D:4:A:N7	2.15	0.61
1:B:27:ASN:O	1:B:28:THR:HG23	2.00	0.61
1:A:351:SER:HA	1:A:399:ARG:HE	1.65	0.61
1:A:365:VAL:CG1	1:A:376:LYS:HD3	2.27	0.61
1:A:413:PRO:HD2	1:B:370:PHE:HB2	1.82	0.61
1:B:38:LEU:HD22	1:B:39:PHE:CE2	2.35	0.61
1:A:8:ALA:HB3	1:A:48:ILE:HG23	1.83	0.61
1:B:154:THR:CG2	1:B:178:ALA:O	2.48	0.61
1:C:131:ILE:HD12	1:C:131:ILE:H	1.66	0.61
1:A:55:ASP:HB2	1:A:103:GLU:O	2.00	0.61
1:A:270:VAL:HG13	1:A:332:LYS:HB3	1.81	0.61
1:A:235:PHE:CE1	1:A:240:LYS:CB	2.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:VAL:HG12	1:C:86:VAL:HG23	1.81	0.61
1:C:407:LEU:HD23	1:C:407:LEU:H	1.66	0.61
1:C:415:VAL:HG22	1:C:421:ILE:CG2	2.30	0.61
1:A:267:VAL:HG23	1:A:268:ASN:N	2.15	0.61
1:A:309:LEU:O	1:B:131:ILE:HD13	2.01	0.61
1:C:337:LEU:HD23	1:C:441:ARG:HH11	1.65	0.61
1:A:361:CYS:HB2	1:A:451:LEU:CD2	2.31	0.61
1:C:392:TYR:OH	1:C:446:LYS:HD3	1.99	0.61
1:B:137:ILE:O	1:B:140:ILE:HG13	2.01	0.60
1:B:260:ASN:O	1:B:265:PHE:N	2.30	0.60
1:C:365:VAL:HG23	1:C:365:VAL:O	2.01	0.60
1:C:350:LEU:CD2	1:C:440:LEU:HD13	2.32	0.60
1:C:154:THR:HG21	1:C:178:ALA:HB3	1.84	0.60
1:B:74:LEU:HD12	1:B:74:LEU:O	2.01	0.60
1:A:276:LEU:HA	1:A:279:ILE:HD12	1.84	0.60
1:B:165:MET:HE3	1:B:199:VAL:CG2	2.32	0.60
1:B:320:VAL:HG23	1:B:323:LEU:HD12	1.82	0.60
1:B:232:PRO:HG2	1:B:306:GLU:OE2	2.02	0.59
1:B:276:LEU:HA	1:B:279:ILE:HD12	1.84	0.59
1:A:45:ILE:HD12	1:A:45:ILE:H	1.65	0.59
1:A:347:ASP:N	1:A:402:LEU:HD13	2.18	0.59
1:A:249:THR:OG1	1:A:283:LEU:CD1	2.49	0.59
1:A:249:THR:HG21	1:A:283:LEU:HD11	1.85	0.59
1:B:53:VAL:HG22	1:B:102:CYS:SG	2.42	0.59
1:A:270:VAL:HG21	1:A:333:LEU:CD2	2.32	0.59
1:B:73:GLU:C	1:B:74:LEU:HG	2.28	0.59
1:C:251:VAL:O	1:C:254:VAL:HG12	2.03	0.59
1:A:304:GLN:NE2	1:B:126:GLU:OE2	2.36	0.59
1:A:307:THR:HA	1:B:131:ILE:CG1	2.32	0.59
1:B:287:LEU:HD22	1:B:318:LEU:HD11	1.85	0.59
1:B:31:ALA:HB3	1:B:152:ASP:OD2	2.02	0.59
1:C:427:VAL:HG23	1:C:427:VAL:O	2.01	0.59
1:A:235:PHE:HE1	1:A:240:LYS:HA	1.68	0.58
1:A:285:GLU:O	1:A:288:GLU:CB	2.51	0.58
1:C:276:LEU:HA	1:C:279:ILE:HD12	1.85	0.58
1:C:48:ILE:HD12	1:C:63:TYR:HB2	1.84	0.58
1:C:310:VAL:HG12	1:C:313:ASP:H	1.68	0.58
1:A:114:GLU:OE1	1:A:114:GLU:N	2.37	0.58
1:A:131:ILE:HD12	1:A:131:ILE:H	1.67	0.58
1:B:218:ARG:O	1:B:218:ARG:HG2	2.03	0.58
1:B:232:PRO:O	1:B:235:PHE:CD1	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:LYS:CG	1:C:116:ARG:HA	2.32	0.58
1:C:276:LEU:HD23	1:C:279:ILE:CD1	2.27	0.58
1:A:283:LEU:HA	1:A:286:ASP:OD1	2.04	0.58
