Full wwPDB X-ray Structure Validation Report (i)

Apr 12, 2023 – 04:13 PM EDT

PDB ID	:	4SBV
Title	:	The REFINEMENT OF SOUTHERN BEAN MOSAIC VIRUS IN RECIPROCAL SPACE
Authors	:	Rossmann, M.G.
Deposited on	:	1985-04-01
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

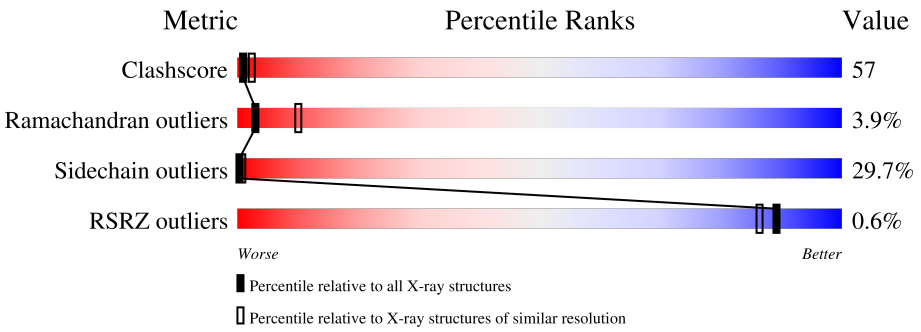
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	260	.% 17% 34% 16% 9% 23%
1	B	260	17% 32% 19% 8% 23%
1	C	260	21% 35% 22% 8% 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4723 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 SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	199	1506	956	249	292	9	0	0	0
1	B	199	1506	956	249	292	9	0	0	0
1	C	222	1674	1062	281	319	12	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0

- Molecule 3 is water.

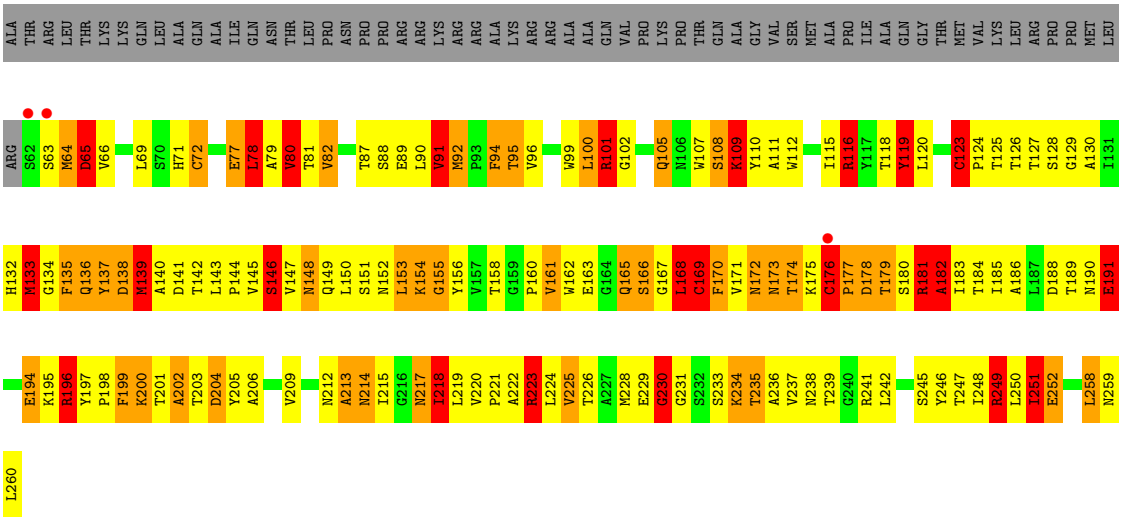
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	15	15	15	0	0
3	B	10	10	10	0	0
3	C	9	9	9	0	0

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.

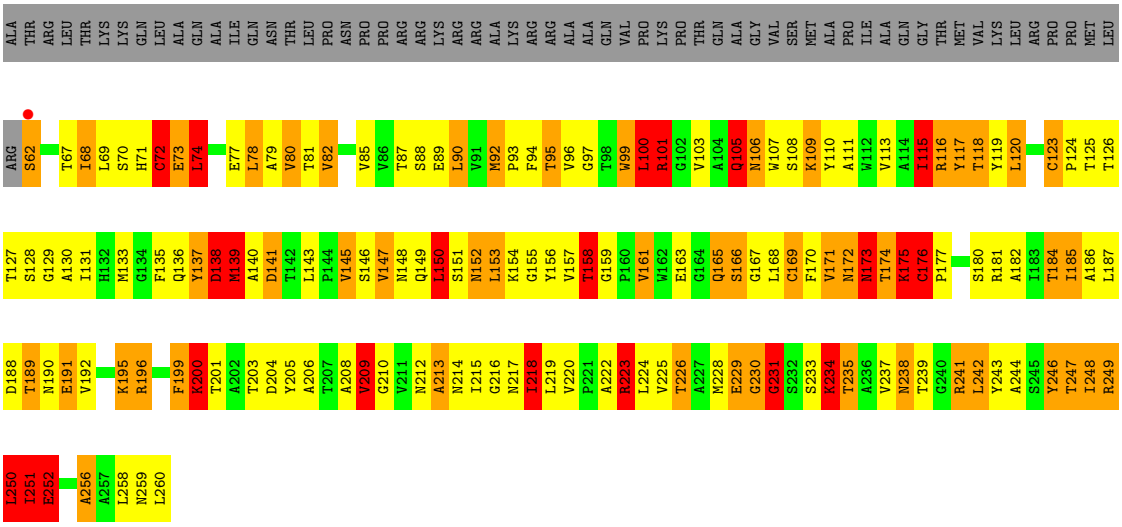
• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain A:



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain B:



• Molecule 1: SOUTHERN BEAN MOSAIC VIRUS COAT PROTEIN

Chain C: 21% 35% 22% 8% 15%

ALA THR ARG LEU THR LYS LYS GLN LEU ALA GLN ALA ILE GLN ASN THR LEU PRO ASN PRO PRO ARG ARG LYS ARG ARG ALA LYS ARG ARG ALA ALA GLN VAL PRO LYS PRO THR Q39 I47 A48 Q49 M52 V53 K54 L55 R56 P57 P58 M59 L60 R61 S62 S63 M64 D65 V66 T67

I68 L69 S70 H71 C72 E73 L74 S75 T76 E77 L78 A79 V80 T81 V82 T83 I84 V85 V86 T87 S88 E89 L90 V91 M92 P93 F94 T95 V96 G97 T98 W99 L100 R101 G102 W107 S108 K109 Y110 V113 A114 I115 R116 Y117 T118 Y119 L120 P121 S122 C123 P124 T125 T126 T127 S128 G129 A130 I131

H132 M133 G134 F135 Q136 Y137 D138 M139 A140 L143 P144 V145 S146 Q149 L150 S151 N152 L153 K154 G155 Y156 V157 T158 V161 W162 E163 G164 Q165 S166 G167 L168 C169 F170 V171 N172 N173 T174 K175 C176 P177 D178 T179 S180 R181 A182 I183 T184 I185 A186 L187 D188 T189 N190 E191 V192 S193 E194

K195 R196 Y197 P198 F199 K200 T201 A202 T203 D204 Y205 A206 T207 A208 V209 N212 A213 N214 I215 G216 N217 I218 L219 V220 P221 A222 R223 L224 V225 T226 A227 M228 E229 G230 G231 S232 S233 K234 T235 N238 T239 G240 R241 L242 Y243 A244 S245 Y246 T247 I248 R249 L250 I251 E252 P253 A256 A257

L258 N259 L260

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	334.30Å 334.30Å 757.50Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.80 142.18 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.80) 75.4 (142.18-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	0.254 , (Not available) 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.6	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 49.7	EDS
L-test for twinning[1]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	4723	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.47	8/1537 (0.5%)	2.64	103/2104 (4.9%)
1	B	1.43	7/1537 (0.5%)	2.46	106/2104 (5.0%)
1	C	1.48	11/1708 (0.6%)	2.55	96/2335 (4.1%)
All	All	1.46	26/4782 (0.5%)	2.55	305/6543 (4.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	4
All	All	0	10

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	252	GLU	N-CA	10.24	1.66	1.46
1	C	155	GLY	N-CA	9.11	1.59	1.46
1	B	231	GLY	N-CA	-8.84	1.32	1.46
1	C	231	GLY	N-CA	-8.78	1.32	1.46
1	A	230	GLY	N-CA	8.31	1.58	1.46
1	A	155	GLY	N-CA	7.50	1.57	1.46
1	A	252	GLU	N-CA	6.94	1.60	1.46
1	C	251	ILE	C-O	6.74	1.36	1.23
1	C	231	GLY	CA-C	-6.66	1.41	1.51
1	B	251	ILE	C-O	6.58	1.35	1.23
1	A	194	GLU	CB-CG	6.31	1.64	1.52
1	C	231	GLY	C-O	6.04	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	GLU	CD-OE1	-5.74	1.19	1.25
1	A	109	LYS	CA-CB	-5.73	1.41	1.53
1	B	252	GLU	CA-CB	-5.72	1.41	1.53
1	A	168	LEU	C-O	5.68	1.34	1.23
1	B	252	GLU	N-CA	5.66	1.57	1.46
1	B	176	CYS	CB-SG	5.57	1.91	1.82
1	B	137	TYR	C-O	5.52	1.33	1.23
1	C	252	GLU	CA-CB	-5.46	1.42	1.53
1	C	252	GLU	CB-CG	-5.34	1.42	1.52
1	C	133	MET	CA-CB	-5.32	1.42	1.53
1	C	64	MET	CA-CB	-5.31	1.42	1.53
1	B	97	GLY	N-CA	5.17	1.53	1.46
1	C	56	ARG	CZ-NH2	5.05	1.39	1.33
1	A	123	CYS	CB-SG	-5.02	1.73	1.81

