



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:15 AM UTC

PDB ID : 3N6V / pdb_00003n6v
Title : Structure of the GluA2 NTD-dimer interface mutant, T78A
Authors : Rossmann, M.; Sukumaran, M.; Greger, I.H.
Deposited on : 2010-05-26
Resolution : 3.20 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

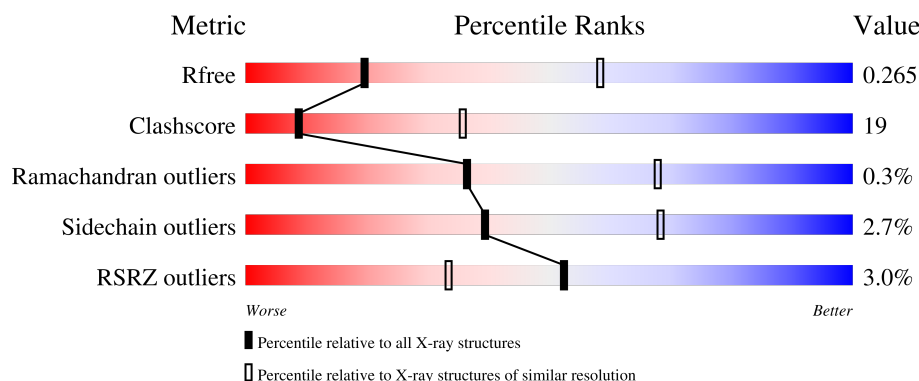
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	374	2% 69% 27% ..
1	B	374	3% 67% 29% ..
1	C	374	3% 66% 29% ..
1	D	374	2% 67% 29% ..
1	E	374	3% 72% 23% ..

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Mol	Chain	Length	Quality of chain
1	F	374	6% 66% 29%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17102 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	0	0	0
			2892	1846	487	551	8			
1	B	372	Total	C	N	O	S	0	0	0
			2923	1865	493	557	8			
1	C	369	Total	C	N	O	S	0	0	0
			2826	1810	461	547	8			
1	D	368	Total	C	N	O	S	0	0	0
			2854	1822	476	548	8			
1	E	366	Total	C	N	O	S	0	0	1
			2678	1713	429	527	9			
1	F	364	Total	C	N	O	S	0	0	0
			2791	1779	467	537	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ALA	THR	engineered mutation	UNP P19491
B	78	ALA	THR	engineered mutation	UNP P19491
C	78	ALA	THR	engineered mutation	UNP P19491
D	78	ALA	THR	engineered mutation	UNP P19491
E	78	ALA	THR	engineered mutation	UNP P19491
F	78	ALA	THR	engineered mutation	UNP P19491

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		
2	B	41	Total	O	0	0
			41	41		
2	C	26	Total	O	0	0
			26	26		

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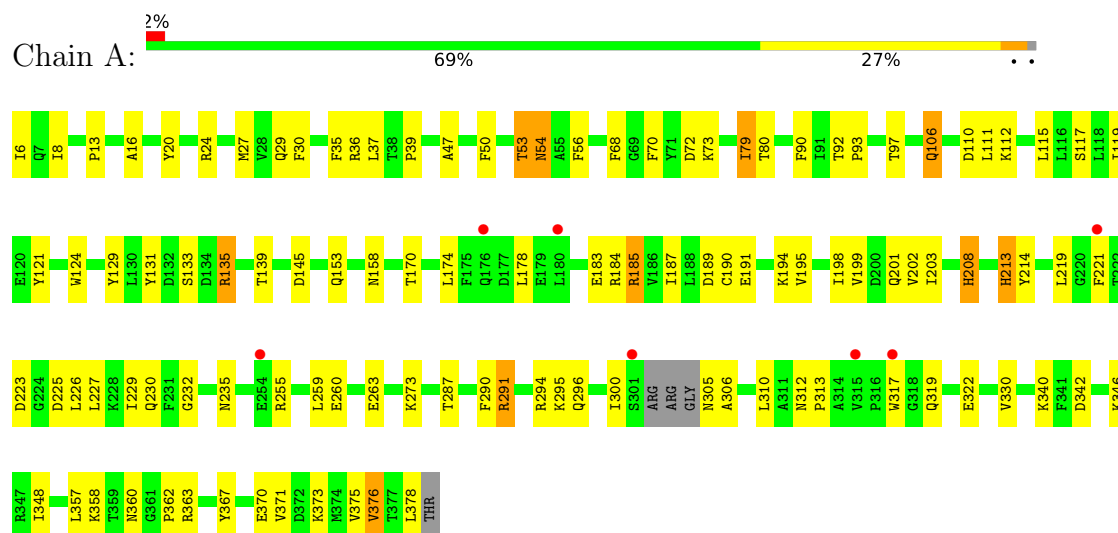
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	26	Total 26	O 26	0	0
2	E	11	Total 11	O 11	0	0
2	F	11	Total 11	O 11	0	0

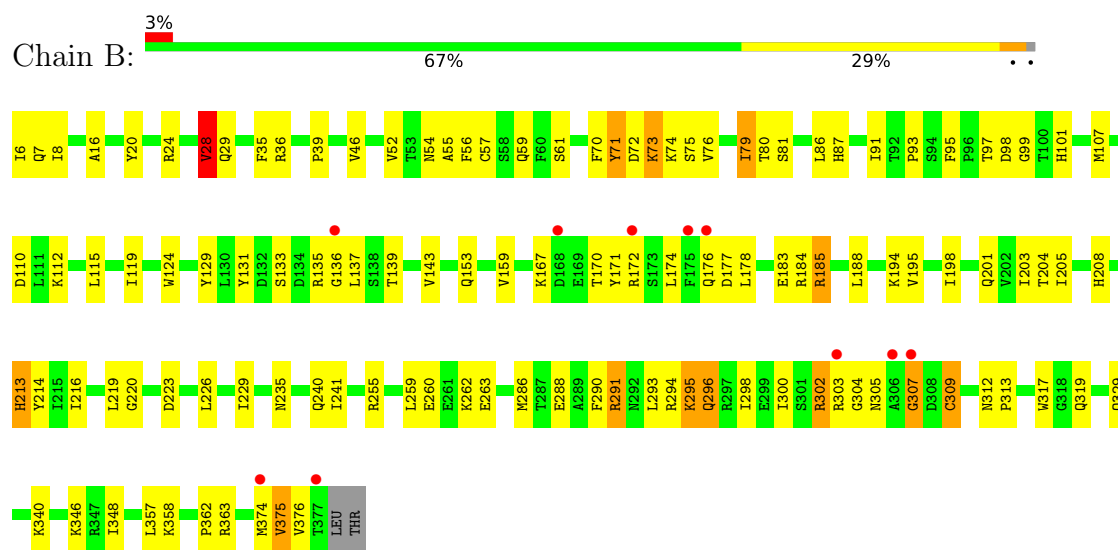
3 Residue-property plots [i](#)

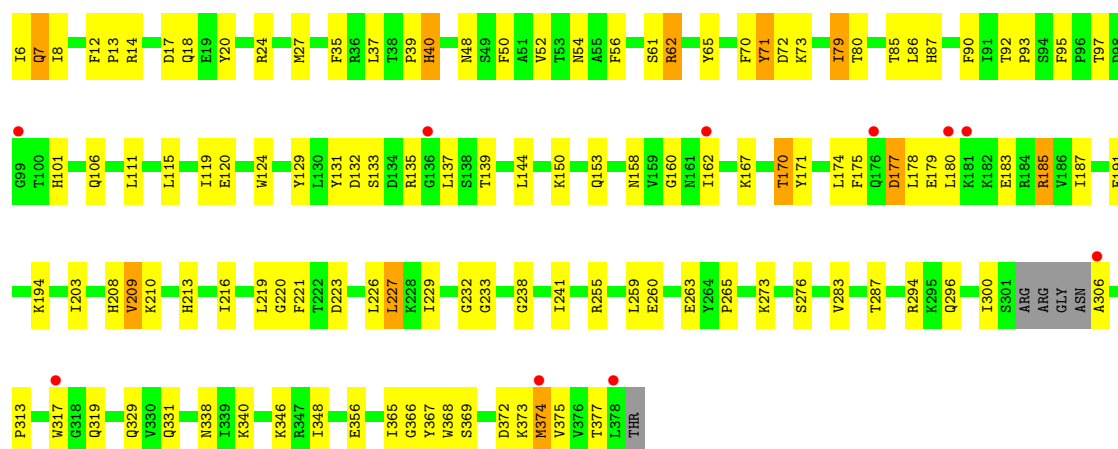
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate receptor 2