1:A:33:HIS:ND1	1:A:79:MET:HE1	2.11	0.58
1:B:310:VAL:CG1	1:B:313:ASP:CG	2.77	0.58
1:B:7:ILE:HG12	1:B:47:LEU:HD22	1.86	0.58
1:B:217:GLU:OE2	1:B:262:ARG:HD2	2.03	0.58
1:B:365:VAL:O	1:B:365:VAL:HG22	2.04	0.58
1:B:414:ASN:O	1:B:415:VAL:HG12	2.04	0.58
1:C:257:PHE:HB2	1:C:276:LEU:HD11	1.85	0.57
1:B:230:LEU:HB3	1:B:247:LYS:HG3	1.85	0.57
1:B:301:LYS:HG3	1:B:304:GLN:HB3	1.86	0.57
1:A:17:VAL:HG12	1:A:188:SER:CB	2.19	0.57
1:A:266:THR:CG2	1:A:336:LEU:CD2	2.65	0.57
1:A:310:VAL:O	1:A:314:LEU:HD13	2.04	0.57
1:C:358:VAL:HG22	1:C:384:VAL:HG21	1.86	0.57
1:A:17:VAL:CG1	1:A:184:PRO:HB2	2.34	0.57
1:A:365:VAL:HG12	1:A:376:LYS:CD	2.31	0.57
1:C:230:LEU:HD11	1:C:309:LEU:HB2	1.86	0.57
1:A:75:ASN:C	1:A:76:PHE:CD1	2.82	0.57
1:A:303:PHE:O	1:B:132:PHE:CD1	2.58	0.57
1:B:266:THR:HG21	1:B:352:LEU:HD13	1.86	0.57
1:A:21:LEU:C	1:A:22:ASN:OD1	2.47	0.57
1:A:96:ILE:CG1	1:B:180:VAL:HG12	2.35	0.57
1:A:251:VAL:O	1:A:254:VAL:HG12	2.04	0.57
1:C:234:ILE:CG2	1:C:302:ASN:HD22	2.17	0.57
1:A:320:VAL:HG23	1:A:323:LEU:HD12	1.87	0.57
1:B:251:VAL:O	1:B:254:VAL:HG12	2.05	0.57
1:A:415:VAL:HB	1:A:421:ILE:HG12	1.87	0.56
1:B:16:ILE:HD13	1:B:29:PHE:HB3	1.87	0.56
1:C:57:VAL:HG13	1:C:58:SER:H	1.70	0.56
1:A:266:THR:HB	1:A:333:LEU:CD2	2.35	0.56
1:B:51:SER:CB	1:B:124:TYR:CE1	2.88	0.56
1:B:31:ALA:CB	1:B:152:ASP:OD2	2.54	0.56
1:B:217:GLU:HG3	1:B:259:TRP:HD1	1.71	0.56
1:C:356:LEU:CD2	1:C:444:PHE:HZ	2.09	0.56
1:A:370:PHE:HD2	1:B:413:PRO:O	1.89	0.56
1:B:215:LEU:HD22	1:B:261:ILE:HG21	1.88	0.56
1:C:356:LEU:HG	1:C:360:ILE:HD12	1.87	0.56
1:C:387:TYR:CZ	1:C:391:ARG:CG	2.89	0.56
1:A:366:GLY:HA2	1:B:417:LYS:HG3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:HB2	1:A:276:LEU:HD11	1.88	0.55
1:A:300:HIS:HB3	1:A:303:PHE:HE2	1.71	0.55
1:B:18:ASN:CB	1:B:27:ASN:HB3	2.36	0.55
1:C:253:VAL:HG12	1:C:276:LEU:HD21	1.87	0.55
1:A:54:LYS:HG3	1:A:54:LYS:O	2.06	0.55
1:A:421:ILE:O	1:B:271:LYS:HE2	2.06	0.55
1:B:1:MET:HB3	1:B:147:ASP:CG	2.32	0.55
1:B:97:ALA:O	1:B:122:LEU:HD23	2.06	0.55
1:C:267:VAL:HG13	1:C:268:ASN:N	2.20	0.55
1:A:69:ASN:OD1	1:A:69:ASN:O	2.25	0.55
1:B:111:LYS:HD2	1:B:116:ARG:HG2	1.87	0.55
1:B:310:VAL:HG12	1:B:310:VAL:O	2.06	0.55
1:A:50:ASP:HA	1:A:90:LYS:HE2	1.89	0.55
1:A:235:PHE:HE1	1:A:240:LYS:CA	2.20	0.55
1:B:38:LEU:HD22	1:B:39:PHE:CZ	2.42	0.55
1:B:69:ASN:HD22	1:B:107:PRO:CG	2.20	0.55
1:B:119:LEU:HD12	1:B:120:LYS:H	1.72	0.55
1:B:303:PHE:HA	1:B:306:GLU:CG	2.36	0.55
1:A:21:LEU:HD22	1:A:38:LEU:HD13	1.88	0.55