All (305) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	196	ARG	NE-CZ-NH1	31.26	135.93	120.30
1	C	101	ARG	NE-CZ-NH1	26.07	133.33	120.30
1	A	109	LYS	CA-CB-CG	25.73	170.01	113.40
1	A	196	ARG	NE-CZ-NH2	-18.91	110.84	120.30
1	A	125	THR	N-CA-CB	17.77	144.05	110.30
1	B	241	ARG	NE-CZ-NH2	-17.49	111.55	120.30
1	C	231	GLY	N-CA-C	16.71	154.88	113.10
1	C	101	ARG	NE-CZ-NH2	-16.55	112.03	120.30
1	C	252	GLU	CA-CB-CG	15.44	147.37	113.40
1	C	196	ARG	NE-CZ-NH2	-15.35	112.62	120.30
1	C	241	ARG	NE-CZ-NH1	-13.62	113.49	120.30
1	C	56	ARG	NE-CZ-NH1	13.23	126.92	120.30
1	B	231	GLY	N-CA-C	12.93	145.43	113.10
1	A	196	ARG	CD-NE-CZ	12.61	141.26	123.60
1	A	223	ARG	CD-NE-CZ	-12.52	106.08	123.60
1	C	173	ASN	C-N-CA	12.14	152.04	121.70
1	B	252	GLU	OE1-CD-OE2	-11.59	109.40	123.30
1	A	181	ARG	NE-CZ-NH1	11.47	126.03	120.30
1	B	251	ILE	CA-C-N	11.33	142.13	117.20
1	A	101	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	C	249	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	C	241	ARG	NE-CZ-NH2	10.99	125.80	120.30
1	C	251	ILE	CA-C-N	10.80	140.97	117.20
1	C	252	GLU	CB-CA-C	10.77	131.94	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	74	LEU	N-CA-CB	10.75	131.90	110.40
1	A	168	LEU	CA-C-N	10.60	140.51	117.20
1	A	176	CYS	CA-CB-SG	10.29	132.52	114.00
1	B	251	ILE	CA-C-O	-10.26	98.55	120.10
1	A	178	ASP	C-N-CA	10.19	147.18	121.70
1	C	153	LEU	CA-CB-CG	10.05	138.43	115.30
1	A	168	LEU	CA-C-O	-10.04	99.02	120.10
1	A	191	GLU	CA-CB-CG	9.92	135.22	113.40
1	A	169	CYS	CA-CB-SG	9.89	131.81	114.00
1	C	214	ASN	CB-CA-C	9.84	130.08	110.40
1	B	90	LEU	CA-CB-CG	9.81	137.88	115.30
1	C	133	MET	CA-CB-CG	9.77	129.91	113.30
1	B	72	CYS	CA-CB-SG	-9.76	96.44	114.00
1	A	241	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	C	178	ASP	CB-CG-OD1	9.55	126.89	118.30
1	B	223	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	B	101	ARG	CG-CD-NE	9.31	131.36	111.80
1	B	74	LEU	O-C-N	9.27	137.54	122.70
1	C	73	GLU	CA-CB-CG	9.21	133.65	113.40
1	C	59	MET	CA-CB-CG	-9.07	97.88	113.30
1	B	138	ASP	O-C-N	8.90	136.94	122.70
1	A	181	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	A	123	CYS	CB-CA-C	-8.63	93.14	110.40
1	C	251	ILE	CA-C-O	-8.63	101.98	120.10
1	C	154	LYS	CA-C-N	8.54	133.29	116.20
1	A	178	ASP	CB-CA-C	8.49	127.38	110.40
1	C	249	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	204	ASP	CB-CG-OD1	8.42	125.88	118.30
1	A	69	LEU	O-C-N	8.42	136.17	122.70
1	A	138	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	A	146	SER	N-CA-CB	-8.36	97.96	110.50
1	A	249	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	A	218	ILE	CB-CA-C	-8.30	95.01	111.60
1	B	163	GLU	CG-CD-OE2	-8.25	101.81	118.30
1	C	196	ARG	N-CA-CB	8.14	125.26	110.60
1	B	223	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	B	230	GLY	C-N-CA	8.04	139.19	122.30
1	B	176	CYS	CA-CB-SG	-8.03	99.54	114.00
1	A	80	VAL	CB-CA-C	-7.98	96.23	111.40
1	B	252	GLU	CG-CD-OE1	7.94	134.18	118.30
1	B	223	ARG	NH1-CZ-NH2	7.94	128.13	119.40
1	B	246	TYR	CB-CG-CD2	7.88	125.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	165	GLN	CA-CB-CG	-7.82	96.20	113.40
1	A	190	ASN	CB-CA-C	-7.81	94.78	110.40
1	C	110	TYR	CB-CG-CD1	7.80	125.68	121.00
1	B	196	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	B	251	ILE	N-CA-C	7.75	131.94	111.00
1	A	251	ILE	CA-C-N	7.75	134.24	117.20
1	C	214	ASN	N-CA-CB	-7.73	96.69	110.60
1	C	65	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	B	158	THR	O-C-N	7.48	135.92	123.20
1	C	95	THR	CA-CB-OG1	-7.39	93.48	109.00
1	C	248	ILE	N-CA-CB	-7.34	93.92	110.80
1	A	111	ALA	N-CA-CB	7.33	120.36	110.10
1	B	252	GLU	CA-CB-CG	7.31	129.48	113.40
1	A	175	LYS	N-CA-CB	7.26	123.68	110.60
1	C	154	LYS	CA-C-O	-7.19	105.01	120.10
1	A	101	ARG	CD-NE-CZ	7.17	133.63	123.60
1	A	252	GLU	CB-CA-C	7.13	124.66	110.40
1	C	230	GLY	N-CA-C	7.11	130.88	113.10
1	B	139	MET	CA-CB-CG	-7.05	101.31	113.30
1	C	196	ARG	CA-CB-CG	7.03	128.85	113.40
1	B	241	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	141	ASP	CB-CA-C	7.02	124.44	110.40
1	B	241	ARG	CD-NE-CZ	-7.00	113.80	123.60
1	C	64	MET	CA-CB-CG	6.99	125.19	113.30
1	A	179	THR	CA-C-N	-6.99	101.82	117.20
1	B	150	LEU	CA-CB-CG	6.98	131.36	115.30
1	C	133	MET	CB-CA-C	6.97	124.35	110.40
1	C	61	ARG	CA-CB-CG	6.93	128.65	113.40
1	A	251	ILE	CA-C-O	-6.93	105.55	120.10
1	A	170	PHE	CB-CA-C	6.92	124.23	110.40
1	B	246	TYR	CB-CG-CD1	-6.88	116.87	121.00
1	C	62	SER	N-CA-CB	-6.87	100.20	110.50
1	C	56	ARG	CD-NE-CZ	6.86	133.20	123.60
1	C	217	ASN	CA-C-O	-6.85	105.71	120.10
1	B	92	MET	CA-CB-CG	6.84	124.93	113.30
1	B	243	TYR	CB-CG-CD2	-6.84	116.90	121.00
1	B	252	GLU	N-CA-C	-6.83	92.56	111.00
1	A	168	LEU	CA-CB-CG	6.83	131.00	115.30
1	B	191	GLU	CG-CD-OE1	6.80	131.90	118.30
1	B	185	ILE	CB-CG1-CD1	6.79	132.90	113.90
1	C	213	ALA	C-N-CA	-6.79	104.74	121.70
1	C	73	GLU	CG-CD-OE1	6.76	131.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	169	CYS	CA-CB-SG	-6.75	101.85	114.00
1	A	252	GLU	CG-CD-OE1	6.75	131.80	118.30
1	B	115	ILE	CA-CB-CG1	-6.75	98.18	111.00
1	A	153	LEU	CB-CA-C	6.73	123.00	110.20
1	A	178	ASP	CA-C-O	6.71	134.20	120.10
1	B	130	ALA	CB-CA-C	-6.71	100.03	110.10
1	A	258	LEU	N-CA-CB	-6.70	96.99	110.40
1	A	136	GLN	CB-CA-C	6.67	123.73	110.40
1	B	105	GLN	CA-CB-CG	6.54	127.78	113.40
1	C	146	SER	N-CA-CB	-6.54	100.69	110.50
1	A	116	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	B	96	VAL	CA-CB-CG1	6.47	120.60	110.90
1	A	249	ARG	NE-CZ-NH1	-6.43	117.08	120.30
1	C	73	GLU	CG-CD-OE2	-6.43	105.44	118.30
1	B	138	ASP	N-CA-C	-6.43	93.65	111.00
1	C	242	LEU	CB-CA-C	6.43	122.41	110.20
1	B	145	VAL	C-N-CA	6.41	137.73	121.70
1	C	56	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	194	GLU	CG-CD-OE2	-6.41	105.49	118.30
1	C	188	ASP	CB-CA-C	6.40	123.20	110.40
1	B	168	LEU	CA-CB-CG	6.37	129.94	115.30
1	A	154	LYS	CA-C-N	6.35	128.90	116.20
1	C	251	ILE	CA-CB-CG1	-6.35	98.94	111.00
1	A	178	ASP	CA-CB-CG	6.34	127.35	113.40
1	B	195	LYS	CD-CE-NZ	6.28	126.15	111.70
1	B	117	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	B	138	ASP	CA-CB-CG	6.26	127.17	113.40
1	A	78	LEU	O-C-N	6.25	132.70	122.70
1	A	125	THR	CB-CA-C	-6.24	94.74	111.60
1	A	69	LEU	CA-C-N	-6.24	103.47	117.20
1	B	68	ILE	O-C-N	6.23	132.66	122.70
1	C	206	ALA	N-CA-CB	-6.23	101.38	110.10
1	B	251	ILE	CA-CB-CG1	-6.22	99.17	111.00
1	B	166	SER	O-C-N	6.22	133.78	123.20
1	C	77	GLU	N-CA-CB	6.21	121.78	110.60
1	B	89	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	C	188	ASP	N-CA-C	-6.19	94.29	111.00
1	C	204	ASP	N-CA-CB	6.18	121.73	110.60
1	A	133	MET	O-C-N	6.18	133.70	123.20
1	C	196	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	72	CYS	CA-CB-SG	-6.14	102.95	114.00
1	B	96	VAL	CB-CA-C	6.13	123.05	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	215	ILE	CA-C-O	6.12	132.96	120.10
1	C	94	PHE	CA-C-N	-6.10	103.78	117.20
1	A	169	CYS	O-C-N	6.08	132.44	122.70