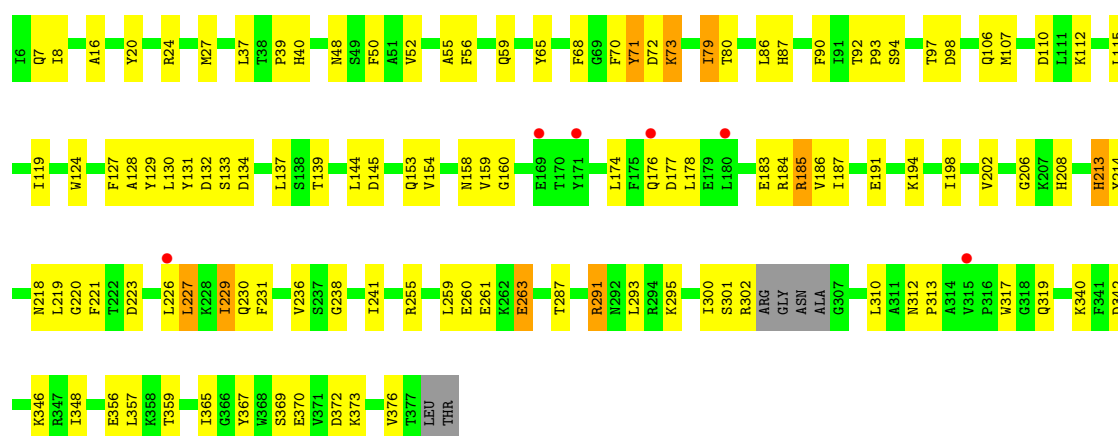


• Molecule 1: Glutamate receptor 2

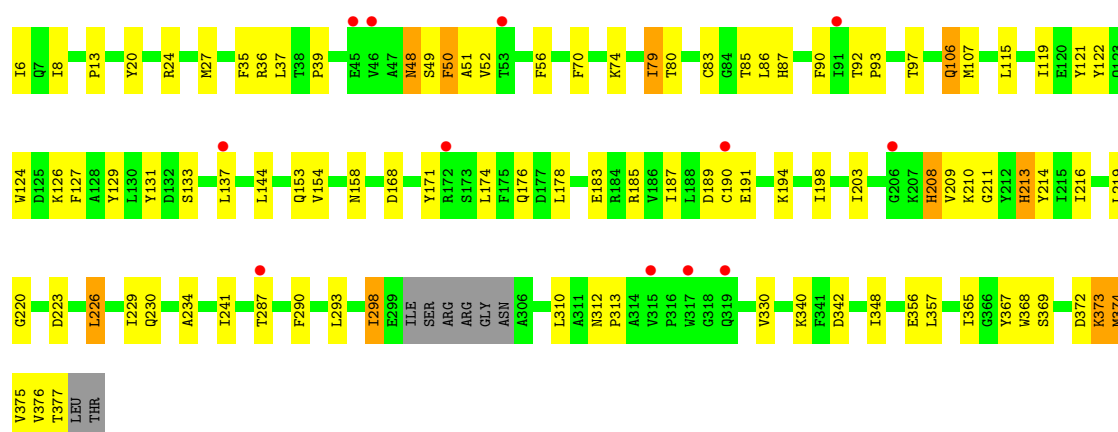




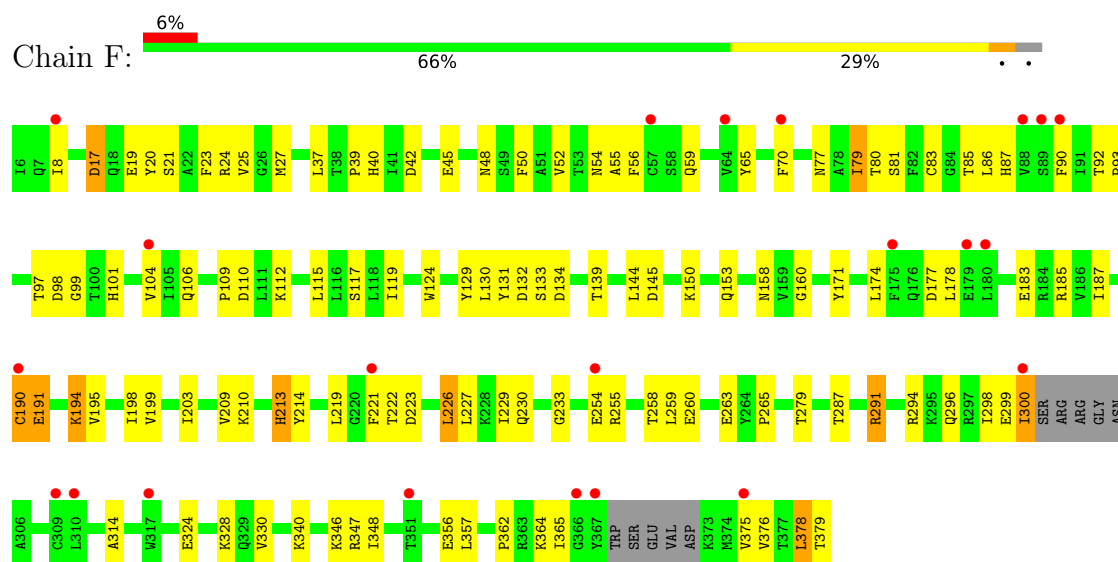
• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.21Å 120.15Å 360.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	53.78 – 3.20 53.78 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (53.78-3.20) 99.8 (53.78-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.6.1 _357	Depositor
R, R_{free}	0.235 , 0.265 0.231 , 0.265	Depositor DCC
R_{free} test set	1890 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.410	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17102	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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	0.69	7/2953 (0.2%)	0.96	13/4009 (0.3%)
1	B	0.74	7/2985 (0.2%)	1.03	25/4047 (0.6%)
1	C	0.75	10/2887 (0.3%)	0.96	13/3931 (0.3%)
1	D	0.71	4/2914 (0.1%)	0.98	12/3960 (0.3%)
1	E	0.66	4/2734 (0.1%)	0.90	7/3745 (0.2%)
1	F	0.67	3/2843 (0.1%)	0.95	9/3856 (0.2%)
All	All	0.70	35/17316 (0.2%)	0.96	79/23548 (0.3%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	GLN	CD-OE1	5.90	1.34	1.23
1	F	213	HIS	ND1-CE1	5.73	1.38	1.32
1	E	213	HIS	ND1-CE1	5.63	1.38	1.32
1	A	106	GLN	CD-NE2	-5.62	1.21	1.33
1	A	213	HIS	ND1-CE1	5.59	1.38	1.32
1	F	40	HIS	ND1-CE1	5.56	1.38	1.32
1	C	329	GLN	CD-OE1	5.55	1.34	1.23
1	E	106	GLN	CD-OE1	5.52	1.34	1.23
1	C	213	HIS	ND1-CE1	5.49	1.38	1.32
1	A	54	ASN	CG-ND2	-5.42	1.21	1.33
1	C	208	HIS	ND1-CE1	5.38	1.38	1.32
1	B	213	HIS	ND1-CE1	5.37	1.38	1.32
1	A	153	GLN	CD-OE1	5.32	1.33	1.23
1	C	153	GLN	CD-OE1	5.30	1.33	1.23
1	C	331	GLN	CD-OE1	5.30	1.33	1.23
1	A	360	ASN	CG-OD1	5.28	1.33	1.23
1	B	213	HIS	CD2-NE2	-5.27	1.32	1.37
1	F	153	GLN	CD-OE1	5.27	1.33	1.23
1	B	329	GLN	CD-OE1	5.26	1.33	1.23
1	A	53	THR	CA-CB	-5.24	1.44	1.53
1	C	338	ASN	CG-OD1	5.20	1.33	1.23
1	B	101	HIS	ND1-CE1	5.20	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	GLN	CD-OE1	5.18	1.33	1.23
1	C	101	HIS	ND1-CE1	5.16	1.37	1.32
1	A	208	HIS	ND1-CE1	5.15	1.37	1.32
1	D	106	GLN	CD-NE2	-5.14	1.22	1.33
1	D	153	GLN	CD-OE1	5.14	1.33	1.23
1	E	153	GLN	CD-OE1	5.12	1.33	1.23
1	B	7	GLN	CD-OE1	5.12	1.33	1.23
1	C	40	HIS	ND1-CE1	5.11	1.37	1.32
1	C	106	GLN	CD-NE2	-5.10	1.22	1.33
1	D	213	HIS	ND1-CE1	5.08	1.37	1.32
1	B	208	HIS	CD2-NE2	-5.03	1.32	1.37
1	E	208	HIS	ND1-CE1	5.02	1.37	1.32
1	D	213	HIS	CD2-NE2	-5.01	1.32	1.37

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	222	THR	N-CA-C	14.54	130.28	112.54
1	B	303	ARG	N-CA-C	-12.07	98.52	113.97
1	D	229	ILE	N-CA-C	11.41	122.06	111.91
1	D	229	ILE	N-CA-CB	-10.47	100.14	112.39
1	D	263	GLU	N-CA-C	-9.86	101.76	113.88
1	B	307	GLY	N-CA-C	9.79	132.64	115.61
1	B	375	VAL	N-CA-C	-8.29	98.18	109.37
1	B	135	ARG	N-CA-C	8.09	122.10	111.75
1	D	227	LEU	N-CA-C	-7.80	103.03	112.54
1	B	309	CYS	N-CA-CB	-7.72	98.31	110.28
1	C	135	ARG	N-CA-C	7.71	119.69	111.28
1	F	134	ASP	N-CA-C	7.49	121.34	111.75
1	A	29	GLN	N-CA-C	7.06	120.99	112.38
1	D	191	GLU	N-CA-C	-7.01	100.81	110.35
1	A	306	ALA	N-CA-C	-6.98	99.04	109.86
1	E	191	GLU	N-CA-C	-6.78	101.55	110.43
1	B	208	HIS	CB-CG-CD2	-6.62	122.60	131.20
1	B	195	VAL	N-CA-C	-6.57	103.93	110.30
1	C	101	HIS	CB-CG-CD2	-6.56	122.68	131.20
1	A	305	ASN	CB-CA-C	6.56	122.56	110.10
1	C	40	HIS	CB-CG-CD2	-6.55	122.68	131.20
1	B	101	HIS	CB-CG-CD2	-6.55	122.69	131.20
1	C	208	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	A	208	HIS	CB-CG-CD2	-6.53	122.71	131.20
1	E	208	HIS	CB-CG-CD2	-6.53	122.72	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	B	213	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	F	40	HIS	CB-CG-CD2	-6.46	122.80	131.20
1	B	302	ARG	N-CA-C	-6.44	101.42	110.50
1	B	79	ILE	N-CA-C	6.39	117.14	110.62
1	A	213	HIS	CB-CG-CD2	-6.34	122.95	131.20
1	C	191	GLU	N-CA-C	-6.29	101.80	110.35
1	C	213	HIS	CB-CG-CD2	-6.26	123.06	131.20
1	B	305	ASN	N-CA-C	6.26	119.14	109.07
1	D	263	GLU	N-CA-CB	6.23	118.88	110.59
1	F	213	HIS	CB-CG-CD2	-6.22	123.12	131.20
1	E	213	HIS	CB-CG-CD2	-6.08	123.30	131.20
1	B	195	VAL	N-CA-CB	5.96	117.12	110.62
1	A	135	ARG	N-CA-C	5.86	117.67	111.28
1	F	191	GLU	N-CA-C	-5.86	102.38	110.35
1	B	208	HIS	CB-CG-ND1	5.79	131.38	122.70
1	D	261	GLU	N-CA-C	5.78	119.81	112.87
1	B	213	HIS	CB-CG-ND1	5.77	131.36	122.70
1	F	40	HIS	CB-CG-ND1	5.70	131.24	122.70
1	B	101	HIS	CB-CG-ND1	5.68	131.22	122.70
1	C	40	HIS	CB-CG-ND1	5.67	131.20	122.70
1	C	101	HIS	CB-CG-ND1	5.66	131.18	122.70
1	A	322	GLU	N-CA-C	-5.63	105.04	111.07
1	D	213	HIS	CB-CG-ND1	5.62	131.14	122.70
1	C	208	HIS	CB-CG-ND1	5.60	131.10	122.70
1	B	307	GLY	CA-C-N	-5.60	114.82	122.93
1	B	307	GLY	C-N-CA	-5.60	114.82	122.93
1	F	17	ASP	N-CA-C	5.59	117.37	111.28
1	C	213	HIS	CB-CG-ND1	5.58	131.07	122.70
1	B	176	GLN	N-CA-C	-5.58	106.24	113.16
1	C	50	PHE	N-CA-C	-5.57	105.13	111.14
1	E	126	LYS	N-CA-CB	5.57	119.44	110.86
1	A	208	HIS	CB-CG-ND1	5.57	131.05	122.70
1	F	213	HIS	CB-CG-ND1	5.56	131.04	122.70
1	B	172	ARG	N-CA-C	-5.55	105.31	111.36
1	E	208	HIS	CB-CG-ND1	5.55	131.02	122.70
1	D	16	ALA	N-CA-C	-5.53	103.68	110.65
1	B	170	THR	N-CA-C	5.50	119.99	113.28
1	B	28	VAL	CB-CA-C	-5.49	104.94	111.97
1	A	30	PHE	N-CA-CB	5.49	118.60	110.53
1	A	213	HIS	CB-CG-ND1	5.48	130.93	122.70
1	A	145	ASP	N-CA-C	-5.43	105.36	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	HIS	CB-CG-ND1	5.41	130.81	122.70
1	D	177	ASP	N-CA-C	-5.37	107.39	114.31
1	A	170	THR	N-CA-C	5.36	119.87	113.23
1	C	62	ARG	N-CA-C	-5.31	105.49	111.28
1	E	176	GLN	N-CA-C	-5.29	106.60	113.16
1	B	296	GLN	N-CA-C	-5.20	104.62	112.99
1	F	177	ASP	N-CA-C	-5.17	107.64	114.31
1	B	16	ALA	N-CA-C	-5.09	104.23	110.65
1	A	16	ALA	N-CA-C	-5.07	104.26	110.65
1	B	177	ASP	N-CA-C	-5.04	107.81	114.31
1	C	227	LEU	N-CA-C	5.02	121.50	110.80
1	D	176	GLN	N-CA-C	-5.02	106.93	113.16