1:A:26:GLN:HG2	1:A:34:ALA:HA	1.88	0.55
1:A:212:ILE:HD13	1:A:319:LYS:HB3	1.89	0.55
1:B:407:LEU:HD12	1:B:407:LEU:N	2.22	0.55
1:C:79:MET:HE2	1:C:79:MET:HA	1.88	0.55
1:A:303:PHE:HA	1:A:306:GLU:HG2	1.89	0.54
1:A:415:VAL:HA	1:A:420:ASN:O	2.07	0.54
1:B:51:SER:O	1:B:51:SER:OG	2.24	0.54
2:E:2:A:H2'	2:E:2:A:N3	2.21	0.54
1:A:370:PHE:CD2	1:B:413:PRO:O	2.60	0.54
1:B:154:THR:HG23	1:B:178:ALA:O	2.06	0.54
1:A:330:LEU:CD1	1:B:421:ILE:HD11	2.36	0.54
1:B:362:LEU:O	1:B:367:GLY:N	2.40	0.54
1:C:94:VAL:HG13	1:C:128:ARG:H	1.72	0.54
1:B:212:ILE:HD13	1:B:319:LYS:HB3	1.89	0.54
1:A:192:ILE:CG2	1:A:193:VAL:N	2.70	0.54
1:B:50:ASP:HA	1:B:90:LYS:HE2	1.90	0.54
1:C:48:ILE:HD11	1:C:53:VAL:HG12	1.88	0.54
1:A:270:VAL:HG21	1:A:333:LEU:HD23	1.90	0.54
1:C:53:VAL:CG2	1:C:102:CYS:SG	2.96	0.54
1:C:1:MET:HB3	1:C:147:ASP:CG	2.33	0.53
1:C:6:TYR:CB	1:C:152:ASP:HB3	2.38	0.53
1:C:350:LEU:HD23	1:C:440:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:GLN:H	1:A:24:GLN:CD	2.15	0.53
1:C:48:ILE:HG23	1:C:90:LYS:HA	1.89	0.53
1:B:18:ASN:HB3	1:B:27:ASN:HB3	1.89	0.53
1:A:6:TYR:CB	1:A:152:ASP:HB3	2.39	0.53
1:A:8:ALA:HB3	1:A:48:ILE:CG2	2.38	0.53
1:C:101:GLN:HG3	1:C:108:LYS:HD3	1.91	0.53
1:A:365:VAL:HG12	1:A:365:VAL:O	2.08	0.53
1:A:120:LYS:HB3	1:A:122:LEU:HD22	1.90	0.52
1:B:217:GLU:OE1	1:B:262:ARG:CB	2.57	0.52
1:C:122:LEU:N	1:C:123:PRO:HD3	2.25	0.52
2:E:2:A:N3	2:E:2:A:C2'	2.72	0.52
1:A:366:GLY:O	1:B:417:LYS:HB2	2.10	0.52
1:B:165:MET:CE	1:B:199:VAL:HG22	2.40	0.52
1:C:52:LEU:O	1:C:100:ILE:CD1	2.58	0.52
1:A:370:PHE:CD2	1:B:413:PRO:HD2	2.44	0.52
1:B:94:VAL:HG13	1:B:128:ARG:H	1.73	0.52
1:B:430:ASN:HA	1:B:433:GLU:HB2	1.92	0.52
1:C:47:LEU:HD23	1:C:91:ILE:HG21	1.91	0.52
1:B:234:ILE:HG23	1:B:302:ASN:HD22	1.74	0.52
1:C:203:ASN:HB2	3:C:523:HOH:O	2.10	0.52
1:C:354:ARG:HG2	1:C:399:ARG:NH1	2.25	0.52
1:A:38:LEU:HD23	1:A:38:LEU:C	2.35	0.52
1:A:94:VAL:HG13	1:A:128:ARG:H	1.74	0.52
1:A:98:SER:HA	1:A:122:LEU:O	2.10	0.52
1:A:230:LEU:CD2	1:A:243:LEU:HD21	2.40	0.52
1:A:347:ASP:HA	1:A:402:LEU:HD13	1.93	0.51
1:B:35:LEU:HD22	1:B:39:PHE:HE2	1.75	0.51
1:C:356:LEU:HG	1:C:360:ILE:HD11	1.91	0.51
1:B:180:VAL:CG1	1:B:190:VAL:CG2	2.84	0.51
1:C:199:VAL:O	1:C:202:THR:HG22	2.10	0.51
1:A:307:THR:O	1:A:307:THR:OG1	2.18	0.51
1:A:1:MET:HB2	1:A:147:ASP:CG	2.35	0.51
1:A:336:LEU:HA	1:A:339:LEU:HD12	1.92	0.51
1:B:415:VAL:HA	1:B:421:ILE:HG23	1.91	0.51
1:A:17:VAL:HG12	1:A:184:PRO:HB2	1.93	0.51