1	A	137	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	235	THR	CA-CB-OG1	-6.01	96.38	109.00
1	A	174	THR	CA-CB-CG2	6.01	120.81	112.40
1	C	173	ASN	CA-CB-CG	6.01	126.62	113.40
1	A	182	ALA	O-C-N	6.00	132.29	122.70
1	B	89	GLU	CB-CG-CD	5.98	130.36	114.20
1	B	226	THR	CA-CB-CG2	5.97	120.75	112.40
1	B	174	THR	N-CA-C	-5.96	94.91	111.00
1	A	166	SER	N-CA-CB	-5.95	101.57	110.50
1	A	217	ASN	CB-CG-OD1	5.95	133.50	121.60
1	B	209	VAL	CB-CA-C	5.95	122.70	111.40
1	C	252	GLU	N-CA-C	-5.94	94.97	111.00
1	B	181	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	109	LYS	CG-CD-CE	5.92	129.67	111.90
1	A	251	ILE	N-CA-C	5.92	126.98	111.00
1	C	163	GLU	CG-CD-OE2	-5.91	106.49	118.30
1	B	128	SER	N-CA-CB	-5.88	101.68	110.50
1	B	186	ALA	CB-CA-C	5.88	118.92	110.10
1	B	96	VAL	CA-CB-CG2	-5.85	102.12	110.90
1	B	173	ASN	CA-C-N	-5.82	104.40	117.20
1	B	224	LEU	CA-C-O	-5.81	107.89	120.10
1	A	179	THR	CA-C-O	5.81	132.30	120.10
1	C	186	ALA	N-CA-CB	-5.81	101.97	110.10
1	B	163	GLU	OE1-CD-OE2	5.78	130.24	123.30
1	C	76	THR	CA-C-O	-5.77	107.98	120.10
1	C	146	SER	CA-CB-OG	5.77	126.78	111.20
1	A	91	VAL	CB-CA-C	5.75	122.33	111.40
1	A	116	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	B	95	THR	CA-CB-CG2	5.72	120.41	112.40
1	A	196	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
1	A	65	ASP	N-CA-CB	5.71	120.88	110.60
1	A	241	ARG	NH1-CZ-NH2	5.71	125.67	119.40
1	B	200	LYS	CD-CE-NZ	5.70	124.81	111.70
1	B	138	ASP	CA-C-O	-5.67	108.19	120.10
1	B	99	TRP	CA-CB-CG	5.67	124.47	113.70
1	B	158	THR	N-CA-CB	5.67	121.07	110.30
1	C	119	TYR	N-CA-CB	-5.66	100.41	110.60
1	C	234	LYS	C-N-CA	5.66	135.86	121.70
1	C	152	ASN	CA-CB-CG	5.65	125.83	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	SER	CB-CA-C	5.64	120.82	110.10
1	C	154	LYS	C-N-CA	-5.64	110.45	122.30
1	B	234	LYS	CA-CB-CG	5.57	125.66	113.40
1	A	169	CYS	N-CA-C	-5.57	95.96	111.00
1	C	110	TYR	CB-CG-CD2	-5.56	117.66	121.00
1	B	73	GLU	CA-CB-CG	5.55	125.61	113.40
1	A	178	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	191	GLU	CG-CD-OE2	-5.53	107.23	118.30
1	A	223	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	80	VAL	O-C-N	5.53	131.55	122.70
1	C	99	TRP	O-C-N	5.53	131.55	122.70
1	B	99	TRP	CB-CA-C	5.51	121.42	110.40
1	A	230	GLY	N-CA-C	-5.50	99.36	113.10
1	B	246	TYR	O-C-N	5.50	131.49	122.70
1	C	143	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	B	77	GLU	CG-CD-OE1	5.49	129.28	118.30
1	C	110	TYR	O-C-N	5.48	131.47	122.70
1	A	174	THR	CA-CB-OG1	-5.46	97.54	109.00
1	B	184	THR	CA-CB-CG2	-5.46	104.76	112.40
1	A	213	ALA	O-C-N	5.45	131.42	122.70
1	C	95	THR	CA-CB-CG2	5.45	120.03	112.40
1	A	252	GLU	CG-CD-OE2	-5.45	107.41	118.30
1	B	243	TYR	CB-CG-CD1	5.45	124.27	121.00
1	B	120	LEU	CB-CA-C	5.44	120.54	110.20
1	A	105	GLN	O-C-N	5.43	131.39	122.70
1	A	116	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	C	138	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	B	152	ASN	CA-C-O	-5.40	108.76	120.10
1	C	163	GLU	CG-CD-OE1	5.40	129.09	118.30
1	A	241	ARG	CD-NE-CZ	-5.39	116.05	123.60
1	B	174	THR	O-C-N	5.39	131.32	122.70
1	B	123	CYS	CA-CB-SG	-5.38	104.31	114.00
1	C	87	THR	N-CA-CB	-5.37	100.09	110.30
1	A	229	GLU	CA-C-O	-5.37	108.83	120.10
1	C	173	ASN	N-CA-CB	5.37	120.26	110.60
1	A	252	GLU	N-CA-C	-5.36	96.52	111.00
1	C	138	ASP	CB-CA-C	5.36	121.12	110.40
1	C	161	VAL	N-CA-CB	-5.36	99.71	111.50
1	C	101	ARG	NH1-CZ-NH2	-5.36	113.51	119.40
1	C	222	ALA	N-CA-CB	-5.35	102.60	110.10
1	B	182	ALA	O-C-N	5.35	131.26	122.70
1	A	115	ILE	O-C-N	5.35	131.25	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	250	LEU	CB-CA-C	5.34	120.35	110.20
1	B	252	GLU	CB-CA-C	5.34	121.08	110.40
1	B	141	ASP	N-CA-CB	-5.34	100.99	110.60
1	C	89	GLU	CB-CA-C	-5.34	99.72	110.40
1	A	217	ASN	C-N-CA	5.33	135.04	121.70
1	A	188	ASP	CB-CG-OD2	5.33	123.09	118.30
1	A	247	THR	N-CA-CB	5.33	120.42	110.30
1	C	191	GLU	CG-CD-OE2	-5.32	107.66	118.30
1	B	100	LEU	O-C-N	5.32	131.21	122.70
1	B	173	ASN	CA-C-O	5.30	131.24	120.10
1	C	174	THR	CA-CB-CG2	5.29	119.81	112.40
1	C	230	GLY	O-C-N	-5.29	114.21	123.20
1	A	82	VAL	CA-CB-CG1	5.29	118.83	110.90
1	A	137	TYR	N-CA-CB	-5.28	101.09	110.60
1	B	256	ALA	CA-C-N	-5.28	105.58	117.20
1	A	251	ILE	N-CA-CB	-5.27	98.67	110.80
1	B	218	ILE	N-CA-CB	5.27	122.92	110.80
1	C	168	LEU	CA-CB-CG	-5.27	103.19	115.30
1	C	217	ASN	CB-CG-OD1	-5.27	111.06	121.60
1	A	72	CYS	O-C-N	5.26	131.12	122.70
1	A	111	ALA	O-C-N	5.26	131.11	122.70
1	B	247	THR	O-C-N	5.25	131.10	122.70
1	B	252	GLU	CB-CG-CD	5.25	128.36	114.20
1	A	77	GLU	CG-CD-OE1	5.24	128.77	118.30
1	A	247	THR	O-C-N	5.23	131.06	122.70
1	A	204	ASP	OD1-CG-OD2	-5.22	113.38	123.30
1	C	188	ASP	CA-CB-CG	5.22	124.89	113.40
1	C	116	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	222	ALA	N-CA-CB	-5.21	102.80	110.10
1	B	238	ASN	CA-C-O	-5.21	109.16	120.10
1	A	135	PHE	O-C-N	5.21	131.03	122.70
1	B	73	GLU	CA-C-O	-5.20	109.17	120.10
1	A	116	ARG	N-CA-CB	-5.20	101.24	110.60
1	C	78	LEU	N-CA-CB	-5.20	100.00	110.40
1	C	223	ARG	O-C-N	5.17	130.98	122.70
1	B	204	ASP	CA-CB-CG	-5.17	102.03	113.40
1	C	195	LYS	CA-CB-CG	5.17	124.76	113.40
1	A	95	THR	CB-CA-C	-5.16	97.67	111.60
1	A	128	SER	CA-C-O	-5.15	109.28	120.10
1	B	77	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	C	208	ALA	CA-C-O	5.15	130.92	120.10
1	C	132	HIS	O-C-N	5.15	130.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	250	LEU	O-C-N	5.14	130.92	122.70
1	B	77	GLU	CA-CB-CG	5.13	124.69	113.40
1	B	175	LYS	CB-CA-C	5.12	120.65	110.40
1	C	73	GLU	CB-CA-C	5.12	120.64	110.40
1	A	119	TYR	O-C-N	5.12	130.89	122.70
1	B	165	GLN	OE1-CD-NE2	5.12	133.67	121.90
1	C	77	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	A	168	LEU	N-CA-C	-5.11	97.20	111.00
1	B	67	THR	CA-CB-OG1	-5.10	98.28	109.00
1	C	216	GLY	O-C-N	5.10	130.85	122.70
1	A	218	ILE	O-C-N	5.09	130.85	122.70
1	C	116	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	182	ALA	CB-CA-C	5.09	117.73	110.10
1	A	133	MET	N-CA-CB	5.08	119.74	110.60
1	C	199	PHE	CB-CG-CD1	-5.08	117.25	120.80
1	B	206	ALA	CB-CA-C	5.07	117.71	110.10
1	A	194	GLU	OE1-CD-OE2	5.07	129.39	123.30
1	A	213	ALA	CA-C-O	-5.07	109.46	120.10
1	B	206	ALA	N-CA-CB	-5.06	103.02	110.10
1	C	181	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	174	THR	N-CA-CB	5.04	119.89	110.30
1	B	229	GLU	C-N-CA	-5.04	111.71	122.30
1	C	235	THR	CA-CB-OG1	-5.03	98.44	109.00
1	B	74	LEU	N-CA-C	-5.02	97.44	111.00
1	A	112	TRP	CA-C-O	-5.02	109.56	120.10
1	A	78	LEU	CA-C-N	-5.01	106.18	117.20
1	A	236	ALA	N-CA-CB	-5.01	103.09	110.10
1	A	77	GLU	OE1-CD-OE2	-5.00	117.30	123.30
1	B	109	LYS	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	116	ARG	Sidechain
1	A	223	ARG	Sidechain
1	A	249	ARG	Sidechain
1	B	101	ARG	Sidechain
1	B	241	ARG	Sidechain
1	B	249	ARG	Sidechain
1	C	101	ARG	Sidechain
1	C	181	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	196	ARG	Sidechain
1	C	223	ARG	Sidechain