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	2892	0	2783	97	0
1	B	2923	0	2836	93	3
1	C	2826	0	2657	99	3
1	D	2854	0	2720	99	0
1	E	2678	0	2401	135	0
1	F	2791	0	2666	121	0
2	A	23	0	0	3	0
2	B	41	0	0	4	0
2	C	26	0	0	3	0
2	D	26	0	0	4	0
2	E	11	0	0	7	0
2	F	11	0	0	3	0
All	All	17102	0	16063	617	3

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 19.

All (617) 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:E:124:TRP:CZ3	1:E:185:ARG:HB3	1.53	1.41
1:C:62:ARG:HD2	2:C:401:HOH:O	1.37	1.23
1:F:112:LYS:HG2	1:F:139:THR:HG22	1.27	1.14
1:B:57:CYS:CB	1:B:309:CYS:SG	2.38	1.10
1:F:50:PHE:O	1:F:54:ASN:ND2	1.83	1.10
1:C:367:TYR:CZ	1:C:375:VAL:HG21	1.88	1.08
1:D:227:LEU:O	1:D:227:LEU:HD23	1.54	1.07
1:D:160:GLY:HA2	1:D:194:LYS:HE2	1.36	1.07
1:E:369:SER:HB3	1:E:372:ASP:HB2	1.40	1.03
1:C:72:ASP:OD1	1:C:73:LYS:N	1.90	1.03
1:E:85:THR:HG21	1:F:50:PHE:CE1	1.94	1.01
1:E:124:TRP:CH2	1:E:185:ARG:HB3	1.94	1.00
1:F:50:PHE:CD2	1:F:54:ASN:ND2	2.30	0.99
1:E:293:LEU:HB3	1:E:298:ILE:CG1	1.93	0.98
1:D:40:HIS:HB2	2:D:394:HOH:O	1.63	0.98
1:E:368:TRP:CD1	1:E:374:MET:HB2	1.98	0.98
1:E:293:LEU:HB3	1:E:298:ILE:HG12	1.45	0.95
1:E:124:TRP:CZ3	1:E:185:ARG:CB	2.49	0.95
1:B:72:ASP:OD1	1:B:73:LYS:N	1.99	0.95
1:B:57:CYS:SG	1:B:309:CYS:CB	2.58	0.91
1:E:368:TRP:HA	1:E:374:MET:HA	1.54	0.88
1:A:371:VAL:HG23	2:A:393:HOH:O	1.73	0.87
1:D:194:LYS:O	1:D:198:ILE:HG13	1.73	0.87
1:D:112:LYS:HG3	1:D:139:THR:HG22	1.56	0.86
1:B:159:VAL:O	1:B:194:LYS:HE2	1.74	0.86
1:E:298:ILE:HD12	1:E:298:ILE:O	1.74	0.86
1:F:50:PHE:HD2	1:F:54:ASN:ND2	1.71	0.86
1:B:112:LYS:HG3	1:B:139:THR:HG22	1.57	0.84
1:C:367:TYR:CE2	1:C:375:VAL:HG21	2.13	0.83
1:E:168:ASP:HB3	2:E:390:HOH:O	1.78	0.83
1:F:42:ASP:OD2	1:F:59:GLN:NE2	2.11	0.82
1:E:210:LYS:CA	1:E:211:GLY:N	2.42	0.82
1:C:368:TRP:CD1	1:C:374:MET:HB2	2.14	0.82
1:B:312:ASN:OD1	1:B:313:PRO:HA	1.78	0.82
1:A:194:LYS:O	1:A:198:ILE:HG13	1.79	0.81
1:C:160:GLY:HA2	1:C:194:LYS:HE2	1.62	0.81
1:E:368:TRP:HD1	1:E:374:MET:HB2	1.40	0.81
1:C:373:LYS:O	1:C:374:MET:HB3	1.80	0.81
1:E:312:ASN:OD1	1:E:313:PRO:HA	1.79	0.81
1:E:373:LYS:O	1:E:374:MET:HB3	1.78	0.81
1:D:367:TYR:CZ	1:D:376:VAL:HG21	2.14	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:TYR:CZ	1:C:375:VAL:CG2	2.64	0.80
1:A:376:VAL:HG12	1:A:376:VAL:O	1.79	0.80
1:E:312:ASN:OD1	1:E:313:PRO:CA	2.30	0.80
1:D:367:TYR:O	1:D:376:VAL:HG22	1.81	0.80
1:E:298:ILE:O	1:E:298:ILE:CD1	2.30	0.80
1:E:85:THR:CG2	1:F:50:PHE:CE1	2.65	0.79
1:D:367:TYR:CE2	1:D:376:VAL:HG21	2.17	0.79
1:E:377:THR:O	1:E:377:THR:HG22	1.81	0.78
1:A:112:LYS:HG3	1:A:139:THR:HG22	1.64	0.78
1:F:364:LYS:HG2	1:F:378:LEU:HD21	1.62	0.78
1:F:112:LYS:CG	1:F:139:THR:HG22	2.11	0.78
1:C:18:GLN:OE1	1:C:276:SER:OG	2.01	0.77
1:C:366:GLY:HA2	1:C:377:THR:HG23	1.66	0.77
1:A:221:PHE:O	1:A:226:LEU:HD11	1.84	0.77
1:E:293:LEU:O	1:E:298:ILE:HG13	1.86	0.76
1:A:190:CYS:HB3	1:A:194:LYS:HB3	1.66	0.76
1:C:177:ASP:OD1	1:C:177:ASP:C	2.30	0.75
1:D:301:SER:O	1:D:302:ARG:HB3	1.85	0.75
1:C:167:LYS:O	1:C:171:TYR:CD2	2.41	0.73
1:E:129:TYR:HE1	1:E:131:TYR:HB3	1.52	0.73
1:A:72:ASP:OD1	1:A:73:LYS:N	2.22	0.73
1:A:195:VAL:O	1:A:199:VAL:HG23	1.90	0.72
1:C:221:PHE:CD1	1:C:238:GLY:HA3	2.24	0.72
1:F:221:PHE:HE2	1:F:362:PRO:HB3	1.54	0.72
1:F:65:TYR:CE2	1:F:300:ILE:HG21	2.25	0.72
1:A:35:PHE:HZ	1:A:290:PHE:HB2	1.55	0.71
1:C:373:LYS:O	1:C:374:MET:CB	2.37	0.71
1:A:124:TRP:CE2	1:A:185:ARG:HG2	2.26	0.71
1:E:48:ASN:OD1	1:E:48:ASN:C	2.34	0.71
1:D:367:TYR:CE1	1:D:376:VAL:HG21	2.25	0.70
1:C:129:TYR:HE1	1:C:131:TYR:HB3	1.55	0.70
1:E:376:VAL:O	1:E:377:THR:C	2.35	0.70
1:A:367:TYR:CZ	1:A:376:VAL:HG11	2.26	0.70
1:B:171:TYR:OH	1:B:194:LYS:HE3	1.92	0.69
1:E:310:LEU:HD22	1:F:54:ASN:OD1	1.93	0.69
1:E:293:LEU:CB	1:E:298:ILE:HG12	2.20	0.69
1:B:112:LYS:CG	1:B:139:THR:HG22	2.22	0.69
1:A:225:ASP:OD1	1:A:225:ASP:C	2.35	0.69
1:E:210:LYS:CA	1:E:210:LYS:O	2.40	0.69
1:A:221:PHE:HE2	1:A:362:PRO:HB3	1.56	0.69
1:C:283:VAL:O	1:C:287:THR:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:ASP:O	1:C:373:LYS:CB	2.41	0.69
1:B:129:TYR:HE1	1:B:131:TYR:HB3	1.56	0.69
1:B:298:ILE:HG22	1:B:300:ILE:HG23	1.74	0.69
1:D:129:TYR:HE1	1:D:131:TYR:HB3	1.57	0.68
1:D:198:ILE:O	1:D:202:VAL:HG23	1.93	0.68
1:B:291:ARG:HH11	1:B:291:ARG:HG2	1.58	0.68
1:C:124:TRP:CE2	1:C:185:ARG:HG2	2.29	0.68
1:E:210:LYS:O	1:E:211:GLY:N	2.26	0.68
1:C:367:TYR:CE2	1:C:375:VAL:CG2	2.77	0.68
1:B:219:LEU:HD22	1:B:241:ILE:HG23	1.76	0.68
1:D:301:SER:O	1:D:302:ARG:CB	2.41	0.68
1:B:35:PHE:HZ	1:B:290:PHE:HB2	1.58	0.68
1:F:129:TYR:HE1	1:F:131:TYR:HB3	1.58	0.68
1:E:121:TYR:CE2	1:E:376:VAL:HG21	2.29	0.67
1:D:227:LEU:HD23	1:D:227:LEU:C	2.19	0.67
1:D:367:TYR:CD2	1:D:376:VAL:HG21	2.30	0.67
1:E:50:PHE:CD1	1:E:50:PHE:C	2.73	0.67
1:D:129:TYR:CE1	1:D:131:TYR:HB3	2.30	0.67
1:F:203:ILE:HD11	1:F:229:ILE:CG2	2.24	0.67
1:E:48:ASN:OD1	1:E:51:ALA:N	2.22	0.66
1:E:129:TYR:CE1	1:E:131:TYR:HB3	2.30	0.66
1:A:291:ARG:HG2	1:A:291:ARG:HH11	1.61	0.66
1:E:226:LEU:H	1:E:226:LEU:HD12	1.61	0.66
1:A:129:TYR:HE1	1:A:131:TYR:HB3	1.60	0.66
1:D:112:LYS:CG	1:D:139:THR:HG22	2.24	0.66
1:D:124:TRP:CE2	1:D:185:ARG:HG2	2.32	0.65
1:B:255:ARG:HD3	1:B:255:ARG:O	1.96	0.65
1:E:122:TYR:HB3	1:E:124:TRP:HE1	1.60	0.65
1:A:110:ASP:OD1	1:A:112:LYS:HE3	1.94	0.65
1:B:98:ASP:OD1	1:B:99:GLY:N	2.30	0.65
1:E:372:ASP:O	1:E:373:LYS:CB	2.44	0.65
1:E:312:ASN:OD1	1:E:313:PRO:N	2.30	0.65
1:A:198:ILE:O	1:A:202:VAL:HG23	1.96	0.65