1:A:66:LEU:HD12	1:A:66:LEU:C	2.35	0.51
1:B:130:PRO:HA	1:B:133:ILE:HD12	1.93	0.51
1:A:81:GLU:C	1:A:83:MET:H	2.19	0.51
1:A:284:GLU:OE1	1:A:321:LYS:NZ	2.40	0.51
1:B:266:THR:HB	1:B:333:LEU:HD21	1.92	0.51
1:B:266:THR:CB	1:B:333:LEU:HD21	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLU:CD	1:B:262:ARG:HD2	2.36	0.51
1:C:236:GLU:O	1:C:240:LYS:HB2	2.11	0.51
1:A:267:VAL:CG2	1:A:268:ASN:H	2.24	0.50
1:B:61:GLU:OE1	1:B:65:ASN:ND2	2.44	0.50
1:A:103:GLU:CG	1:A:104:ASN:N	2.67	0.50
1:A:192:ILE:HG22	1:A:193:VAL:N	2.26	0.50
1:B:358:VAL:HG22	1:B:384:VAL:CG2	2.35	0.50
1:A:270:VAL:HG13	1:A:332:LYS:CB	2.40	0.50
1:A:287:LEU:HD21	1:A:291:LYS:HE2	1.89	0.50
1:C:9:GLY:HA3	1:C:14:TYR:OH	2.11	0.50
1:A:98:SER:C	1:A:122:LEU:HB3	2.37	0.50
1:A:100:ILE:HD13	1:A:122:LEU:HD21	1.92	0.50
1:A:310:VAL:HG13	1:A:313:ASP:H	1.77	0.50
1:A:401:THR:HG23	1:A:411:MET:HE3	1.94	0.50
1:A:47:LEU:HD23	1:A:90:LYS:N	2.27	0.50
1:A:235:PHE:CZ	1:A:240:LYS:HG3	2.46	0.50
1:A:400:ASN:HB3	1:A:410:ASP:OD1	2.12	0.50
1:B:217:GLU:CD	1:B:259:TRP:HA	2.37	0.50
1:A:361:CYS:CB	1:A:451:LEU:HD21	2.40	0.50
1:C:415:VAL:CA	1:C:421:ILE:HG23	2.41	0.50
1:B:150:LEU:HD23	1:B:174:LYS:HB2	1.94	0.50
1:A:57:VAL:HB	1:A:104:ASN:O	2.12	0.49
1:A:428:THR:HB	1:A:431:LYS:CB	2.42	0.49
1:B:217:GLU:OE2	1:B:259:TRP:CD1	2.64	0.49
1:B:267:VAL:CG2	1:B:268:ASN:HD22	2.09	0.49
1:B:294:TYR:CD2	1:B:311:LEU:HD11	2.47	0.49
1:B:415:VAL:HG23	1:B:421:ILE:CD1	2.42	0.49
1:C:294:TYR:CE2	1:C:311:LEU:HD11	2.47	0.49
1:A:403:MET:CG	1:B:403:MET:HG2	2.42	0.49
1:B:110:GLU:CB	1:B:119:LEU:HD13	2.42	0.49
1:C:151:VAL:HG12	1:C:173:ALA:HB1	1.93	0.49
1:A:57:VAL:CG1	1:A:58:SER:N	2.69	0.49
1:A:235:PHE:CE1	1:A:240:LYS:CA	2.95	0.49
1:C:387:TYR:CZ	1:C:391:ARG:HG2	2.40	0.49
1:C:415:VAL:HA	1:C:421:ILE:HG23	1.93	0.49
1:C:408:SER:C	1:C:410:ASP:H	2.20	0.49
1:A:294:TYR:OH	1:A:309:LEU:HD23	2.13	0.49
1:A:398:PHE:HD2	1:A:435:PHE:HD2	1.50	0.49
1:C:266:THR:HB	1:C:333:LEU:CD2	2.43	0.49
1:B:21:LEU:HB3	1:B:192:ILE:HD11	1.95	0.49
1:A:199:VAL:O	1:A:202:THR:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:MET:CE	1:C:199:VAL:HG22	2.39	0.48
1:A:47:LEU:HB2	1:A:88:ILE:HG22	1.95	0.48
1:A:130:PRO:HA	1:A:133:ILE:HD12	1.94	0.48
1:B:49:PRO:HD2	1:B:52:LEU:CD2	2.44	0.48
1:C:26:GLN:HG2	1:C:34:ALA:HA	1.96	0.48
1:C:53:VAL:HG22	1:C:102:CYS:SG	2.53	0.48
1:C:408:SER:C	1:C:410:ASP:N	2.70	0.48
1:A:153:LEU:HD12	1:A:153:LEU:O	2.13	0.48
1:B:11:VAL:HB	1:B:66:LEU:HD21	1.96	0.48