5.2 Too-close contacts (i)

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	1506	0	1504	208	0
1	B	1506	0	1504	180	0
1	C	1674	0	1691	181	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	15	0	0	1	0
3	B	10	0	0	0	0
3	C	9	0	0	0	0
All	All	4723	0	4699	536	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 57.

All (536) 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:212:ASN:ND2	1:C:214:ASN:H	1.42	1.14
1:C:145:VAL:H	1:C:149:GLN:NE2	1.46	1.12
1:C:161:VAL:HG22	1:C:239:THR:CG2	1.82	1.09
1:C:161:VAL:HG22	1:C:239:THR:HG21	1.09	1.08
1:C:131:ILE:HG13	1:C:228:MET:HE2	1.34	1.05
1:C:187:LEU:HD22	1:C:188:ASP:H	1.19	1.05
1:A:165:GLN:HE21	1:A:165:GLN:HA	1.21	1.04
1:A:168:LEU:O	1:A:169:CYS:HB2	1.57	1.01
1:A:201:THR:HG22	1:A:260:LEU:OXT	1.61	0.99
1:C:145:VAL:H	1:C:149:GLN:HE22	1.07	0.98
1:C:195:LYS:HB3	1:C:195:LYS:HZ3	1.26	0.95
1:A:105:GLN:HA	1:A:199:PHE:CE1	2.01	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:LYS:H	1:C:172:ASN:HD21	0.99	0.94
1:C:212:ASN:HD22	1:C:214:ASN:N	1.66	0.93
1:C:119:TYR:OH	1:C:239:THR:HG22	1.68	0.93
1:C:125:THR:HG22	1:C:162:TRP:CE3	2.04	0.91
1:C:161:VAL:CG2	1:C:239:THR:HG21	2.01	0.90
1:C:139:MET:H	1:C:217:ASN:HD21	0.94	0.89
1:C:187:LEU:HD22	1:C:188:ASP:N	1.87	0.89
1:B:248:ILE:HD12	1:B:250:LEU:HD13	1.52	0.89
1:A:251:ILE:HG23	1:A:252:GLU:HG2	1.52	0.89
1:A:178:ASP:HB2	1:A:180:SER:OG	1.72	0.89
1:A:205:TYR:CE2	1:A:209:VAL:HG21	2.08	0.88
1:C:187:LEU:CD2	1:C:188:ASP:H	1.86	0.88
1:A:137:TYR:CE1	1:B:252:GLU:HG3	2.10	0.87
1:B:150:LEU:HA	1:B:153:LEU:HD12	1.53	0.87
1:A:148:ASN:O	1:A:151:SER:HB3	1.74	0.87
1:C:115:ILE:HG23	1:C:187:LEU:HB2	1.55	0.86
1:B:82:VAL:HG22	1:B:234:LYS:HA	1.57	0.86
1:C:195:LYS:HB3	1:C:195:LYS:NZ	1.90	0.86
1:C:90:LEU:HB2	1:C:95:THR:HG21	1.57	0.85
1:C:139:MET:H	1:C:217:ASN:ND2	1.74	0.85
1:C:129:GLY:O	1:C:161:VAL:HB	1.77	0.84
1:C:212:ASN:ND2	1:C:214:ASN:N	2.25	0.84
1:C:129:GLY:HA2	1:C:230:GLY:HA3	1.58	0.83
1:A:168:LEU:O	1:A:169:CYS:CB	2.20	0.83
1:B:103:VAL:O	1:B:106:ASN:ND2	2.11	0.82
1:B:140:ALA:O	1:C:260:LEU:HD12	1.79	0.81
1:C:146:SER:H	1:C:149:GLN:HE21	1.28	0.81
1:A:136:GLN:HE21	1:A:223:ARG:HH11	1.25	0.81
1:C:212:ASN:HD22	1:C:214:ASN:H	0.81	0.80
1:B:124:PRO:HD2	1:B:127:THR:OG1	1.82	0.80
1:A:165:GLN:HA	1:A:165:GLN:NE2	1.97	0.79
1:A:92:MET:O	1:A:96:VAL:HG23	1.83	0.79
1:B:131:ILE:O	1:B:158:THR:HG23	1.80	0.79
1:A:105:GLN:HA	1:A:199:PHE:HE1	1.42	0.79
1:B:100:LEU:HG	1:B:246:TYR:CE2	2.17	0.78
1:B:212:ASN:ND2	1:B:214:ASN:HB2	1.98	0.78
1:B:151:SER:HA	1:B:156:TYR:CD2	2.18	0.78
1:A:144:PRO:HA	1:B:258:LEU:HD11	1.66	0.78
1:B:120:LEU:HD11	1:B:171:VAL:HG21	1.64	0.78
1:C:145:VAL:N	1:C:149:GLN:NE2	2.29	0.78
1:C:119:TYR:OH	1:C:239:THR:CG2	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:N	1:A:143:LEU:HD12	2.00	0.77
1:B:78:LEU:HB2	1:B:228:MET:HE2	1.66	0.77
1:B:214:ASN:HD21	1:C:200:LYS:NZ	1.82	0.77
1:C:163:GLU:HG3	1:C:164:GLY:N	1.99	0.77
1:A:105:GLN:CA	1:A:199:PHE:HE1	1.98	0.77
1:C:139:MET:N	1:C:217:ASN:HD21	1.77	0.77
1:A:123:CYS:HB3	1:A:124:PRO:HD2	1.67	0.77
1:C:49:GLN:NE2	1:C:165:GLN:HG2	2.00	0.76
1:B:117:TYR:HB3	1:B:242:LEU:HD21	1.65	0.76
1:A:181:ARG:HG2	1:A:181:ARG:O	1.84	0.76
1:A:90:LEU:HD13	1:A:92:MET:HE1	1.68	0.75
1:A:136:GLN:HE21	1:A:223:ARG:NH1	1.86	0.74
1:A:161:VAL:HB	1:A:239:THR:OG1	1.86	0.74
1:C:131:ILE:CG1	1:C:228:MET:HE2	2.16	0.74
1:C:169:CYS:O	1:C:173:ASN:N	2.20	0.73
1:A:109:LYS:HE3	1:A:252:GLU:OE1	1.88	0.73
1:A:129:GLY:HA2	1:A:230:GLY:CA	2.18	0.73
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.24	0.73
1:C:150:LEU:HD13	1:C:150:LEU:O	1.89	0.73
1:C:60:LEU:HD12	1:C:69:LEU:HD13	1.70	0.72
1:A:79:ALA:HA	1:A:237:VAL:O	1.89	0.72
1:C:101:ARG:HG2	1:C:102:GLY:N	2.03	0.72
1:C:54:LYS:H	1:C:172:ASN:ND2	1.81	0.72
1:C:66:VAL:HG12	1:C:251:ILE:HD11	1.70	0.71
1:A:129:GLY:HA2	1:A:230:GLY:HA2	1.72	0.71
1:B:146:SER:OG	1:B:148:ASN:HB2	1.89	0.71
1:C:125:THR:HG22	1:C:162:TRP:CD2	2.24	0.70
1:C:239:THR:HG22	1:C:240:GLY:N	2.06	0.70
1:A:105:GLN:HA	1:A:199:PHE:CD1	2.26	0.70
1:B:110:TYR:HB2	1:B:248:ILE:HD11	1.74	0.70
1:A:258:LEU:HD11	1:C:144:PRO:HA	1.74	0.70
1:A:200:LYS:HE3	1:A:260:LEU:C	2.11	0.70
1:C:81:THR:HG23	1:C:83:THR:O	1.92	0.69
1:B:139:MET:H	1:B:217:ASN:HD21	1.40	0.69
1:C:205:TYR:O	1:C:209:VAL:HG23	1.93	0.69
1:B:118:THR:O	1:B:242:LEU:HD23	1.93	0.69
1:B:138:ASP:HA	1:B:217:ASN:HD21	1.58	0.69
1:C:116:ARG:HH21	1:C:184:THR:HG21	1.57	0.69
1:B:174:THR:HG22	1:B:175:LYS:H	1.58	0.68
1:C:78:LEU:HG	1:C:228:MET:HE3	1.75	0.68
1:A:155:GLY:HA3	1:A:185:ILE:HG13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:GLU:HG3	1:C:164:GLY:H	1.58	0.68
1:C:234:LYS:HE3	1:C:234:LYS:H	1.58	0.68
1:B:94:PHE:CE1	1:B:101:ARG:HD2	2.29	0.68
1:A:201:THR:HG22	1:A:260:LEU:C	2.14	0.67
1:B:125:THR:HG22	1:B:125:THR:O	1.95	0.67
1:A:148:ASN:C	1:A:148:ASN:HD22	1.98	0.67
1:C:195:LYS:NZ	1:C:195:LYS:CB	2.57	0.67
1:C:118:THR:HB	1:C:184:THR:OG1	1.94	0.67
1:A:218:ILE:HD11	1:B:218:ILE:HD12	1.77	0.67
1:B:175:LYS:O	1:B:177:PRO:HD3	1.94	0.67
1:B:218:ILE:HG12	1:B:219:LEU:CD1	2.25	0.67
1:A:94:PHE:HB2	1:A:199:PHE:HE2	1.59	0.66
1:A:116:ARG:NE	1:A:170:PHE:HD1	1.92	0.66
1:A:108:SER:HB2	1:A:252:GLU:O	1.96	0.66
1:B:195:LYS:HE3	1:C:195:LYS:HZ1	1.61	0.66
1:C:69:LEU:HD12	1:C:70:SER:N	2.10	0.66
1:B:73:GLU:OE1	1:B:99:TRP:HB3	1.96	0.66
1:B:137:TYR:CD1	1:C:252:GLU:HG3	2.31	0.66
1:C:92:MET:O	1:C:96:VAL:HG23	1.94	0.66
1:A:81:THR:O	1:A:231:GLY:HA2	1.95	0.66
1:B:166:SER:O	1:B:176:CYS:SG	2.54	0.66
1:A:160:PRO:HG2	1:A:163:GLU:HB2	1.78	0.65
1:A:110:TYR:CD1	1:A:248:ILE:HD11	2.31	0.65
1:B:106:ASN:ND2	1:B:106:ASN:H	1.94	0.65
1:B:119:TYR:O	1:B:120:LEU:HD23	1.96	0.65
1:A:71:HIS:HB3	1:A:246:TYR:CZ	2.31	0.65
1:B:71:HIS:HD2	1:B:99:TRP:CZ3	2.13	0.65
1:B:136:GLN:HE22	1:B:143:LEU:HD23	1.61	0.65
1:A:66:VAL:HG21	1:A:249:ARG:HH21	1.61	0.65
1:B:150:LEU:HA	1:B:153:LEU:CD1	2.25	0.65
1:B:115:ILE:HG13	1:B:246:TYR:HB3	1.79	0.64
1:C:124:PRO:O	1:C:127:THR:OG1	2.14	0.64
1:B:189:THR:HA	1:B:192:VAL:HG23	1.79	0.64
1:A:174:THR:HG22	1:A:176:CYS:SG	2.38	0.64
1:B:138:ASP:O	1:B:141:ASP:HB2	1.97	0.64