1:B:124:TRP:CE2	1:B:185:ARG:HG2	2.32	0.65
1:E:373:LYS:O	1:E:374:MET:CB	2.45	0.65
1:E:122:TYR:HB3	1:E:124:TRP:NE1	2.12	0.65
1:C:124:TRP:CZ3	1:C:185:ARG:HB3	2.32	0.64
1:C:129:TYR:CE1	1:C:131:TYR:HB3	2.31	0.64
1:A:124:TRP:CZ3	1:A:185:ARG:HB3	2.32	0.64
1:D:158:ASN:OD1	1:D:159:VAL:N	2.30	0.64
1:D:291:ARG:HH11	1:D:291:ARG:HG2	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:TRP:CZ3	1:D:185:ARG:HB3	2.33	0.64
1:B:110:ASP:OD1	1:B:112:LYS:HE3	1.96	0.64
1:B:129:TYR:CE1	1:B:131:TYR:HB3	2.32	0.64
1:E:124:TRP:CE3	1:E:185:ARG:HB3	2.28	0.64
1:E:50:PHE:CZ	1:F:314:ALA:HB2	2.32	0.64
1:F:291:ARG:HG2	1:F:291:ARG:HH11	1.61	0.64
1:C:162:ILE:CG2	1:C:167:LYS:HA	2.28	0.64
1:F:255:ARG:O	1:F:255:ARG:HD3	1.98	0.63
1:C:368:TRP:HD1	1:C:374:MET:HB2	1.62	0.63
1:E:312:ASN:HA	1:E:313:PRO:C	2.23	0.63
1:E:377:THR:O	1:E:377:THR:CG2	2.45	0.63
1:C:368:TRP:HA	1:C:374:MET:HA	1.80	0.63
1:D:312:ASN:OD1	1:D:313:PRO:HA	1.99	0.63
1:A:35:PHE:HZ	1:A:290:PHE:CB	2.12	0.63
1:F:110:ASP:OD1	1:F:112:LYS:HE2	1.99	0.62
1:C:162:ILE:HG21	1:C:167:LYS:HA	1.81	0.62
1:B:70:PHE:CE2	1:B:93:PRO:HG2	2.34	0.62
1:B:71:TYR:OH	1:B:95:PHE:O	2.09	0.62
1:F:144:LEU:CA	1:F:145:ASP:N	2.62	0.62
1:B:46:VAL:O	1:B:75:SER:OG	2.18	0.62
1:E:293:LEU:CB	1:E:298:ILE:CG1	2.75	0.62
1:F:117:SER:HB3	1:F:375:VAL:CG1	2.30	0.62
1:C:175:PHE:O	1:C:179:GLU:N	2.31	0.62
1:E:50:PHE:HZ	1:F:314:ALA:HB2	1.63	0.62
1:E:293:LEU:C	1:E:298:ILE:HG13	2.24	0.62
1:B:188:LEU:HD12	1:B:216:ILE:CD1	2.30	0.62
1:D:110:ASP:OD1	1:D:112:LYS:HE3	2.00	0.62
1:E:374:MET:CG	1:E:375:VAL:N	2.63	0.62
1:C:61:SER:O	1:C:306:ALA:N	2.33	0.61
1:C:177:ASP:O	1:C:180:LEU:HB2	2.01	0.61
1:F:50:PHE:CE2	1:F:54:ASN:ND2	2.62	0.61
1:E:115:LEU:HD11	1:E:187:ILE:HD13	1.82	0.60
1:C:70:PHE:CE2	1:C:93:PRO:HG2	2.36	0.60
1:F:226:LEU:HD12	1:F:226:LEU:H	1.65	0.60
1:A:133:SER:OG	1:A:158:ASN:ND2	2.35	0.60
1:D:219:LEU:HD22	1:D:241:ILE:HG23	1.82	0.60
1:C:72:ASP:OD1	1:C:72:ASP:C	2.40	0.60
1:E:124:TRP:CH2	1:E:185:ARG:CB	2.78	0.60
1:D:48:ASN:O	1:D:52:VAL:HG23	2.02	0.60
1:D:255:ARG:O	1:D:255:ARG:HD3	2.01	0.60
1:B:124:TRP:CZ3	1:B:185:ARG:HB3	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LYS:HE2	1:A:133:SER:O	2.01	0.59
1:D:79:ILE:HG22	1:D:80:THR:N	2.16	0.59
1:E:48:ASN:O	1:E:52:VAL:HG23	2.02	0.59
1:E:85:THR:CB	1:F:50:PHE:CE1	2.85	0.59
1:F:97:THR:O	1:F:346:LYS:HE3	2.02	0.59
1:F:99:GLY:HA3	1:F:101:HIS:CE1	2.37	0.59
1:E:310:LEU:CD2	1:F:54:ASN:OD1	2.50	0.59
1:A:35:PHE:CZ	1:A:290:PHE:HB2	2.35	0.59
1:C:255:ARG:O	1:C:255:ARG:HD3	2.02	0.59
1:A:112:LYS:CG	1:A:139:THR:HG22	2.30	0.59
1:B:35:PHE:HZ	1:B:290:PHE:CB	2.15	0.59
1:D:367:TYR:CD1	1:D:376:VAL:HG21	2.38	0.59
1:E:374:MET:HE2	1:E:376:VAL:CG2	2.33	0.59
1:F:376:VAL:HG23	1:F:376:VAL:O	2.02	0.59
1:A:300:ILE:HG13	1:A:300:ILE:O	2.03	0.58
1:F:255:ARG:HD2	1:F:259:LEU:HD21	1.85	0.58
1:E:35:PHE:HZ	1:E:290:PHE:CB	2.16	0.58
1:E:122:TYR:CB	1:E:124:TRP:CD1	2.87	0.58
1:A:317:TRP:NE1	1:A:319:GLN:OE1	2.34	0.58
1:A:35:PHE:HD1	1:A:36:ARG:N	2.01	0.58
1:B:72:ASP:OD1	1:B:72:ASP:C	2.47	0.58
1:F:117:SER:HB3	1:F:375:VAL:HG13	1.85	0.58
1:B:97:THR:O	1:B:346:LYS:HE3	2.04	0.58
1:B:35:PHE:CZ	1:B:290:PHE:HB2	2.39	0.58
1:D:65:TYR:CD2	1:D:300:ILE:HD12	2.39	0.57
1:B:374:MET:O	1:B:375:VAL:C	2.47	0.57
1:B:302:ARG:HB3	1:B:304:GLY:O	2.04	0.57
1:F:48:ASN:O	1:F:52:VAL:HG23	2.05	0.57
1:F:195:VAL:O	1:F:199:VAL:HG23	2.04	0.57
1:A:367:TYR:CE2	1:A:376:VAL:HG11	2.40	0.57
1:C:367:TYR:CE1	1:C:375:VAL:CG2	2.88	0.57
1:E:374:MET:HE2	1:E:376:VAL:HG23	1.85	0.57
1:F:194:LYS:O	1:F:198:ILE:HG13	2.05	0.57
1:B:255:ARG:HD3	1:B:255:ARG:C	2.28	0.57
1:E:190:CYS:HB3	1:E:194:LYS:CB	2.35	0.57
1:D:71:TYR:CE1	1:D:94:SER:HB2	2.41	0.56
1:F:65:TYR:HE2	1:F:300:ILE:HG21	1.69	0.56
1:C:367:TYR:CE1	1:C:375:VAL:HG22	2.41	0.56
1:B:133:SER:HA	1:B:137:LEU:HD11	1.88	0.56
1:C:97:THR:O	1:C:346:LYS:HE3	2.05	0.56
1:A:97:THR:O	1:A:346:LYS:HE3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:LEU:O	1:E:178:LEU:HB2	2.05	0.56
1:D:367:TYR:CG	1:D:376:VAL:HG21	2.41	0.56
1:D:70:PHE:CE2	1:D:93:PRO:HG2	2.41	0.56
1:B:28:VAL:HG12	1:B:29:GLN:N	2.21	0.56
1:B:188:LEU:HD12	1:B:216:ILE:HD11	1.88	0.56
1:A:129:TYR:CE1	1:A:131:TYR:HB3	2.41	0.55
1:A:178:LEU:HD23	1:A:183:GLU:HB3	1.88	0.55
1:C:167:LYS:HA	1:C:170:THR:OG1	2.05	0.55
1:F:203:ILE:HD11	1:F:229:ILE:HG23	1.88	0.55
1:B:260:GLU:OE2	1:B:262:LYS:HG2	2.06	0.55
1:F:129:TYR:CE1	1:F:131:TYR:HB3	2.40	0.55
1:A:35:PHE:HD1	1:A:35:PHE:C	2.15	0.55
1:B:35:PHE:HD1	1:B:36:ARG:N	2.04	0.55
1:F:133:SER:OG	1:F:158:ASN:ND2	2.40	0.55
1:E:144:LEU:HD11	1:F:144:LEU:HD11	1.87	0.55
1:F:79:ILE:HG22	1:F:80:THR:N	2.21	0.55
1:F:255:ARG:HD3	1:F:255:ARG:C	2.30	0.55
1:B:61:SER:OG	1:B:307:GLY:O	2.23	0.55
1:C:124:TRP:CH2	1:C:185:ARG:HB3	2.42	0.55
1:F:190:CYS:CB	1:F:194:LYS:HB3	2.36	0.55
1:B:71:TYR:CD1	1:B:71:TYR:C	2.85	0.55
1:C:178:LEU:HD23	1:C:183:GLU:HB3	1.89	0.55
1:D:115:LEU:O	1:D:119:ILE:HG13	2.07	0.55
1:D:174:LEU:O	1:D:178:LEU:HB2	2.07	0.55
1:A:53:THR:HG22	1:A:53:THR:O	2.07	0.54
1:A:213:HIS:CD2	1:A:235:ASN:HB3	2.42	0.54
1:B:174:LEU:O	1:B:178:LEU:HB2	2.07	0.54
1:D:132:ASP:OD1	1:D:160:GLY:HA2	2.07	0.54
1:B:35:PHE:HD1	1:B:35:PHE:C	2.15	0.54
1:C:8:ILE:O	1:C:39:PRO:HA	2.07	0.54
1:F:132:ASP:OD1	1:F:160:GLY:HA3	2.07	0.54
1:F:178:LEU:HD23	1:F:183:GLU:HB3	1.88	0.54
1:A:111:LEU:HD13	1:A:219:LEU:CD2	2.37	0.54
1:A:174:LEU:O	1:A:178:LEU:HB2	2.07	0.54
1:F:144:LEU:CA	1:F:144:LEU:O	2.56	0.54