1:B:217:GLU:CD	1:B:262:ARG:HE	2.22	0.48
1:B:266:THR:O	1:B:270:VAL:HB	2.12	0.48
1:C:387:TYR:O	1:C:391:ARG:CB	2.58	0.48
1:A:234:ILE:O	1:A:234:ILE:CD1	2.60	0.48
1:A:234:ILE:O	1:A:234:ILE:CG1	2.61	0.48
1:C:111:LYS:CE	1:C:116:ARG:HB2	2.35	0.48
1:C:122:LEU:O	1:C:122:LEU:HG	2.13	0.48
1:A:267:VAL:CG1	1:B:407:LEU:HD12	2.44	0.48
1:A:232:PRO:CG	1:A:235:PHE:CD2	2.83	0.48
1:B:165:MET:HE3	1:B:199:VAL:HG22	1.96	0.48
1:A:98:SER:HA	1:A:122:LEU:HB3	1.95	0.48
1:B:217:GLU:OE1	1:B:262:ARG:CD	2.62	0.48
1:B:389:ARG:HG2	1:B:396:MET:HG3	1.96	0.48
1:A:47:LEU:HG	1:A:90:LYS:HA	1.96	0.47
1:A:154:THR:HG23	1:A:178:ALA:HB3	1.96	0.47
1:A:303:PHE:HA	1:A:306:GLU:HG3	1.96	0.47
1:A:253:VAL:HG12	1:A:276:LEU:HD21	1.96	0.47
1:A:297:TRP:HH2	1:B:50:ASP:HB3	1.80	0.47
1:B:232:PRO:O	1:B:235:PHE:HD1	1.95	0.47
1:A:33:HIS:ND1	1:A:79:MET:CE	2.71	0.47
1:A:153:LEU:HB2	1:A:161:VAL:HG13	1.95	0.47
1:C:48:ILE:HD11	1:C:53:VAL:CG1	2.44	0.47
1:B:57:VAL:CG2	1:B:58:SER:N	2.59	0.47
1:B:178:ALA:HB2	1:B:192:ILE:HG22	1.97	0.47
1:C:96:ILE:HA	1:C:124:TYR:O	2.15	0.47
1:B:231:ASN:N	1:B:232:PRO:HD3	2.30	0.47
1:C:180:VAL:CG1	2:E:2:A:C8	2.97	0.47
1:A:189:ILE:HG23	1:A:189:ILE:O	2.15	0.47
1:A:308:LEU:HA	1:A:308:LEU:HD13	1.73	0.47
1:B:28:THR:HG22	1:B:76:PHE:HZ	1.77	0.47
1:C:51:SER:HA	1:C:124:TYR:CD1	2.50	0.47
1:C:52:LEU:HA	2:E:1:A:N6	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:VAL:HG23	1:C:376:LYS:HD3	1.95	0.47
1:A:47:LEU:CD1	1:A:48:ILE:CG1	2.80	0.47
1:B:216:ASP:HB3	1:B:219:TYR:HD2	1.80	0.47
1:C:130:PRO:HA	1:C:133:ILE:HD12	1.97	0.47
1:A:101:GLN:O	1:A:102:CYS:HB3	2.14	0.47
1:B:362:LEU:HA	1:B:365:VAL:HG12	1.96	0.47
1:C:16:ILE:HB	1:C:186:LYS:HG2	1.97	0.47
1:A:24:GLN:CD	1:A:24:GLN:N	2.73	0.47
1:A:354:ARG:HH21	1:A:384:VAL:HG23	1.80	0.47
1:B:182:GLY:HA2	2:D:2:A:O2'	2.15	0.47
1:C:242:VAL:HG22	1:C:289:LYS:HD2	1.97	0.47
1:B:20:GLU:O	1:B:20:GLU:HG3	2.15	0.46
1:A:266:THR:HB	1:A:333:LEU:HD21	1.97	0.46
1:A:302:ASN:C	1:A:304:GLN:H	2.23	0.46
1:A:11:VAL:HG11	1:A:67:VAL:HA	1.97	0.46
1:B:154:THR:HG21	1:B:178:ALA:O	2.15	0.46
1:B:217:GLU:CD	1:B:262:ARG:CD	2.88	0.46
1:A:214:ASN:HD22	1:B:218:ARG:HD3	1.79	0.46
1:A:243:LEU:HD23	1:A:243:LEU:C	2.40	0.46
1:A:249:THR:CB	1:A:283:LEU:HD11	2.45	0.46
1:B:21:LEU:CB	1:B:192:ILE:CG1	2.89	0.46
1:C:236:GLU:CD	1:C:237:GLU:N	2.73	0.46
1:C:407:LEU:N	1:C:407:LEU:CD2	2.73	0.46
1:A:11:VAL:HG21	1:A:67:VAL:HG23	1.97	0.46
1:B:362:LEU:HD13	1:B:368:GLY:O	2.14	0.46
1:C:54:LYS:HD2	1:C:54:LYS:HA	1.74	0.46