1:A:215:ILE:O	1:A:219:LEU:HD12	1.99	0.63
1:A:155:GLY:O	1:A:156:TYR:C	2.36	0.63
1:B:135:PHE:HE2	1:B:187:LEU:HA	1.64	0.63
1:B:78:LEU:HB2	1:B:228:MET:CE	2.29	0.63
1:C:78:LEU:HG	1:C:228:MET:CE	2.29	0.63
1:B:248:ILE:HD13	1:B:249:ARG:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:CYS:O	1:C:173:ASN:HA	1.99	0.62
1:A:100:LEU:HG	1:A:246:TYR:CE2	2.34	0.62
1:C:144:PRO:CG	1:C:150:LEU:HD23	2.29	0.62
1:B:81:THR:O	1:B:231:GLY:HA3	2.00	0.62
1:C:155:GLY:HA3	1:C:185:ILE:HG13	1.82	0.62
1:C:169:CYS:O	1:C:173:ASN:CA	2.48	0.62
1:A:116:ARG:NE	1:A:170:PHE:CD1	2.68	0.62
1:B:78:LEU:N	1:B:78:LEU:HD12	2.15	0.61
1:B:79:ALA:HB1	1:B:237:VAL:O	2.00	0.61
1:A:144:PRO:CA	1:B:258:LEU:HD11	2.29	0.61
1:A:71:HIS:CG	1:A:72:CYS:H	2.18	0.61
1:B:139:MET:CE	1:B:223:ARG:HB3	2.31	0.61
1:A:109:LYS:CE	1:A:252:GLU:OE1	2.49	0.61
1:C:66:VAL:CG1	1:C:251:ILE:HD11	2.31	0.61
1:A:260:LEU:N	1:A:260:LEU:HD23	2.16	0.60
1:B:71:HIS:ND1	1:B:72:CYS:N	2.49	0.60
1:C:74:LEU:HD12	1:C:75:SER:N	2.16	0.60
1:C:146:SER:H	1:C:149:GLN:NE2	1.97	0.60
1:C:192:VAL:HG13	1:C:197:TYR:OH	2.01	0.60
1:A:138:ASP:O	1:A:140:ALA:N	2.35	0.60
1:A:129:GLY:C	1:A:161:VAL:HG13	2.22	0.60
1:A:137:TYR:CE2	1:B:252:GLU:OE1	2.55	0.60
1:B:212:ASN:HD21	1:B:214:ASN:HB2	1.67	0.60
1:C:145:VAL:N	1:C:149:GLN:HE22	1.88	0.60
1:A:135:PHE:HE1	1:A:185:ILE:HG12	1.67	0.59
1:B:94:PHE:O	1:B:101:ARG:NH1	2.35	0.59
1:C:187:LEU:CD2	1:C:188:ASP:N	2.56	0.59
1:C:115:ILE:CG2	1:C:187:LEU:HB2	2.27	0.59
1:B:74:LEU:HD12	1:B:74:LEU:H	1.67	0.59
1:B:195:LYS:HE3	1:C:195:LYS:CE	2.32	0.59
1:A:135:PHE:CE1	1:A:185:ILE:HG12	2.37	0.59
1:A:196:ARG:HD2	1:A:196:ARG:N	2.18	0.59
1:B:218:ILE:HG12	1:B:219:LEU:HD12	1.85	0.59
1:A:129:GLY:HA2	1:A:230:GLY:HA3	1.85	0.59
1:B:158:THR:HG22	1:B:159:GLY:H	1.66	0.59
1:C:125:THR:CG2	1:C:162:TRP:CE3	2.81	0.59
1:C:133:MET:HA	1:C:225:VAL:O	2.03	0.59
1:A:248:ILE:HG23	1:A:250:LEU:HD13	1.85	0.58
1:B:139:MET:H	1:B:217:ASN:ND2	2.01	0.58
1:B:71:HIS:HB3	1:B:246:TYR:CZ	2.38	0.58
1:A:137:TYR:CD1	1:B:252:GLU:HG3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:GLN:NE2	1:B:143:LEU:HD23	2.19	0.58
1:A:123:CYS:CB	1:A:124:PRO:CD	2.79	0.58
1:A:212:ASN:OD1	1:A:214:ASN:HB2	2.02	0.58
1:A:71:HIS:HD2	1:A:99:TRP:CE3	2.23	0.57
1:C:52:MET:SD	1:C:52:MET:N	2.76	0.57
1:A:179:THR:O	1:A:180:SER:C	2.43	0.57
1:A:200:LYS:CE	1:A:260:LEU:OXT	2.51	0.57
1:B:155:GLY:O	1:B:157:VAL:HG23	2.04	0.57
1:B:195:LYS:HE3	1:C:195:LYS:NZ	2.19	0.57
1:B:214:ASN:HD21	1:C:200:LYS:HZ2	1.49	0.57
1:C:80:VAL:HG13	1:C:81:THR:N	2.19	0.57
1:A:92:MET:HE2	1:A:220:VAL:CG1	2.34	0.57
1:B:248:ILE:HD13	1:B:249:ARG:N	2.20	0.57
1:C:114:ALA:O	1:C:246:TYR:HA	2.04	0.57
1:A:123:CYS:CB	1:A:124:PRO:HD2	2.35	0.57
1:A:141:ASP:HB3	1:B:258:LEU:O	2.04	0.57
1:B:158:THR:HG22	1:B:159:GLY:N	2.20	0.57
1:A:251:ILE:CG2	1:A:252:GLU:HG2	2.32	0.57
1:B:73:GLU:OE1	1:B:99:TRP:N	2.30	0.57
1:A:123:CYS:HB3	1:A:124:PRO:CD	2.34	0.57
1:A:142:THR:HB	1:B:258:LEU:HD22	1.87	0.57
1:B:82:VAL:HG21	1:B:234:LYS:HG3	1.86	0.57
1:B:139:MET:N	1:B:217:ASN:HD21	2.03	0.57
1:B:145:VAL:N	1:B:149:GLN:OE1	2.33	0.57
1:B:246:TYR:CD1	1:B:246:TYR:N	2.72	0.57
1:B:135:PHE:CE2	1:B:187:LEU:HA	2.40	0.56
1:A:248:ILE:HG23	1:A:250:LEU:CD1	2.35	0.56
1:B:216:GLY:O	1:B:219:LEU:N	2.37	0.56
1:A:160:PRO:O	1:A:162:TRP:N	2.39	0.56
1:A:200:LYS:HE3	1:A:260:LEU:OXT	2.05	0.56
1:C:144:PRO:HG3	1:C:150:LEU:CD2	2.35	0.56
1:A:137:TYR:CZ	1:B:252:GLU:OE1	2.58	0.56
1:B:138:ASP:HA	1:B:217:ASN:ND2	2.21	0.56
1:C:135:PHE:O	1:C:153:LEU:HG	2.05	0.56
1:A:116:ARG:HG3	1:A:186:ALA:HB2	1.86	0.56
1:A:138:ASP:C	1:A:140:ALA:N	2.57	0.56
1:A:143:LEU:N	1:A:143:LEU:CD1	2.68	0.56
1:A:195:LYS:C	1:A:196:ARG:HD2	2.26	0.56
1:B:189:THR:HA	1:B:192:VAL:CG2	2.35	0.56
1:B:251:ILE:HG23	1:B:252:GLU:OE2	2.06	0.56
1:B:70:SER:OG	1:B:247:THR:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:VAL:CG2	1:B:234:LYS:HA	2.33	0.56
1:B:156:TYR:C	1:B:157:VAL:HG23	2.26	0.56
1:A:71:HIS:CG	1:A:72:CYS:N	2.74	0.55
1:C:49:GLN:CD	1:C:165:GLN:HG2	2.26	0.55
1:A:119:TYR:O	1:A:120:LEU:HD23	2.06	0.55
1:A:251:ILE:HG23	1:A:252:GLU:CG	2.31	0.55
1:B:199:PHE:C	1:B:199:PHE:CD2	2.80	0.55
1:A:155:GLY:HA3	1:A:185:ILE:CG1	2.36	0.55
1:C:234:LYS:H	1:C:234:LYS:CE	2.19	0.55
1:A:199:PHE:O	1:A:200:LYS:HD2	2.05	0.55
1:A:223:ARG:O	1:A:223:ARG:HG2	2.07	0.55
1:B:169:CYS:HA	1:B:172:ASN:HB2	1.89	0.55
1:B:199:PHE:C	1:B:199:PHE:HD2	2.10	0.55
1:C:90:LEU:HD11	1:C:205:TYR:CE1	2.41	0.55
1:C:101:ARG:CG	1:C:102:GLY:N	2.69	0.55
1:C:234:LYS:H	1:C:234:LYS:CD	2.19	0.55
1:A:91:VAL:HG13	1:A:222:ALA:O	2.05	0.55
1:A:92:MET:HE2	1:A:220:VAL:HG12	1.89	0.55
1:A:259:ASN:C	1:A:260:LEU:HD23	2.27	0.55
1:A:200:LYS:HZ2	1:C:140:ALA:HB3	1.70	0.55
1:B:106:ASN:ND2	1:B:106:ASN:N	2.54	0.55
1:C:80:VAL:CG1	1:C:81:THR:N	2.70	0.55
1:C:256:ALA:O	1:C:257:ALA:C	2.43	0.55
1:B:150:LEU:HD12	1:B:150:LEU:O	2.07	0.54
1:A:123:CYS:HB2	1:A:124:PRO:O	2.07	0.54
1:A:81:THR:O	1:A:231:GLY:CA	2.56	0.54
1:A:138:ASP:C	1:A:140:ALA:H	2.09	0.54
1:B:195:LYS:HE3	1:C:195:LYS:HE3	1.89	0.54
1:C:218:ILE:O	1:C:220:VAL:N	2.41	0.54
1:B:123:CYS:HB2	1:B:124:PRO:CD	2.38	0.54
1:C:60:LEU:CD1	1:C:69:LEU:HD13	2.36	0.54
1:C:146:SER:N	1:C:149:GLN:NE2	2.56	0.53
1:A:204:ASP:O	1:A:205:TYR:C	2.46	0.53
1:B:137:TYR:CE1	1:C:252:GLU:HG3	2.43	0.53
1:B:131:ILE:O	1:B:158:THR:CG2	2.52	0.53
1:C:144:PRO:HG3	1:C:150:LEU:HD23	1.89	0.53
1:C:178:ASP:OD1	1:C:180:SER:HB2	2.08	0.53
1:A:78:LEU:HB2	1:A:228:MET:CE	2.38	0.53
1:A:139:MET:N	1:A:217:ASN:OD1	2.40	0.53
1:B:139:MET:HE2	1:B:223:ARG:HB3	1.90	0.53
1:C:205:TYR:CE1	1:C:209:VAL:HG21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HB2	1:A:228:MET:HE2	1.91	0.53
1:C:90:LEU:O	1:C:95:THR:CG2	2.57	0.53
1:A:139:MET:HG3	1:A:205:TYR:OH	2.08	0.53
1:A:218:ILE:CD1	1:B:218:ILE:HD12	2.38	0.53
1:C:131:ILE:HG12	1:C:132:HIS:N	2.24	0.53
1:A:212:ASN:OD1	1:A:213:ALA:N	2.42	0.52
1:A:250:LEU:CD1	1:A:250:LEU:N	2.72	0.52
1:A:63:SER:HA	1:A:66:VAL:O	2.09	0.52
1:A:71:HIS:ND1	1:A:72:CYS:N	2.51	0.52
1:A:147:VAL:HG12	1:A:148:ASN:N	2.24	0.52
1:A:195:LYS:HB3	1:A:196:ARG:HD2	1.92	0.52