1:A:27:MET:HE1	1:A:37:LEU:O	2.08	0.54
1:D:367:TYR:CG	1:D:376:VAL:CG2	2.90	0.54
1:D:255:ARG:HD3	1:D:255:ARG:C	2.33	0.54
1:E:293:LEU:CA	1:E:298:ILE:HG13	2.38	0.54
1:F:298:ILE:HG22	1:F:299:GLU:N	2.23	0.54
1:F:115:LEU:HD11	1:F:187:ILE:HD13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:TYR:CD2	1:D:376:VAL:CG2	2.91	0.53
1:E:122:TYR:HB3	1:E:124:TRP:CD1	2.43	0.53
1:B:115:LEU:O	1:B:119:ILE:HG13	2.07	0.53
1:B:226:LEU:HD12	1:B:362:PRO:HG3	1.91	0.53
1:C:255:ARG:HD2	1:C:259:LEU:HD21	1.90	0.53
1:C:174:LEU:O	1:C:178:LEU:HB2	2.09	0.53
1:F:70:PHE:CE2	1:F:93:PRO:HG2	2.44	0.53
1:A:35:PHE:C	1:A:35:PHE:CD1	2.85	0.53
1:F:45:GLU:HG3	2:F:380:HOH:O	2.08	0.53
1:B:36:ARG:HG2	2:B:417:HOH:O	2.07	0.53
1:B:240:GLN:NE2	2:B:418:HOH:O	2.41	0.53
1:A:178:LEU:HD23	1:A:178:LEU:O	2.09	0.53
1:A:229:ILE:HA	2:E:385:HOH:O	2.08	0.53
1:E:122:TYR:HB2	1:E:124:TRP:CD1	2.43	0.53
1:E:203:ILE:HD11	1:E:229:ILE:CG2	2.38	0.53
1:D:8:ILE:O	1:D:39:PRO:HA	2.08	0.53
1:E:374:MET:HG2	2:E:389:HOH:O	2.07	0.53
1:B:35:PHE:C	1:B:35:PHE:CD1	2.86	0.53
1:B:291:ARG:HH11	1:B:291:ARG:CG	2.20	0.53
1:D:291:ARG:NH2	2:D:395:HOH:O	2.42	0.53
1:C:17:ASP:HB3	1:C:265:PRO:HB2	1.91	0.53
1:E:35:PHE:HD1	1:E:36:ARG:N	2.07	0.53
1:A:340:LYS:O	1:A:348:ILE:HG12	2.09	0.53
1:E:178:LEU:HD23	1:E:183:GLU:HB3	1.91	0.53
1:F:144:LEU:O	1:F:145:ASP:N	2.42	0.53
1:A:111:LEU:HD13	1:A:219:LEU:HD21	1.91	0.52
1:A:203:ILE:HD11	1:A:229:ILE:CG2	2.39	0.52
1:A:295:LYS:O	1:A:295:LYS:HG2	2.09	0.52
1:B:71:TYR:C	1:B:71:TYR:HD1	2.17	0.52
1:B:203:ILE:HD11	1:B:229:ILE:CG2	2.39	0.52
1:D:178:LEU:HD23	1:D:183:GLU:HB3	1.90	0.52
1:E:35:PHE:HD1	1:E:35:PHE:C	2.17	0.52
1:F:65:TYR:HE2	1:F:300:ILE:CG2	2.22	0.52
1:F:174:LEU:O	1:F:178:LEU:HB2	2.10	0.52
1:D:295:LYS:O	1:D:295:LYS:HG2	2.10	0.52
1:F:178:LEU:HD23	1:F:178:LEU:O	2.10	0.52
1:E:85:THR:CB	1:F:50:PHE:CD1	2.93	0.52
1:D:158:ASN:OD1	1:D:158:ASN:C	2.53	0.52
1:D:291:ARG:HH11	1:D:291:ARG:CG	2.23	0.52
1:A:79:ILE:HG22	1:A:80:THR:N	2.25	0.52
1:B:178:LEU:HD23	1:B:183:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ARG:HD3	1:C:255:ARG:C	2.34	0.52
1:D:7:GLN:NE2	2:D:394:HOH:O	2.40	0.52
1:D:56:PHE:CD1	1:D:56:PHE:C	2.87	0.52
1:D:97:THR:O	1:D:346:LYS:HE3	2.10	0.52
1:E:85:THR:HG21	1:F:50:PHE:CZ	2.44	0.52
1:E:85:THR:OG1	1:F:50:PHE:CD1	2.62	0.52
1:E:122:TYR:CB	1:E:124:TRP:NE1	2.73	0.52
1:E:356:GLU:HG3	1:E:365:ILE:HD13	1.91	0.52
1:E:20:TYR:CE2	1:E:24:ARG:HD2	2.45	0.51
1:F:340:LYS:O	1:F:348:ILE:HG12	2.10	0.51
1:C:356:GLU:HG3	1:C:365:ILE:HD13	1.91	0.51
1:D:86:LEU:O	1:D:87:HIS:HB2	2.10	0.51
1:D:227:LEU:C	1:D:227:LEU:CD2	2.84	0.51
1:E:298:ILE:CD1	1:E:298:ILE:C	2.80	0.51
1:B:8:ILE:O	1:B:39:PRO:HA	2.10	0.51
1:B:235:ASN:ND2	2:B:391:HOH:O	2.43	0.51
1:B:312:ASN:HA	1:B:313:PRO:C	2.35	0.51
1:C:115:LEU:O	1:C:119:ILE:HG13	2.10	0.51
1:D:221:PHE:O	1:D:226:LEU:HD13	2.11	0.51
1:F:80:THR:HG22	1:F:104:VAL:HG21	1.92	0.51
1:A:191:GLU:O	1:A:195:VAL:HG23	2.11	0.51
1:C:115:LEU:HD11	1:C:187:ILE:HD13	1.91	0.51
1:E:144:LEU:HD11	1:F:144:LEU:CD1	2.41	0.51
1:F:376:VAL:O	1:F:376:VAL:CG2	2.59	0.51
1:F:213:HIS:HD2	1:F:214:TYR:N	2.09	0.51
1:A:190:CYS:CB	1:A:194:LYS:HB3	2.37	0.51
1:E:49:SER:HB2	1:F:81:SER:CB	2.41	0.51
1:E:115:LEU:O	1:E:119:ILE:HG13	2.10	0.51
1:A:201:GLN:HA	1:A:201:GLN:OE1	2.10	0.51
1:B:57:CYS:CA	1:B:309:CYS:SG	2.97	0.51
1:B:295:LYS:O	1:B:295:LYS:HG2	2.10	0.51
1:C:79:ILE:HG22	1:C:80:THR:N	2.25	0.51
1:E:85:THR:HB	1:F:50:PHE:CE1	2.46	0.51
1:F:291:ARG:HH11	1:F:291:ARG:CG	2.24	0.50
1:F:8:ILE:O	1:F:39:PRO:HA	2.11	0.50
1:C:132:ASP:OD1	1:C:160:GLY:HA3	2.10	0.50
1:C:177:ASP:OD1	1:C:177:ASP:O	2.30	0.50
1:E:35:PHE:C	1:E:35:PHE:CD1	2.88	0.50
1:E:293:LEU:HD22	1:E:298:ILE:HG12	1.93	0.50
1:F:50:PHE:O	1:F:50:PHE:HD2	1.95	0.50
1:A:291:ARG:HH11	1:A:291:ARG:CG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:HD23	1:C:178:LEU:O	2.11	0.50
1:C:340:LYS:O	1:C:348:ILE:HG12	2.11	0.50
1:A:115:LEU:HD11	1:A:187:ILE:HD13	1.94	0.50
1:B:136:GLY:O	1:B:137:LEU:HB2	2.11	0.50
1:C:71:TYR:CD1	1:C:71:TYR:C	2.89	0.50
1:A:47:ALA:HB2	1:A:72:ASP:OD2	2.12	0.50
1:A:115:LEU:O	1:A:119:ILE:HG13	2.12	0.50
1:C:111:LEU:HD13	1:C:219:LEU:HD21	1.93	0.50
1:E:189:ASP:OD1	1:E:189:ASP:O	2.30	0.50
1:A:255:ARG:O	1:A:255:ARG:HD3	2.12	0.50
1:D:221:PHE:CD1	1:D:238:GLY:HA3	2.47	0.50
1:D:255:ARG:HD2	1:D:259:LEU:HD21	1.94	0.50
1:E:374:MET:HG2	1:E:375:VAL:N	2.26	0.50
1:F:191:GLU:O	1:F:195:VAL:HG23	2.12	0.50
1:A:376:VAL:O	1:A:376:VAL:CG1	2.52	0.50
1:D:227:LEU:O	1:D:227:LEU:CD2	2.44	0.50
1:E:8:ILE:O	1:E:39:PRO:HA	2.11	0.50
1:A:35:PHE:CZ	1:A:290:PHE:CB	2.95	0.49
1:C:20:TYR:CE2	1:C:24:ARG:HD2	2.47	0.49
1:C:175:PHE:O	1:C:179:GLU:HB2	2.12	0.49
1:E:70:PHE:CE2	1:E:93:PRO:HG2	2.46	0.49
1:F:115:LEU:O	1:F:119:ILE:HG13	2.11	0.49
1:D:55:ALA:O	1:D:59:GLN:HG2	2.12	0.49
1:E:230:GLN:HA	1:E:357:LEU:HD21	1.93	0.49
1:E:298:ILE:O	1:E:298:ILE:HD13	2.12	0.49
1:F:190:CYS:HB3	1:F:194:LYS:HB3	1.93	0.49
1:D:132:ASP:OD2	1:D:134:ASP:HB2	2.12	0.49
1:A:56:PHE:CD1	1:A:56:PHE:C	2.90	0.49
1:C:133:SER:HA	1:C:137:LEU:HD11	1.94	0.49
1:D:71:TYR:CD1	1:D:71:TYR:C	2.90	0.49
1:F:375:VAL:O	1:F:375:VAL:HG23	2.12	0.49
1:A:310:LEU:CD2	1:B:54:ASN:OD1	2.61	0.49
1:B:52:VAL:CG1	1:B:79:ILE:HD13	2.42	0.49
1:D:340:LYS:O	1:D:348:ILE:HG12	2.13	0.49
1:F:199:VAL:O	1:F:203:ILE:HG13	2.13	0.49
1:A:20:TYR:CE2	1:A:24:ARG:HD2	2.47	0.49
1:F:260:GLU:HB3	1:F:263:GLU:HB3	1.94	0.49
1:D:71:TYR:C	1:D:71:TYR:HD1	2.20	0.49