1:C:83:MET:HA	1:C:86:VAL:HG12	1.98	0.46
1:B:283:LEU:HD11	1:B:314:LEU:HD23	1.98	0.46
1:C:264:GLY:CA	1:C:348:LYS:HD2	2.46	0.46
1:A:399:ARG:CZ	1:A:403:MET:HE1	2.46	0.46
1:B:266:THR:CB	1:B:333:LEU:CD2	2.93	0.46
1:A:267:VAL:HG12	1:B:407:LEU:HD12	1.97	0.45
1:C:121:ARG:HB3	1:C:123:PRO:HD3	1.98	0.45
1:A:151:VAL:HG12	1:A:173:ALA:HB1	1.98	0.45
1:B:401:THR:HG23	1:B:411:MET:HE3	1.97	0.45
1:A:55:ASP:HB3	1:A:102:CYS:HB3	1.98	0.45
1:C:28:THR:HG21	1:C:33:HIS:HB3	1.98	0.45
1:A:64:LYS:HE3	1:A:84:ASN:HA	1.98	0.45
1:A:309:LEU:O	1:B:131:ILE:CD1	2.64	0.45
1:B:287:LEU:CD2	1:B:318:LEU:HD11	2.46	0.45
1:A:8:ALA:CB	1:A:48:ILE:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:THR:O	1:A:270:VAL:HG23	2.17	0.45
1:A:6:TYR:CE1	1:A:46:ALA:HB2	2.52	0.45
1:A:347:ASP:CA	1:A:402:LEU:HD13	2.47	0.45
1:C:100:ILE:HG23	1:C:118:VAL:CG1	2.47	0.45
1:C:391:ARG:HD3	1:C:391:ARG:HA	1.62	0.45
1:A:181:MET:CG	2:D:1:A:N1	2.75	0.44
1:A:237:GLU:HG2	1:A:238:GLU:N	2.32	0.44
1:B:404:HIS:N	1:B:404:HIS:CD2	2.83	0.44
1:B:444:PHE:HA	1:B:447:ILE:HD12	1.98	0.44
1:C:155:HIS:CE1	2:E:2:A:C8	3.05	0.44
1:A:403:MET:HG3	1:B:403:MET:HG2	2.00	0.44
1:A:28:THR:CG2	1:A:33:HIS:ND1	2.79	0.44
1:B:21:LEU:CB	1:B:192:ILE:HD11	2.47	0.44
1:B:217:GLU:OE1	1:B:262:ARG:NE	2.51	0.44
1:C:234:ILE:HG21	1:C:302:ASN:HD22	1.82	0.44
1:A:259:TRP:HH2	1:B:432:ILE:HD13	1.83	0.44
1:C:401:THR:O	1:C:405:GLY:N	2.49	0.44
1:C:341:ILE:HD11	1:C:440:LEU:HD23	2.00	0.44
1:A:287:LEU:HD23	1:A:291:LYS:HE3	2.00	0.44
1:B:16:ILE:CD1	1:B:74:LEU:HD21	2.47	0.44
1:B:362:LEU:O	1:B:365:VAL:HG12	2.18	0.44
1:A:310:VAL:O	1:A:314:LEU:CD1	2.66	0.43
1:B:361:CYS:HB2	1:B:451:LEU:HD22	2.00	0.43
1:A:237:GLU:HA	1:A:240:LYS:HB3	2.00	0.43
1:B:20:GLU:C	1:B:20:GLU:CD	2.86	0.43
1:B:47:LEU:HD12	1:B:140:ILE:HD11	2.00	0.43
1:C:97:ALA:HB3	1:C:124:TYR:HB3	2.00	0.43
1:A:370:PHE:CE2	1:B:415:VAL:HB	2.52	0.43
1:B:199:VAL:C	1:B:201:ALA:H	2.26	0.43
1:A:215:LEU:HD11	1:A:323:LEU:HD22	2.00	0.43
1:A:350:LEU:HD23	1:A:440:LEU:HD22	1.99	0.43
1:A:365:VAL:CG1	1:A:376:LYS:CD	2.94	0.43
1:B:445:ASP:HA	1:B:448:VAL:HG22	2.00	0.43
1:B:266:THR:HB	1:B:333:LEU:HD23	2.00	0.43
1:C:165:MET:HE3	1:C:199:VAL:CG2	2.46	0.43
1:A:230:LEU:HD21	1:A:243:LEU:HD11	2.00	0.43
1:B:21:LEU:HD22	1:B:22:ASN:N	2.34	0.43
1:B:230:LEU:CB	1:B:247:LYS:HG3	2.49	0.43
1:A:350:LEU:CD2	1:A:440:LEU:HD13	2.49	0.43
1:B:180:VAL:HG13	1:B:190:VAL:CG2	2.35	0.43