1:B:248:ILE:HG23	1:B:250:LEU:HD22	1.91	0.52
1:A:92:MET:CE	1:A:220:VAL:HG11	2.39	0.52
1:B:103:VAL:HG12	1:B:107:TRP:HZ3	1.74	0.52
1:B:161:VAL:HB	1:B:239:THR:HB	1.89	0.52
1:A:94:PHE:HB2	1:A:199:PHE:CE2	2.43	0.52
1:C:233:SER:HA	1:C:234:LYS:HE3	1.90	0.52
1:C:107:TRP:CE3	1:C:250:LEU:HD23	2.45	0.52
1:B:73:GLU:OE1	1:B:99:TRP:CB	2.57	0.52
1:A:124:PRO:HB2	1:A:126:THR:HG22	1.90	0.52
1:A:200:LYS:CG	1:A:219:LEU:HD23	2.39	0.52
1:B:80:VAL:HG22	1:B:239:THR:CG2	2.39	0.52
1:A:134:GLY:HA3	1:A:153:LEU:HB3	1.91	0.52
1:B:175:LYS:O	1:B:177:PRO:CD	2.58	0.51
1:C:73:GLU:OE1	1:C:99:TRP:N	2.32	0.51
1:C:101:ARG:HG2	1:C:102:GLY:H	1.73	0.51
1:A:194:GLU:HB2	1:A:197:TYR:CZ	2.45	0.51
1:A:132:HIS:CE1	1:A:147:VAL:CG2	2.93	0.51
1:A:201:THR:CG2	1:A:260:LEU:HA	2.41	0.51
1:A:212:ASN:OD1	1:A:212:ASN:C	2.48	0.51
1:C:84:ILE:HG23	1:C:85:VAL:N	2.24	0.51
1:C:90:LEU:CB	1:C:95:THR:HG21	2.35	0.51
1:A:165:GLN:O	1:A:167:GLY:N	2.38	0.51
1:A:200:LYS:HE3	1:A:260:LEU:O	2.10	0.51
1:C:133:MET:HG3	1:C:185:ILE:HG21	1.92	0.51
1:B:129:GLY:HA2	1:B:230:GLY:CA	2.40	0.51
1:A:201:THR:HG22	1:A:260:LEU:CA	2.41	0.51
1:A:218:ILE:HG22	1:A:218:ILE:O	2.09	0.51
1:B:138:ASP:CA	1:B:217:ASN:HD21	2.23	0.51
1:C:116:ARG:NH2	1:C:184:THR:HG21	2.24	0.51
1:A:142:THR:HG22	1:A:143:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HG23	1:B:184:THR:HB	1.93	0.51
1:B:131:ILE:O	1:B:158:THR:HA	2.11	0.51
1:B:185:ILE:HG23	1:B:185:ILE:O	2.11	0.51
1:C:218:ILE:O	1:C:219:LEU:C	2.49	0.51
1:B:205:TYR:O	1:B:208:ALA:HB3	2.11	0.51
1:A:139:MET:N	1:A:139:MET:SD	2.80	0.50
1:B:106:ASN:H	1:B:106:ASN:HD22	1.57	0.50
1:B:62:SER:HA	1:B:68:ILE:CD1	2.41	0.50
1:B:138:ASP:OD2	1:B:140:ALA:HB3	2.11	0.50
1:B:214:ASN:HD22	1:C:219:LEU:HD11	1.76	0.50
1:A:129:GLY:CA	1:A:230:GLY:HA3	2.41	0.50
1:A:94:PHE:O	1:A:101:ARG:NH1	2.41	0.50
1:C:69:LEU:HD12	1:C:70:SER:H	1.77	0.50
1:C:131:ILE:O	1:C:158:THR:HA	2.11	0.50
1:A:124:PRO:HD2	1:A:127:THR:OG1	2.11	0.50
1:B:213:ALA:O	1:B:214:ASN:C	2.50	0.50
1:A:258:LEU:HD11	1:C:144:PRO:CA	2.40	0.50
1:B:72:CYS:HA	1:B:244:ALA:O	2.12	0.50
1:A:107:TRP:CZ3	1:A:250:LEU:HD23	2.47	0.49
1:B:78:LEU:HD22	1:B:228:MET:HE1	1.93	0.49
1:C:113:VAL:HB	1:C:247:THR:O	2.12	0.49
1:C:116:ARG:NE	1:C:170:PHE:CE2	2.80	0.49
1:C:169:CYS:HB3	1:C:174:THR:HG22	1.93	0.49
1:A:133:MET:HA	1:A:225:VAL:O	2.13	0.49
1:A:116:ARG:HE	1:A:170:PHE:HD1	1.59	0.49
1:A:200:LYS:HE2	1:A:260:LEU:OXT	2.12	0.49
1:C:201:THR:HG23	1:C:260:LEU:HA	1.94	0.49
1:C:146:SER:N	1:C:149:GLN:HE21	2.03	0.49
1:B:105:GLN:HA	1:B:199:PHE:CE1	2.48	0.49
1:C:196:ARG:NH1	1:C:249:ARG:HH21	2.10	0.49
1:B:78:LEU:HD12	1:B:78:LEU:H	1.77	0.49
1:A:92:MET:HE1	1:A:220:VAL:HG11	1.95	0.49
1:A:200:LYS:HZ2	1:C:140:ALA:CB	2.26	0.49
1:A:238:ASN:N	1:A:238:ASN:HD22	2.11	0.49
1:B:74:LEU:HD12	1:B:74:LEU:N	2.28	0.49
1:B:69:LEU:HB3	1:B:248:ILE:CG2	2.43	0.49
1:C:76:THR:CG2	1:C:77:GLU:N	2.75	0.49
1:A:199:PHE:HD2	1:A:200:LYS:N	2.10	0.49
1:A:249:ARG:NH2	1:C:191:GLU:OE1	2.45	0.49
1:A:124:PRO:HG2	1:A:126:THR:HG22	1.95	0.48
1:C:167:GLY:O	1:C:168:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLU:HB2	1:C:197:TYR:CE2	2.48	0.48
1:A:177:PRO:O	1:A:178:ASP:HB3	2.14	0.48
1:B:188:ASP:OD1	1:B:191:GLU:HB2	2.13	0.48
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.14	0.48
1:A:252:GLU:OE2	1:C:137:TYR:CZ	2.67	0.48
1:B:69:LEU:HB3	1:B:248:ILE:HG22	1.95	0.48
1:C:150:LEU:HD22	1:C:153:LEU:HD22	1.95	0.48
1:A:155:GLY:HA3	1:A:185:ILE:CD1	2.44	0.47
1:B:72:CYS:O	1:B:73:GLU:HB2	2.13	0.47
1:B:169:CYS:HB2	1:B:174:THR:HB	1.96	0.47
1:C:56:ARG:HG2	1:C:57:PRO:HD2	1.95	0.47
1:C:99:TRP:O	1:C:100:LEU:C	2.51	0.47
1:C:151:SER:HA	1:C:156:TYR:CD2	2.49	0.47
1:B:70:SER:HA	1:B:246:TYR:O	2.14	0.47
1:A:71:HIS:HB3	1:A:246:TYR:OH	2.15	0.47
1:A:215:ILE:HG22	1:A:219:LEU:HD11	1.95	0.47
1:B:62:SER:HA	1:B:68:ILE:HD12	1.95	0.47
1:B:212:ASN:HD22	1:B:214:ASN:HB2	1.77	0.47
1:A:200:LYS:HG3	1:A:219:LEU:HD23	1.95	0.47
1:B:101:ARG:O	1:B:105:GLN:HB2	2.13	0.47
1:C:116:ARG:HE	1:C:184:THR:HG21	1.79	0.47
1:A:82:VAL:HA	1:A:231:GLY:HA3	1.97	0.47
1:A:92:MET:CE	1:A:220:VAL:CG1	2.93	0.47
1:A:138:ASP:HB3	1:A:141:ASP:OD2	2.15	0.47
1:B:93:PRO:CB	1:B:100:LEU:HD13	2.45	0.47
1:C:84:ILE:O	1:C:85:VAL:HG23	2.14	0.47
1:B:71:HIS:CD2	1:B:99:TRP:CZ3	3.00	0.47
1:C:116:ARG:CZ	1:C:170:PHE:CE2	2.97	0.47
1:C:116:ARG:HD3	1:C:170:PHE:CD2	2.50	0.47
1:A:129:GLY:O	1:A:160:PRO:HA	2.15	0.47
1:A:181:ARG:O	1:A:182:ALA:HB2	2.14	0.47
1:A:105:GLN:CA	1:A:199:PHE:CE1	2.78	0.47
1:A:138:ASP:HB3	1:A:141:ASP:CG	2.35	0.47
1:C:145:VAL:CG2	1:C:149:GLN:HE22	2.28	0.47
1:C:197:TYR:CZ	1:C:221:PRO:HB3	2.50	0.47
1:A:142:THR:CG2	1:B:258:LEU:HD22	2.45	0.46
1:A:146:SER:HB3	1:A:149:GLN:HG3	1.97	0.46
1:A:169:CYS:N	1:A:172:ASN:HB2	2.30	0.46
1:A:133:MET:HB2	1:A:224:LEU:HD11	1.98	0.46
1:B:110:TYR:HB2	1:B:248:ILE:CD1	2.43	0.46
1:C:123:CYS:HB2	1:C:127:THR:OG1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:CG2	1:A:249:ARG:HH21	2.27	0.46
1:A:124:PRO:C	1:A:126:THR:H	2.18	0.46
1:B:145:VAL:HG12	1:B:146:SER:N	2.30	0.46
1:C:201:THR:CG2	1:C:260:LEU:HA	2.46	0.46
1:C:168:LEU:O	1:C:169:CYS:C	2.54	0.46
1:B:71:HIS:HD2	1:B:99:TRP:CH2	2.33	0.46
1:B:172:ASN:HD22	1:B:172:ASN:HA	1.20	0.46
1:A:132:HIS:CE1	1:A:147:VAL:HG22	2.51	0.46
1:A:133:MET:CE	1:A:242:LEU:HD11	2.45	0.46
1:B:219:LEU:O	1:B:220:VAL:HG23	2.16	0.46
1:C:223:ARG:HG3	1:C:223:ARG:O	2.16	0.46
1:A:66:VAL:HG21	1:A:249:ARG:NH2	2.28	0.46
1:C:251:ILE:O	1:C:252:GLU:HB3	2.15	0.46
1:A:64:MET:HA	3:A:262:HOH:O	2.15	0.46
1:A:90:LEU:HD13	1:A:92:MET:CE	2.40	0.46
1:A:108:SER:N	1:A:252:GLU:O	2.42	0.46
1:A:203:THR:O	1:A:206:ALA:HB3	2.16	0.46
1:B:100:LEU:HG	1:B:246:TYR:CZ	2.51	0.46
1:C:119:TYR:CD1	1:C:119:TYR:C	2.88	0.46
1:C:90:LEU:O	1:C:95:THR:HG21	2.16	0.45
1:C:131:ILE:HD12	1:C:228:MET:HE1	1.97	0.45
1:B:78:LEU:HD22	1:B:228:MET:CE	2.46	0.45
1:A:133:MET:HE3	1:A:242:LEU:HD11	1.97	0.45
1:B:213:ALA:O	1:B:216:GLY:N	2.40	0.45
1:C:196:ARG:HH11	1:C:249:ARG:HH21	1.63	0.45
1:C:139:MET:HA	1:C:139:MET:CE	2.46	0.45
1:C:205:TYR:O	1:C:208:ALA:N	2.50	0.45
1:A:201:THR:HG21	1:A:260:LEU:HA	1.99	0.45