1:F:56:PHE:CD1	1:F:56:PHE:C	2.91	0.49
1:A:370:GLU:HB3	2:A:393:HOH:O	2.12	0.49
1:B:124:TRP:CH2	1:B:185:ARG:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ASP:OD1	1:D:160:GLY:CA	2.60	0.49
1:E:79:ILE:HG22	1:E:80:THR:N	2.28	0.49
1:F:65:TYR:CE2	1:F:300:ILE:CG2	2.95	0.49
1:F:178:LEU:CD2	1:F:183:GLU:HB3	2.43	0.49
1:A:133:SER:OG	1:A:158:ASN:OD1	2.30	0.48
1:A:378:LEU:C	1:A:378:LEU:HD12	2.38	0.48
1:B:79:ILE:CG2	1:B:80:THR:N	2.76	0.48
1:B:129:TYR:CE2	1:B:143:VAL:HG21	2.48	0.48
1:C:35:PHE:CD1	1:C:35:PHE:C	2.91	0.48
1:C:317:TRP:NE1	1:C:319:GLN:OE1	2.42	0.48
1:E:213:HIS:HD2	1:E:214:TYR:N	2.11	0.48
1:F:27:MET:HE1	1:F:37:LEU:O	2.13	0.48
1:C:178:LEU:CD2	1:C:183:GLU:HB3	2.44	0.48
1:E:178:LEU:HD23	1:E:178:LEU:O	2.13	0.48
1:E:220:GLY:O	1:E:223:ASP:HB2	2.13	0.48
1:A:255:ARG:HD3	1:A:255:ARG:C	2.38	0.48
1:B:358:LYS:HG3	1:B:363:ARG:HD2	1.95	0.48
1:B:291:ARG:NH2	2:B:409:HOH:O	2.47	0.48
1:F:131:TYR:CZ	1:F:158:ASN:HB2	2.48	0.48
1:C:40:HIS:HB3	2:C:401:HOH:O	2.13	0.48
1:F:55:ALA:O	1:F:59:GLN:HG2	2.14	0.48
1:A:72:ASP:O	1:A:73:LYS:C	2.57	0.47
1:D:133:SER:HA	1:D:137:LEU:HD11	1.96	0.47
1:A:6:ILE:HD12	1:A:35:PHE:CZ	2.48	0.47
1:C:220:GLY:O	1:C:223:ASP:HB2	2.14	0.47
1:D:131:TYR:CZ	1:D:158:ASN:HB2	2.49	0.47
1:F:124:TRP:CZ2	1:F:185:ARG:CB	2.97	0.47
1:A:8:ILE:O	1:A:39:PRO:HA	2.14	0.47
1:B:255:ARG:HD2	1:B:259:LEU:HD21	1.97	0.47
1:E:50:PHE:CE1	1:F:85:THR:HG21	2.50	0.47
1:E:219:LEU:HD22	1:E:241:ILE:HG23	1.96	0.47
1:E:367:TYR:O	1:E:374:MET:HG3	2.15	0.47
1:A:124:TRP:CH2	1:A:185:ARG:HB3	2.50	0.47
1:A:50:PHE:HB2	1:B:81:SER:OG	2.14	0.47
1:A:255:ARG:HD2	1:A:259:LEU:HD21	1.95	0.47
1:E:312:ASN:OD1	1:E:312:ASN:C	2.57	0.47
1:E:375:VAL:HA	2:E:389:HOH:O	2.14	0.47
1:A:178:LEU:CD2	1:A:183:GLU:HB3	2.44	0.47
1:E:293:LEU:HB3	1:E:298:ILE:CD1	2.44	0.47
1:A:213:HIS:HD2	1:A:214:TYR:N	2.13	0.47
1:C:203:ILE:HD11	1:C:229:ILE:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:TYR:HE2	1:E:376:VAL:HG21	1.77	0.47
1:F:230:GLN:HA	1:F:357:LEU:HD21	1.96	0.47
1:A:232:GLY:N	2:E:385:HOH:O	2.47	0.47
1:C:167:LYS:O	1:C:171:TYR:HD2	1.93	0.47
1:D:219:LEU:HD22	1:D:241:ILE:CG2	2.45	0.47
1:C:171:TYR:O	1:C:175:PHE:CD1	2.68	0.47
1:C:71:TYR:C	1:C:71:TYR:HD1	2.23	0.46
1:B:56:PHE:CD1	1:B:56:PHE:C	2.92	0.46
1:B:293:LEU:HD13	1:B:300:ILE:HG21	1.98	0.46
1:E:48:ASN:OD1	1:E:50:PHE:N	2.48	0.46
1:F:150:LYS:CB	2:F:385:HOH:O	2.63	0.46
1:E:13:PRO:HD3	1:E:70:PHE:CD1	2.51	0.46
1:F:98:ASP:N	1:F:98:ASP:OD1	2.49	0.46
1:F:50:PHE:CD2	1:F:50:PHE:C	2.94	0.46
1:E:375:VAL:HG12	1:E:376:VAL:N	2.30	0.46
1:C:6:ILE:HB	1:C:37:LEU:HD23	1.96	0.46
1:E:185:ARG:HD2	2:E:384:HOH:O	2.15	0.46
1:F:19:GLU:O	1:F:279:THR:HG21	2.16	0.46
1:E:50:PHE:CZ	1:F:85:THR:HG21	2.50	0.46
1:E:90:PHE:CE2	1:E:92:THR:HB	2.51	0.46
1:F:203:ILE:CD1	1:F:229:ILE:HG22	2.46	0.46
1:A:13:PRO:HD3	1:A:70:PHE:CD1	2.51	0.46
1:A:208:HIS:HE1	1:E:208:HIS:HE1	1.64	0.46
1:E:340:LYS:O	1:E:348:ILE:HG12	2.16	0.46
1:A:230:GLN:HA	1:A:357:LEU:HD21	1.98	0.46
1:B:35:PHE:CZ	1:B:290:PHE:CB	2.98	0.46
1:B:178:LEU:HD23	1:B:178:LEU:O	2.15	0.46
1:B:226:LEU:CD1	1:B:362:PRO:HG3	2.45	0.46
1:E:178:LEU:CD2	1:E:183:GLU:HB3	2.46	0.46
1:B:55:ALA:O	1:B:59:GLN:HG2	2.16	0.45
1:D:20:TYR:CE2	1:D:24:ARG:HD2	2.51	0.45
1:F:294:ARG:C	1:F:296:GLN:H	2.22	0.45
1:F:20:TYR:CE2	1:F:24:ARG:HD2	2.51	0.45
1:F:190:CYS:HB2	1:F:194:LYS:HB3	1.98	0.45
1:D:178:LEU:HD23	1:D:178:LEU:O	2.17	0.45
1:E:27:MET:HE1	1:E:37:LEU:O	2.15	0.45
1:E:375:VAL:CA	2:E:389:HOH:O	2.64	0.45
1:A:358:LYS:HG3	1:A:363:ARG:HD2	1.99	0.45
1:C:13:PRO:HB3	2:C:404:HOH:O	2.16	0.45
1:D:130:LEU:N	1:D:130:LEU:HD12	2.30	0.45
1:E:133:SER:HA	1:E:137:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:GLU:CG	2:F:380:HOH:O	2.63	0.45
1:A:133:SER:OG	1:A:158:ASN:CG	2.60	0.45
1:B:86:LEU:O	1:B:87:HIS:HB2	2.15	0.45
1:D:220:GLY:O	1:D:223:ASP:HB2	2.15	0.45
1:C:369:SER:HB3	1:C:372:ASP:HB2	1.99	0.45
1:D:27:MET:HE1	1:D:37:LEU:O	2.16	0.45
1:D:127:PHE:CE1	1:D:154:VAL:HG22	2.51	0.45
1:F:210:LYS:HA	1:F:233:GLY:O	2.17	0.45
1:F:356:GLU:O	1:F:362:PRO:HA	2.17	0.45
1:B:72:ASP:O	1:B:73:LYS:C	2.59	0.45
1:B:91:ILE:HD13	1:B:286:MET:SD	2.57	0.45
1:C:294:ARG:C	1:C:296:GLN:H	2.25	0.45
1:F:50:PHE:HD2	1:F:54:ASN:HD22	1.58	0.45
1:F:203:ILE:HD11	1:F:229:ILE:HG22	1.99	0.45
1:A:131:TYR:CZ	1:A:158:ASN:HB2	2.52	0.45
1:C:7:GLN:OE1	1:C:62:ARG:CD	2.65	0.45
1:D:124:TRP:CH2	1:D:185:ARG:HB3	2.52	0.45
1:A:174:LEU:O	1:A:174:LEU:HG	2.16	0.45
1:B:340:LYS:O	1:B:348:ILE:HG12	2.16	0.45
1:D:342:ASP:HB3	1:D:348:ILE:HD13	1.99	0.45
1:E:293:LEU:HD22	1:E:298:ILE:HG21	1.99	0.45
1:C:221:PHE:O	1:C:226:LEU:HD21	2.17	0.44
1:D:98:ASP:OD1	1:D:98:ASP:N	2.50	0.44
1:D:107:MET:HE3	1:D:107:MET:HB3	1.87	0.44
1:A:184:ARG:HD3	1:A:184:ARG:HA	1.74	0.44
1:A:300:ILE:O	1:A:300:ILE:CG1	2.64	0.44
1:C:72:ASP:O	1:C:73:LYS:C	2.60	0.44
1:C:120:GLU:OE2	1:C:150:LYS:HE3	2.17	0.44
1:A:135:ARG:NE	1:A:189:ASP:OD1	2.50	0.44
1:A:370:GLU:O	1:A:373:LYS:CG	2.66	0.44
1:B:213:HIS:HD2	1:B:214:TYR:N	2.16	0.44
1:D:367:TYR:CD1	1:D:376:VAL:CG2	3.00	0.44
1:E:226:LEU:HD12	1:E:226:LEU:N	2.30	0.44
1:A:342:ASP:HB3	1:A:348:ILE:HD13	1.99	0.44
1:B:167:LYS:O	1:B:171:TYR:CD2	2.71	0.44
1:B:219:LEU:HB3	1:B:241:ILE:HG12	1.99	0.44
1:F:99:GLY:HA3	1:F:101:HIS:HE1	1.83	0.44
1:F:356:GLU:HG3	1:F:365:ILE:HD13	1.98	0.44
1:B:194:LYS:O	1:B:198:ILE:HG13	2.17	0.44
1:D:184:ARG:HA	1:D:184:ARG:HD3	1.77	0.44
1:E:131:TYR:CZ	1:E:158:ASN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:MET:O	1:B:376:VAL:HG23	2.18	0.44