1:A:428:THR:HB	1:A:431:LYS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:THR:OG1	1:B:333:LEU:HD21	2.19	0.43
1:C:404:HIS:HB3	1:C:408:SER:HB2	2.01	0.43
1:A:46:ALA:N	1:A:87:GLU:O	2.42	0.43
1:A:362:LEU:HD12	1:A:370:PHE:CE1	2.54	0.43
1:B:350:LEU:HD13	1:B:402:LEU:HD12	2.01	0.43
1:B:401:THR:CG2	1:B:411:MET:HE3	2.49	0.43
1:A:270:VAL:HG21	1:A:333:LEU:HG	2.01	0.42
1:A:405:GLY:O	1:A:408:SER:OG	2.36	0.42
1:A:409:THR:HA	1:B:370:PHE:O	2.19	0.42
1:B:66:LEU:HD23	1:B:66:LEU:O	2.18	0.42
1:B:181:MET:SD	2:D:3:A:C5	3.12	0.42
1:C:337:LEU:HD11	1:C:353:ALA:HB2	2.01	0.42
1:C:361:CYS:HB2	1:C:451:LEU:HD22	2.02	0.42
1:C:387:TYR:CZ	1:C:391:ARG:HG3	2.54	0.42
1:A:21:LEU:CD1	1:A:192:ILE:HB	2.50	0.42
1:B:293:PHE:CB	1:B:300:HIS:CD2	3.00	0.42
1:C:4:LEU:HB2	1:C:41:PRO:HG3	2.01	0.42
1:C:98:SER:HA	1:C:122:LEU:HA	2.01	0.42
1:C:444:PHE:HA	1:C:447:ILE:HD12	2.01	0.42
1:A:21:LEU:HD12	1:A:192:ILE:HB	2.01	0.42
1:B:16:ILE:HD11	1:B:74:LEU:HD21	2.02	0.42
1:B:277:LYS:HD2	1:B:324:LEU:HD23	2.01	0.42
1:C:52:LEU:HD12	1:C:100:ILE:HD13	2.01	0.42
1:A:230:LEU:O	1:A:247:LYS:HE3	2.20	0.42
1:C:267:VAL:CG1	1:C:268:ASN:H	2.32	0.42
1:B:35:LEU:HD12	1:B:152:ASP:CG	2.44	0.42
1:B:309:LEU:HD12	1:B:310:VAL:H	1.83	0.42
1:C:264:GLY:HA3	1:C:348:LYS:HD2	2.00	0.42
1:C:62:CYS:HA	1:C:105:GLY:O	2.20	0.42
1:A:445:ASP:O	1:A:449:ASN:HB2	2.20	0.42
1:B:217:GLU:HG3	1:B:259:TRP:CD1	2.54	0.42
1:C:154:THR:HG23	1:C:178:ALA:HB3	2.00	0.42
1:C:320:VAL:HG23	1:C:323:LEU:HD22	2.02	0.42
1:A:285:GLU:O	1:A:288:GLU:CA	2.68	0.41
1:A:294:TYR:CD2	1:A:311:LEU:HD11	2.55	0.41
1:B:414:ASN:O	1:B:415:VAL:CG1	2.67	0.41
1:C:354:ARG:HH22	1:C:381:ASN:ND2	2.03	0.41
1:A:20:GLU:HB3	1:A:191:ASN:HA	2.03	0.41
1:A:307:THR:HB	1:B:129:SER:HB2	2.02	0.41
1:B:310:VAL:CG1	1:B:313:ASP:CB	2.95	0.41
1:A:365:VAL:HG12	1:A:376:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:O	1:A:240:LYS:HB3	2.21	0.41
1:B:407:LEU:N	1:B:407:LEU:CD1	2.82	0.41
1:C:17:VAL:HG22	1:C:190:VAL:HG12	2.02	0.41
1:A:131:ILE:HD13	1:B:307:THR:OG1	2.20	0.41
1:C:52:LEU:HA	2:E:1:A:H62	1.83	0.41
1:A:49:PRO:HA	1:A:91:ILE:HG13	2.01	0.41
1:B:56:ASN:N	1:B:56:ASN:OD1	2.54	0.41
1:B:308:LEU:H	1:B:308:LEU:HG	1.67	0.41
1:C:361:CYS:O	1:C:364:LYS:HB2	2.21	0.41
1:B:416:ASP:OD1	1:B:417:LYS:N	2.54	0.41
1:B:74:LEU:HD12	1:B:74:LEU:C	2.46	0.41
1:C:102:CYS:HA	1:C:107:PRO:HA	2.03	0.41
1:C:243:LEU:HD23	1:C:243:LEU:C	2.45	0.41
1:A:120:LYS:HA	1:A:122:LEU:HD22	2.03	0.41
1:A:267:VAL:CG2	1:A:268:ASN:N	2.82	0.41
1:B:71:ALA:O	1:B:76:PHE:HB3	2.21	0.41