1:B:110:TYR:C	1:B:110:TYR:CD1	2.90	0.45
1:C:59:MET:HG2	1:C:60:LEU:N	2.31	0.45
1:A:150:LEU:HD12	1:A:150:LEU:O	2.17	0.45
1:A:233:SER:HB3	1:A:235:THR:OG1	2.17	0.45
1:B:212:ASN:O	1:B:213:ALA:C	2.55	0.45
1:C:116:ARG:CD	1:C:170:PHE:CD2	3.00	0.45
1:B:146:SER:OG	1:B:147:VAL:N	2.49	0.45
1:B:151:SER:HA	1:B:156:TYR:CE2	2.52	0.45
1:C:91:VAL:HG12	1:C:91:VAL:O	2.16	0.45
1:B:248:ILE:HD12	1:B:250:LEU:CD1	2.37	0.44
1:C:82:VAL:HB	1:C:234:LYS:HA	1.99	0.44
1:A:138:ASP:O	1:A:139:MET:C	2.56	0.44
1:A:233:SER:CB	1:A:235:THR:OG1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PHE:N	1:A:170:PHE:CD2	2.85	0.44
1:C:144:PRO:HG2	1:C:150:LEU:HD23	1.99	0.44
1:C:248:ILE:HG23	1:C:248:ILE:O	2.18	0.44
1:A:91:VAL:CG1	1:A:222:ALA:O	2.66	0.44
1:A:181:ARG:HD2	1:A:181:ARG:N	2.33	0.44
1:A:107:TRP:CE3	1:A:250:LEU:HD23	2.53	0.44
1:A:191:GLU:HG3	1:B:251:ILE:CD1	2.48	0.44
1:A:238:ASN:N	1:A:238:ASN:ND2	2.66	0.44
1:A:214:ASN:HD21	1:B:200:LYS:CE	2.31	0.44
1:A:228:MET:HE3	1:A:239:THR:HG21	1.99	0.44
1:B:92:MET:HA	1:B:93:PRO:HD2	1.86	0.44
1:B:140:ALA:HB2	1:B:214:ASN:OD1	2.18	0.44
1:B:156:TYR:C	1:B:157:VAL:CG2	2.86	0.44
1:A:90:LEU:HB3	1:A:92:MET:HE3	2.00	0.44
1:C:212:ASN:ND2	1:C:214:ASN:ND2	2.66	0.44
1:C:256:ALA:O	1:C:258:LEU:N	2.50	0.44
1:A:79:ALA:CA	1:A:237:VAL:O	2.61	0.43
1:C:116:ARG:O	1:C:244:ALA:HA	2.18	0.43
1:C:206:ALA:O	1:C:207:THR:C	2.56	0.43
1:B:170:PHE:HE1	1:B:184:THR:HG21	1.82	0.43
1:B:209:VAL:O	1:B:212:ASN:N	2.51	0.43
1:C:179:THR:O	1:C:180:SER:C	2.56	0.43
1:B:92:MET:HG2	1:B:94:PHE:H	1.82	0.43
1:B:229:GLU:O	1:B:229:GLU:CG	2.65	0.43
1:C:116:ARG:NE	1:C:170:PHE:CD2	2.86	0.43
1:A:135:PHE:O	1:A:153:LEU:HG	2.18	0.43
1:B:69:LEU:HD21	1:B:99:TRP:HZ3	1.83	0.43
1:B:72:CYS:SG	1:B:171:VAL:HG13	2.59	0.43
1:C:227:ALA:C	1:C:228:MET:HG2	2.38	0.43
1:A:80:VAL:HG11	1:A:129:GLY:HA3	2.01	0.43
1:B:110:TYR:CD1	1:B:111:ALA:N	2.86	0.43
1:B:167:GLY:C	1:B:169:CYS:N	2.70	0.43
1:A:64:MET:HB2	1:A:65:ASP:H	1.46	0.43
1:C:201:THR:HG23	1:C:260:LEU:CA	2.48	0.43
1:B:115:ILE:HG12	1:B:116:ARG:N	2.34	0.43
1:B:124:PRO:C	1:B:126:THR:H	2.22	0.43
1:C:202:ALA:O	1:C:205:TYR:HB3	2.19	0.43
1:A:88:SER:HA	1:A:224:LEU:O	2.19	0.43
1:B:259:ASN:OD1	1:B:260:LEU:N	2.52	0.43
1:C:80:VAL:CG1	1:C:231:GLY:HA2	2.49	0.43
1:C:82:VAL:HG12	1:C:83:THR:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:HD22	1:A:173:ASN:HA	1.27	0.42
1:C:205:TYR:O	1:C:208:ALA:HB3	2.19	0.42
1:A:153:LEU:HA	1:A:153:LEU:HD12	1.67	0.42
1:A:130:ALA:N	1:A:161:VAL:HG13	2.33	0.42
1:A:179:THR:C	1:A:181:ARG:N	2.70	0.42
1:B:129:GLY:HA2	1:B:230:GLY:HA3	2.00	0.42
1:B:200:LYS:HD2	1:B:260:LEU:O	2.19	0.42
1:C:79:ALA:CB	1:C:238:ASN:HA	2.50	0.42
1:C:155:GLY:O	1:C:156:TYR:C	2.55	0.42
1:C:194:GLU:HG3	1:C:218:ILE:HG23	2.01	0.42
1:A:194:GLU:OE1	1:A:194:GLU:HA	2.19	0.42
1:A:200:LYS:HD2	1:A:200:LYS:HA	1.73	0.42
1:A:185:ILE:O	1:A:185:ILE:HG23	2.19	0.42
1:A:221:PRO:O	1:A:222:ALA:HB2	2.20	0.42
1:A:82:VAL:HG13	1:A:234:LYS:N	2.34	0.42
1:B:116:ARG:HH11	1:B:116:ARG:HD2	1.69	0.42
1:A:82:VAL:HG13	1:A:234:LYS:CA	2.49	0.42
1:A:132:HIS:CE1	1:A:147:VAL:HG21	2.54	0.42
1:B:123:CYS:HB2	1:B:124:PRO:HD2	2.02	0.42
1:C:231:GLY:O	1:C:232:SER:HB3	2.18	0.42
1:B:79:ALA:HB2	1:B:238:ASN:HA	2.00	0.42
1:B:195:LYS:CE	1:C:195:LYS:HE3	2.50	0.42
1:C:172:ASN:HD22	1:C:172:ASN:HA	1.62	0.42
1:C:194:GLU:OE1	1:C:194:GLU:HA	2.20	0.42
1:A:170:PHE:N	1:A:170:PHE:HD2	2.18	0.42
1:A:202:ALA:O	1:A:203:THR:C	2.58	0.42
1:C:116:ARG:CZ	1:C:170:PHE:HE2	2.32	0.42
1:A:219:LEU:HD21	1:C:214:ASN:OD1	2.20	0.41
1:B:125:THR:O	1:B:125:THR:CG2	2.63	0.41
1:B:218:ILE:HG12	1:B:219:LEU:HD13	2.00	0.41
1:A:140:ALA:O	1:B:260:LEU:HD12	2.20	0.41
1:A:233:SER:C	1:A:235:THR:H	2.22	0.41
1:B:82:VAL:HG21	1:B:234:LYS:CG	2.50	0.41
1:B:175:LYS:O	1:B:177:PRO:N	2.53	0.41
1:B:233:SER:HB3	1:B:235:THR:HB	2.01	0.41
1:C:55:LEU:HD23	1:C:55:LEU:HA	1.72	0.41
1:A:71:HIS:HB3	1:A:246:TYR:CE2	2.56	0.41
1:B:74:LEU:H	1:B:74:LEU:CD1	2.32	0.41
1:B:133:MET:HE3	1:B:133:MET:HB2	1.94	0.41
1:B:219:LEU:C	1:B:220:VAL:HG23	2.41	0.41
1:C:109:LYS:HB3	1:C:197:TYR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:THR:HG22	1:B:258:LEU:HD22	2.02	0.41
1:A:250:LEU:N	1:A:250:LEU:HD12	2.35	0.41
1:C:181:ARG:H	1:C:181:ARG:HG2	1.63	0.41
1:A:92:MET:HE2	1:A:92:MET:HB3	1.54	0.41
1:A:167:GLY:O	1:A:168:LEU:C	2.59	0.41
1:A:246:TYR:CD1	1:A:246:TYR:N	2.89	0.41
1:B:133:MET:HA	1:B:225:VAL:O	2.20	0.41
1:A:148:ASN:C	1:A:148:ASN:ND2	2.69	0.41
1:C:69:LEU:O	1:C:248:ILE:HG22	2.20	0.41
1:C:76:THR:HG22	1:C:77:GLU:N	2.36	0.41
1:C:90:LEU:O	1:C:95:THR:HG22	2.21	0.41
1:A:82:VAL:HG13	1:A:233:SER:C	2.41	0.41
1:B:79:ALA:HB2	1:B:238:ASN:HD22	1.86	0.41
1:A:201:THR:HG22	1:A:260:LEU:HA	2.03	0.41
1:B:113:VAL:HB	1:B:247:THR:O	2.20	0.41
1:B:200:LYS:HD2	1:B:200:LYS:HA	1.47	0.41
1:B:213:ALA:O	1:B:215:ILE:N	2.54	0.41
1:B:250:LEU:HD12	1:B:250:LEU:HA	1.79	0.41
1:C:71:HIS:CG	1:C:72:CYS:H	2.38	0.41
1:C:74:LEU:HB2	1:C:243:TYR:CE2	2.55	0.41
1:C:219:LEU:H	1:C:219:LEU:HG	1.49	0.41
1:A:72:CYS:SG	1:A:171:VAL:HA	2.61	0.41
1:B:74:LEU:N	1:B:74:LEU:CD1	2.84	0.41
1:C:154:LYS:O	1:C:154:LYS:HD3	2.21	0.41
1:A:101:ARG:HG3	1:A:102:GLY:N	2.30	0.40
1:C:176:CYS:HA	1:C:177:PRO:HD3	1.83	0.40
1:B:136:GLN:NE2	1:B:143:LEU:CD2	2.84	0.40
1:B:161:VAL:H	1:B:161:VAL:HG22	1.59	0.40
1:B:201:THR:HG23	1:B:260:LEU:HA	2.04	0.40
1:C:252:GLU:HA	1:C:253:PRO:HD2	1.71	0.40
1:A:78:LEU:CB	1:A:228:MET:HE2	2.51	0.40
1:C:201:THR:HG23	1:C:260:LEU:OXT	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	197/260 (76%)	160 (81%)	27 (14%)	10 (5%)	2 6
1	B	197/260 (76%)	163 (83%)	29 (15%)	5 (2%)	5 19
1	C	220/260 (85%)	182 (83%)	29 (13%)	9 (4%)	3 9
All	All	614/780 (79%)	505 (82%)	85 (14%)	24 (4%)	3 10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	189	THR
1	B	231	GLY
1	C	219	LEU
1	C	230	GLY
1	C	231	GLY
1	A	161	VAL
1	A	166	SER
1	A	169	CYS
1	B	210	GLY
1	C	177	PRO
1	A	139	MET
1	A	202	ALA
1	B	173	ASN
1	A	94	PHE
1	A	182	ALA
1	B	213	ALA
1	B	256	ALA
1	C	125	THR
1	C	205	TYR
1	C	257	ALA
1	C	173	ASN
1	C	251	ILE
1	A	177	PRO
1	A	230	GLY