1:C:71:TYR:OH	1:C:95:PHE:O	2.27	0.44
1:E:6:ILE:HD12	1:E:35:PHE:CZ	2.51	0.44
1:F:50:PHE:HD2	1:F:50:PHE:C	2.26	0.44
1:A:6:ILE:HD12	1:A:35:PHE:CE1	2.53	0.44
1:B:300:ILE:HA	1:B:319:GLN:HG2	1.99	0.44
1:D:115:LEU:HD11	1:D:187:ILE:HD13	2.00	0.44
1:E:144:LEU:CD1	1:F:144:LEU:HD11	2.47	0.44
1:B:20:TYR:CE2	1:B:24:ARG:HD2	2.52	0.44
1:C:56:PHE:CD1	1:C:56:PHE:C	2.95	0.44
1:C:90:PHE:CE2	1:C:92:THR:HB	2.53	0.44
1:C:219:LEU:HB3	1:C:241:ILE:HG12	2.00	0.44
1:D:145:ASP:HB3	2:D:382:HOH:O	2.17	0.44
1:D:178:LEU:CD2	1:D:183:GLU:HB3	2.48	0.44
1:D:213:HIS:HD2	1:D:214:TYR:N	2.15	0.44
1:E:50:PHE:CD1	1:F:85:THR:HG21	2.53	0.44
1:B:294:ARG:C	1:B:296:GLN:H	2.26	0.43
1:C:12:PHE:HA	1:C:13:PRO:HD3	1.91	0.43
1:C:132:ASP:OD1	1:C:160:GLY:CA	2.66	0.43
1:D:260:GLU:HB3	1:D:263:GLU:HB3	1.99	0.43
1:E:107:MET:HE3	1:E:107:MET:HB3	1.87	0.43
1:B:178:LEU:CD2	1:B:183:GLU:HB3	2.48	0.43
1:C:209:VAL:HA	1:C:232:GLY:O	2.17	0.43
1:D:229:ILE:HD12	1:D:236:VAL:HG21	1.99	0.43
1:F:298:ILE:CG2	1:F:299:GLU:N	2.82	0.43
1:C:111:LEU:HD13	1:C:219:LEU:CD2	2.47	0.43
1:D:68:PHE:CE1	1:D:93:PRO:HD3	2.53	0.43
1:B:184:ARG:HD3	1:B:184:ARG:HA	1.75	0.43
1:C:27:MET:HE1	1:C:37:LEU:O	2.18	0.43
1:A:68:PHE:CE1	1:A:93:PRO:HD3	2.53	0.43
1:E:6:ILE:HD12	1:E:35:PHE:CE1	2.54	0.43
1:A:20:TYR:HB3	2:A:395:HOH:O	2.18	0.43
1:A:203:ILE:HD11	1:A:229:ILE:HG23	2.01	0.43
1:C:223:ASP:OD2	1:C:273:LYS:HA	2.19	0.43
1:D:370:GLU:O	1:D:373:LYS:CG	2.67	0.43
1:E:48:ASN:CG	1:E:51:ALA:H	2.19	0.43
1:C:65:TYR:CE2	1:C:300:ILE:HD12	2.54	0.43
1:D:317:TRP:NE1	1:D:319:GLN:OE1	2.46	0.43
1:E:50:PHE:CE2	1:F:85:THR:HG21	2.53	0.43
1:B:201:GLN:O	1:B:205:ILE:HG12	2.18	0.43
1:B:226:LEU:HD13	1:B:357:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:374:MET:C	1:C:375:VAL:HG13	2.44	0.42
1:D:206:GLY:HA2	1:D:208:HIS:CE1	2.54	0.42
1:D:230:GLN:HA	1:D:357:LEU:HD21	2.00	0.42
1:A:312:ASN:OD1	1:A:313:PRO:HA	2.19	0.42
1:C:86:LEU:O	1:C:87:HIS:HB2	2.19	0.42
1:C:131:TYR:CZ	1:C:158:ASN:HB2	2.54	0.42
1:C:367:TYR:CD1	1:C:375:VAL:HG22	2.55	0.42
1:A:70:PHE:CE2	1:A:93:PRO:HG2	2.54	0.42
1:A:260:GLU:HB3	1:A:263:GLU:HB3	2.02	0.42
1:C:366:GLY:CA	1:C:377:THR:HG23	2.41	0.42
1:F:375:VAL:O	1:F:375:VAL:CG2	2.67	0.42
1:B:317:TRP:NE1	1:B:319:GLN:OE1	2.43	0.42
1:D:71:TYR:HD1	1:D:71:TYR:O	2.02	0.42
1:E:174:LEU:O	1:E:174:LEU:HG	2.19	0.42
1:E:219:LEU:HB3	1:E:241:ILE:HG12	2.02	0.42
1:A:117:SER:HB3	1:A:375:VAL:HG22	2.02	0.42
1:B:52:VAL:HG12	1:B:79:ILE:HD13	2.02	0.42
1:E:35:PHE:CZ	1:E:290:PHE:CB	3.00	0.42
1:F:90:PHE:CE2	1:F:92:THR:HB	2.55	0.42
1:F:203:ILE:HG12	1:F:229:ILE:HG22	2.01	0.42
1:B:220:GLY:O	1:B:223:ASP:HB2	2.20	0.42
1:C:260:GLU:HB3	1:C:263:GLU:HB3	2.01	0.42
1:D:293:LEU:HD23	1:D:293:LEU:HA	1.92	0.42
1:F:226:LEU:HD12	1:F:226:LEU:N	2.34	0.42
1:C:227:LEU:HD23	1:C:227:LEU:HA	1.87	0.42
1:E:56:PHE:CD1	1:E:56:PHE:C	2.97	0.42
1:E:209:VAL:O	1:E:234:ALA:HB2	2.20	0.42
1:C:129:TYR:OH	1:C:139:THR:OG1	2.11	0.41
1:D:72:ASP:OD1	1:D:73:LYS:N	2.53	0.41
1:B:6:ILE:HD12	1:B:35:PHE:CZ	2.54	0.41
1:B:291:ARG:CG	1:B:291:ARG:NH1	2.82	0.41
1:F:27:MET:CE	1:F:39:PRO:HD3	2.50	0.41
1:F:86:LEU:O	1:F:87:HIS:HB2	2.20	0.41
1:F:129:TYR:C	1:F:130:LEU:HD12	2.45	0.41
1:E:74:LYS:O	1:F:77:ASN:HB3	2.20	0.41
1:B:107:MET:HE3	1:B:107:MET:HB3	1.86	0.41
1:B:288:GLU:OE1	1:B:291:ARG:NH1	2.53	0.41
1:D:90:PHE:CE2	1:D:92:THR:HB	2.56	0.41
1:D:356:GLU:HG3	1:D:365:ILE:HD13	2.02	0.41
1:D:369:SER:HB3	1:D:372:ASP:HB2	2.02	0.41
1:E:83:CYS:SG	1:E:90:PHE:HB2	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:342:ASP:HB3	1:E:348:ILE:HD13	2.01	0.41
1:E:374:MET:HG3	1:E:375:VAL:H	1.85	0.41
1:A:97:THR:HG23	1:A:106:GLN:HE21	1.84	0.41
1:D:231:PHE:CD1	1:D:359:THR:HG23	2.55	0.41
1:E:86:LEU:O	1:E:87:HIS:HB2	2.20	0.41
1:E:203:ILE:HG12	1:E:229:ILE:HG22	2.02	0.41
1:F:17:ASP:HB3	1:F:265:PRO:HB2	2.02	0.41
1:F:254:GLU:O	1:F:258:THR:HG23	2.21	0.41
1:F:364:LYS:HG2	1:F:378:LEU:CD2	2.43	0.41
1:A:121:TYR:HB2	1:A:375:VAL:HG21	2.02	0.41
1:C:120:GLU:OE2	1:C:150:LYS:CE	2.69	0.41
1:A:97:THR:H	1:A:106:GLN:NE2	2.19	0.41
1:D:128:ALA:HB3	1:D:186:VAL:HG22	2.02	0.41
1:E:97:THR:HG23	1:E:106:GLN:HE21	1.85	0.41
1:E:293:LEU:HB3	1:E:298:ILE:HG13	1.93	0.41
1:E:374:MET:HG3	1:E:375:VAL:N	2.35	0.41
1:A:90:PHE:CE2	1:A:92:THR:HB	2.56	0.41
1:C:174:LEU:O	1:C:174:LEU:HG	2.20	0.41
1:C:210:LYS:HA	1:C:233:GLY:O	2.21	0.41
1:D:219:LEU:HB3	1:D:241:ILE:HG12	2.02	0.41
1:D:342:ASP:C	1:D:342:ASP:OD1	2.63	0.41
1:F:104:VAL:HG12	1:F:106:GLN:HG3	2.03	0.41
1:F:109:PRO:HG3	1:F:347:ARG:HD3	2.03	0.41
1:E:194:LYS:O	1:E:198:ILE:HG13	2.21	0.41
1:F:52:VAL:HG11	1:F:79:ILE:HG12	2.03	0.41
1:F:131:TYR:CE2	1:F:158:ASN:HB2	2.56	0.41
1:A:223:ASP:OD2	1:A:273:LYS:HA	2.20	0.40
1:C:216:ILE:HD13	1:C:216:ILE:HA	1.90	0.40
1:F:21:SER:O	1:F:25:VAL:HG23	2.21	0.40
1:C:54:ASN:OD1	1:D:310:LEU:CD2	2.69	0.40
1:B:260:GLU:HB3	1:B:263:GLU:HB3	2.03	0.40
1:C:85:THR:HG21	1:D:50:PHE:CE1	2.55	0.40
1:E:216:ILE:HD13	1:E:216:ILE:HA	1.88	0.40
1:F:324:GLU:HG2	1:F:328:LYS:HE3	2.03	0.40
1:A:203:ILE:HG12	1:A:229:ILE:HG22	2.03	0.40
1:F:83:CYS:SG	1:F:90:PHE:HB2	2.60	0.40
1:A:294:ARG:C	1:A:296:GLN:H	2.28	0.40
1:C:48:ASN:O	1:C:52:VAL:HG23	2.22	0.40
1:C:144:LEU:HD11	1:D:144:LEU:HD11	2.04	0.40
1:D:218:ASN:OD1	1:D:218:ASN:C	2.64	0.40
1:E:50:PHE:CD2	1:F:85:THR:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:PHE:CE1	1:E:154:VAL:HG22	2.56	0.40
1:F:23:PHE:HB2	1:F:279:THR:CG2	2.52	0.40