1:A:365:VAL:HG11	1:A:376:LYS:CG	2.48	0.40
1:B:369:MET:HE3	1:B:369:MET:HB2	1.97	0.40
1:C:215:LEU:HD23	1:C:343:ALA:HB2	2.03	0.40
1:C:215:LEU:HD23	1:C:343:ALA:CB	2.51	0.40
1:C:224:SER:OG	1:C:251:VAL:CG1	2.69	0.40
1:B:243:LEU:C	1:B:243:LEU:HD23	2.46	0.40
1:B:362:LEU:O	1:B:367:GLY:HA2	2.22	0.40
1:A:60:GLU:HB3	1:A:88:ILE:HD13	2.02	0.40
1:C:6:TYR:HB3	1:C:152:ASP:HB3	2.02	0.40
1:A:428:THR:HB	1:A:431:LYS:HB2	2.02	0.40
1:B:21:LEU:C	1:B:21:LEU:HD22	2.46	0.40

There are no symmetry-related clashes.

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	452/454 (100%)	392 (87%)	52 (12%)	8 (2%)	6	26
1	B	452/454 (100%)	404 (89%)	43 (10%)	5 (1%)	11	36
1	C	452/454 (100%)	412 (91%)	37 (8%)	3 (1%)	18	47
All	All	1356/1362 (100%)	1208 (89%)	132 (10%)	16 (1%)	10	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	VAL
1	B	233	THR
1	A	47	LEU
1	A	78	GLY
1	A	415	VAL
1	B	306	GLU
1	C	366	GLY
1	C	409	THR
1	A	46	ALA
1	B	104	ASN
1	A	105	GLY
1	C	122	LEU
1	B	57	VAL
1	A	267	VAL
1	A	123	PRO
1	B	122	LEU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	3/4 (75%)	3 (100%)	1 (33%)
2	E	1/4 (25%)	1 (100%)	0
All	All	4/8 (50%)	4 (100%)	1 (25%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	2	A

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Mol	Chain	Res	Type
2	D	3	A
2	D	4	A
2	E	2	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	3	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

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](#)

There are no chain breaks in this entry.

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	454/454 (100%)	0.17	11 (2%) 59 38	94, 142, 199, 226	0
1	B	454/454 (100%)	0.09	8 (1%) 67 46	79, 135, 199, 213	0
1	C	454/454 (100%)	-0.17	3 (0%) 84 68	58, 106, 147, 166	0
2	D	4/4 (100%)	-0.37	0 100 100	187, 188, 192, 194	0
2	E	2/4 (50%)	-0.42	0 100 100	110, 110, 110, 112	0
All	All	1368/1370 (99%)	0.03	22 (1%) 70 49	58, 126, 195, 226	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	ILE	4.4
1	A	370	PHE	3.5
1	C	427	VAL	3.4
1	A	310	VAL	3.0
1	A	76	PHE	2.7
1	B	47	LEU	2.7
1	C	423	PRO	2.6
1	A	276	LEU	2.5
1	A	118	VAL	2.5
1	B	368	GLY	2.5
1	B	421	ILE	2.4
1	A	119	LEU	2.4
1	A	63	TYR	2.3
1	A	350	LEU	2.3
1	B	189	ILE	2.3
1	B	53	VAL	2.2
1	A	91	ILE	2.2
1	B	222	ASP	2.2
1	B	7	ILE	2.2
1	C	78	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	313	ASP	2.0
1	B	118	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.