5.3.2 Protein sidechains (i)

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	167/217 (77%)	121 (72%)	46 (28%)	0 1
1	B	167/217 (77%)	116 (70%)	51 (30%)	0 1
1	C	185/217 (85%)	128 (69%)	57 (31%)	0 0
All	All	519/651 (80%)	365 (70%)	154 (30%)	0 1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	MET
1	A	65	ASP
1	A	77	GLU
1	A	78	LEU
1	A	80	VAL
1	A	87	THR
1	A	91	VAL
1	A	92	MET
1	A	95	THR
1	A	100	LEU
1	A	101	ARG
1	A	108	SER
1	A	109	LYS
1	A	116	ARG
1	A	118	THR
1	A	119	TYR
1	A	123	CYS
1	A	133	MET
1	A	139	MET
1	A	145	VAL
1	A	146	SER
1	A	148	ASN
1	A	152	ASN
1	A	154	LYS
1	A	158	THR
1	A	165	GLN
1	A	168	LEU
1	A	172	ASN
1	A	173	ASN
1	A	176	CYS
1	A	181	ARG

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Mol	Chain	Res	Type
1	A	183	ILE
1	A	184	THR
1	A	191	GLU
1	A	196	ARG
1	A	198	PRO
1	A	199	PHE
1	A	200	LYS
1	A	214	ASN
1	A	218	ILE
1	A	223	ARG
1	A	225	VAL
1	A	226	THR
1	A	234	LYS
1	A	245	SER
1	A	251	ILE
1	B	62	SER
1	B	72	CYS
1	B	74	LEU
1	B	78	LEU
1	B	82	VAL
1	B	85	VAL
1	B	87	THR
1	B	88	SER
1	B	90	LEU
1	B	95	THR
1	B	100	LEU
1	B	105	GLN
1	B	106	ASN
1	B	108	SER
1	B	109	LYS
1	B	115	ILE
1	B	116	ARG
1	B	118	THR
1	B	138	ASP
1	B	139	MET
1	B	147	VAL
1	B	150	LEU
1	B	152	ASN
1	B	153	LEU
1	B	154	LYS
1	B	158	THR
1	B	161	VAL

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Mol	Chain	Res	Type
1	B	165	GLN
1	B	171	VAL
1	B	172	ASN
1	B	173	ASN
1	B	175	LYS
1	B	176	CYS
1	B	180	SER
1	B	189	THR
1	B	190	ASN
1	B	196	ARG
1	B	199	PHE
1	B	200	LYS
1	B	203	THR
1	B	209	VAL
1	B	218	ILE
1	B	223	ARG
1	B	226	THR
1	B	234	LYS
1	B	235	THR
1	B	242	LEU
1	B	248	ILE
1	B	250	LEU
1	B	251	ILE
1	B	252	GLU
1	C	47	ILE
1	C	52	MET
1	C	54	LYS
1	C	60	LEU
1	C	61	ARG
1	C	65	ASP
1	C	66	VAL
1	C	67	THR
1	C	70	SER
1	C	72	CYS
1	C	74	LEU
1	C	78	LEU
1	C	80	VAL
1	C	82	VAL
1	C	83	THR
1	C	84	ILE
1	C	87	THR
1	C	88	SER

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Mol	Chain	Res	Type
1	C	92	MET
1	C	98	THR
1	C	115	ILE
1	C	118	THR
1	C	121	PRO
1	C	122	SER
1	C	125	THR
1	C	127	THR
1	C	128	SER
1	C	145	VAL
1	C	146	SER
1	C	149	GLN
1	C	150	LEU
1	C	152	ASN
1	C	153	LEU
1	C	161	VAL
1	C	165	GLN
1	C	172	ASN
1	C	173	ASN
1	C	174	THR
1	C	178	ASP
1	C	181	ARG
1	C	184	THR
1	C	187	LEU
1	C	189	THR
1	C	191	GLU
1	C	193	SER
1	C	195	LYS
1	C	196	ARG
1	C	200	LYS
1	C	203	THR
1	C	214	ASN
1	C	228	MET
1	C	234	LYS
1	C	235	THR
1	C	242	LEU
1	C	245	SER
1	C	249	ARG
1	C	251	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	136	GLN
1	A	148	ASN
1	A	165	GLN
1	A	172	ASN
1	A	173	ASN
1	A	190	ASN
1	A	214	ASN
1	A	238	ASN
1	B	106	ASN
1	B	136	GLN
1	B	152	ASN
1	B	165	GLN
1	B	172	ASN
1	B	173	ASN
1	B	190	ASN
1	B	212	ASN
1	B	214	ASN
1	B	217	ASN
1	B	238	ASN
1	C	49	GLN
1	C	149	GLN
1	C	172	ASN
1	C	173	ASN
1	C	212	ASN
1	C	217	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	199/260 (76%)	0.27	3 (1%)	73	68	12, 22, 60, 83	0
1	B	199/260 (76%)	0.22	1 (0%)	91	88	10, 21, 50, 65	0
1	C	222/260 (85%)	0.15	0	100	100	8, 21, 37, 60	0
All	All	620/780 (79%)	0.21	4 (0%)	89	86	8, 21, 46, 83	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	62	SER	11.8
1	A	63	SER	8.5
1	A	176	CYS	3.7
1	B	62	SER	3.4

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 monosaccharides in this entry.

6.4 Ligands (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
2	CA	A	261	1/1	0.95	0.10	27,27,27,27	0
2	CA	C	261	1/1	0.97	0.12	20,20,20,20	0
2	CA	B	261	1/1	0.98	0.12	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.