All (3) 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)
1:B:29:GLN:OE1	1:C:313:PRO:CB[1_455]	1.39	0.81
1:B:29:GLN:OE1	1:C:313:PRO:CA[1_455]	1.57	0.63
1:B:204:THR:O	1:C:14:ARG:NH2[4_455]	1.80	0.40

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	366/374 (98%)	337 (92%)	28 (8%)	1 (0%)	36	68
1	B	370/374 (99%)	342 (92%)	27 (7%)	1 (0%)	36	68
1	C	365/374 (98%)	335 (92%)	28 (8%)	2 (0%)	24	59
1	D	364/374 (97%)	333 (92%)	31 (8%)	0	100	100
1	E	360/374 (96%)	332 (92%)	26 (7%)	2 (1%)	21	56
1	F	356/374 (95%)	327 (92%)	28 (8%)	1 (0%)	36	68
All	All	2181/2244 (97%)	2006 (92%)	168 (8%)	7 (0%)	36	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	MET
1	E	374	MET
1	B	295	LYS
1	A	376	VAL

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Mol	Chain	Res	Type
1	E	373	LYS
1	F	209	VAL
1	C	209	VAL

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	305/322 (95%)	298 (98%)	7 (2%)	44	70
1	B	310/322 (96%)	303 (98%)	7 (2%)	44	70
1	C	292/322 (91%)	287 (98%)	5 (2%)	53	75
1	D	298/322 (92%)	292 (98%)	6 (2%)	48	72
1	E	263/322 (82%)	255 (97%)	8 (3%)	36	66
1	F	290/322 (90%)	276 (95%)	14 (5%)	23	56
All	All	1758/1932 (91%)	1711 (97%)	47 (3%)	39	68

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	79	ILE
1	A	185	ARG
1	A	227	LEU
1	A	287	THR
1	A	291	ARG
1	A	330	VAL
1	B	28	VAL
1	B	71	TYR
1	B	73	LYS
1	B	74	LYS
1	B	76	VAL
1	B	185	ARG
1	B	291	ARG
1	C	71	TYR

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Mol	Chain	Res	Type
1	C	79	ILE
1	C	170	THR
1	C	177	ASP
1	C	185	ARG
1	D	71	TYR
1	D	73	LYS
1	D	79	ILE
1	D	185	ARG
1	D	287	THR
1	D	291	ARG
1	E	48	ASN
1	E	50	PHE
1	E	79	ILE
1	E	171	TYR
1	E	226	LEU
1	E	287	THR
1	E	298	ILE
1	E	330	VAL
1	F	79	ILE
1	F	171	TYR
1	F	190	CYS
1	F	194	LYS
1	F	219	LEU
1	F	223	ASP
1	F	226	LEU
1	F	227	LEU
1	F	287	THR
1	F	291	ARG
1	F	300	ILE
1	F	330	VAL
1	F	378	LEU
1	F	379	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	196	ASN
1	A	284	GLN
1	A	349	ASN
1	B	40	HIS
1	B	235	ASN

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Mol	Chain	Res	Type
1	B	360	ASN
1	C	77	ASN
1	C	284	GLN
1	C	331	GLN
1	C	338	ASN
1	C	349	ASN
1	D	29	GLN
1	D	40	HIS
1	D	284	GLN
1	D	360	ASN
1	E	40	HIS
1	E	284	GLN
1	E	349	ASN
1	F	29	GLN
1	F	230	GLN
1	F	284	GLN
1	F	349	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 ⓘ

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	370/374 (98%)	0.07	7 (1%) 66 46	27, 62, 104, 137	0
1	B	372/374 (99%)	-0.06	10 (2%) 56 36	24, 45, 94, 153	0
1	C	369/374 (98%)	0.12	10 (2%) 56 36	26, 65, 102, 129	0
1	D	368/374 (98%)	-0.06	6 (1%) 70 51	23, 50, 112, 155	0
1	E	366/374 (97%)	0.55	12 (3%) 49 30	42, 87, 121, 142	0
1	F	364/374 (97%)	0.71	22 (6%) 27 17	47, 99, 126, 160	0
All	All	2209/2244 (98%)	0.22	67 (3%) 52 33	23, 68, 119, 160	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	88	VAL	5.9
1	C	176	GLN	4.1
1	F	367	TYR	3.5
1	F	221	PHE	3.5
1	F	89	SER	3.5
1	F	90	PHE	3.5
1	E	319	GLN	3.5
1	E	317	TRP	3.4
1	C	317	TRP	3.1
1	F	309	CYS	3.1
1	A	317	TRP	3.0
1	E	190	CYS	3.0
1	F	57	CYS	2.9
1	F	254	GLU	2.9
1	B	176	GLN	2.9
1	C	378	LEU	2.8
1	B	168	ASP	2.8
1	F	375	VAL	2.8
1	D	180	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	176	GLN	2.7
1	F	64	VAL	2.7
1	C	136	GLY	2.7
1	B	306	ALA	2.7
1	E	287	THR	2.7
1	F	8	ILE	2.6
1	A	254	GLU	2.6
1	B	307	GLY	2.6
1	F	366	GLY	2.6
1	C	374	MET	2.5
1	D	171	TYR	2.5
1	D	169	GLU	2.5
1	C	181	LYS	2.5
1	D	315	VAL	2.5
1	A	221	PHE	2.4
1	B	175	PHE	2.4
1	B	377	THR	2.4
1	D	176	GLN	2.4
1	B	136	GLY	2.4
1	E	172	ARG	2.4
1	A	180	LEU	2.4
1	F	179	GLU	2.4
1	E	91	ILE	2.4
1	D	226	LEU	2.3
1	F	351	THR	2.3
1	E	45	GLU	2.3
1	C	162	ILE	2.2
1	F	70	PHE	2.2
1	F	190	CYS	2.2
1	B	303	ARG	2.2
1	A	301	SER	2.2
1	F	310	LEU	2.2
1	E	137	LEU	2.2
1	C	306	ALA	2.2
1	E	206	GLY	2.2
1	E	315	VAL	2.1
1	F	300	ILE	2.1
1	E	53	THR	2.1
1	C	99	GLY	2.1
1	F	104	VAL	2.1
1	B	374	MET	2.1
1	A	315	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	317	TRP	2.1
1	F	175	PHE	2.1
1	B	172	ARG	2.1
1	C	180	LEU	2.0
1	F	180	LEU	2.0
1	E	46	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.