



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 PM UTC

PDB ID : 3V8F / pdb_00003v8f
Title : Crystal structure of crosslinked GltPh V216C-M385C mutant
Authors : Verdon, G.; Boudker, O.
Deposited on : 2011-12-22
Resolution : 3.80 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 ⓘ symbol.

The types of validation reports are described at

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

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

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

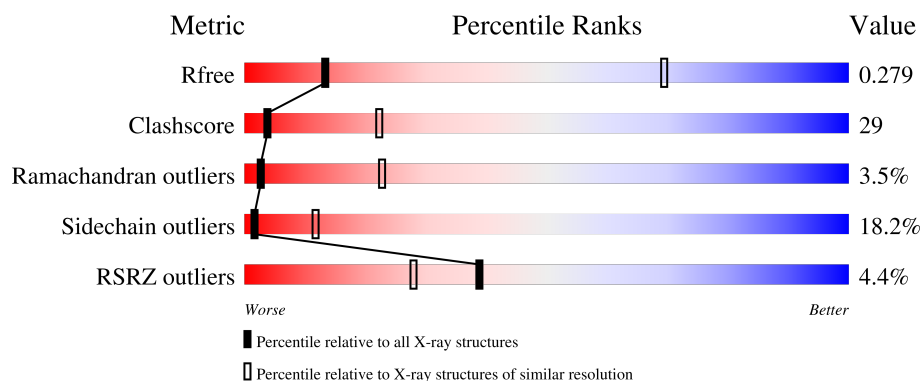
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	422	6% 44% 43% 9% .
1	B	422	4% 45% 41% 12% ..
1	C	422	3% 43% 42% 11% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	C	901	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9155 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 sodium-coupled L-aspartate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3038	1999	490	532	17			
1	B	411	Total	C	N	O	S	0	0	0
			3043	2002	491	533	17			
1	C	410	Total	C	N	O	S	0	0	0
			3038	1999	490	532	17			

There are 45 discrepancies between the modelled and reference sequences:

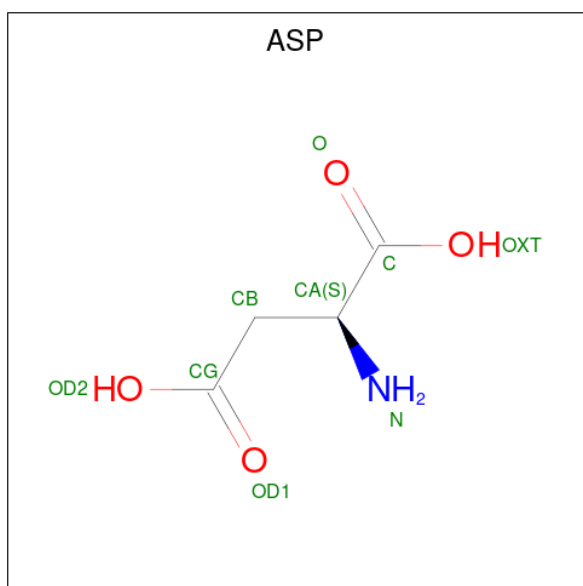
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	216	CYS	VAL	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	385	CYS	MET	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
A	421	PRO	-	expression tag	UNP O59010
A	422	ARG	-	expression tag	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	216	CYS	VAL	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	368	HIS	GLU	engineered mutation	UNP O59010
B	385	CYS	MET	engineered mutation	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
B	421	PRO	-	expression tag	UNP O59010
B	422	ARG	-	expression tag	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	216	CYS	VAL	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	385	CYS	MET	engineered mutation	UNP O59010
C	418	THR	-	expression tag	UNP O59010
C	419	LEU	-	expression tag	UNP O59010
C	420	VAL	-	expression tag	UNP O59010
C	421	PRO	-	expression tag	UNP O59010
C	422	ARG	-	expression tag	UNP O59010

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		

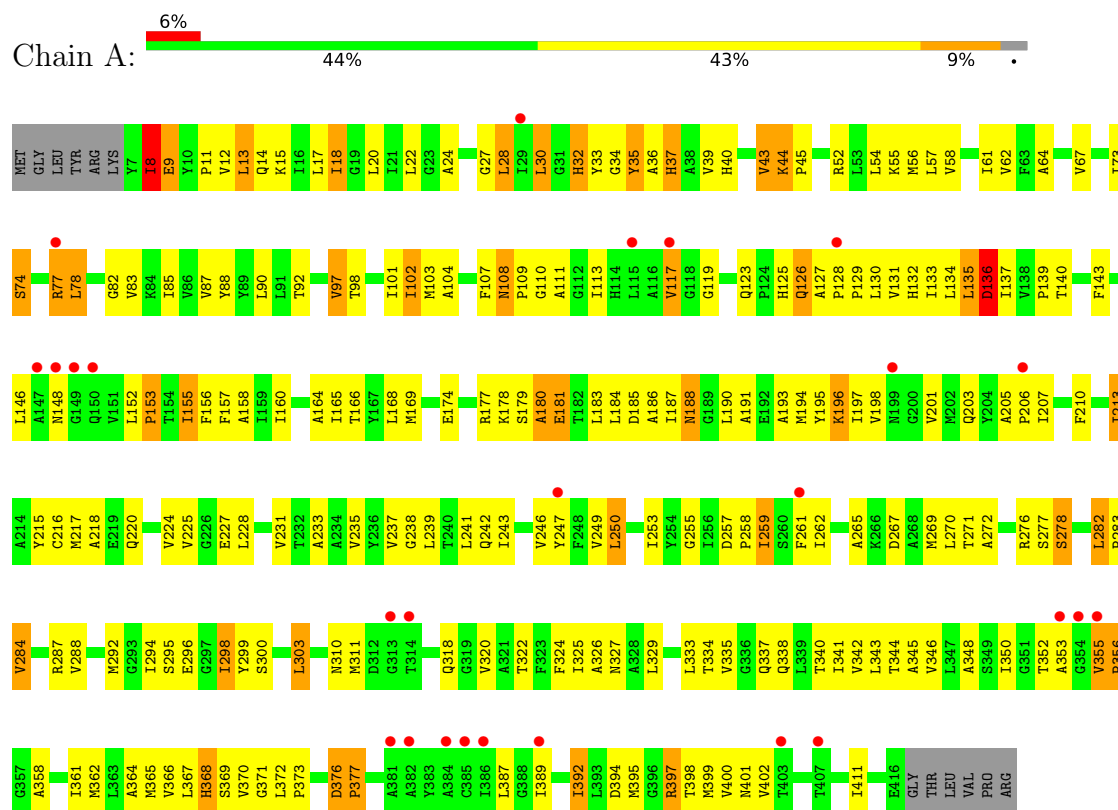
- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Hg	0	0
			1	1		
4	B	1	Total	Hg	0	0
			1	1		
4	C	1	Total	Hg	0	0
			1	1		

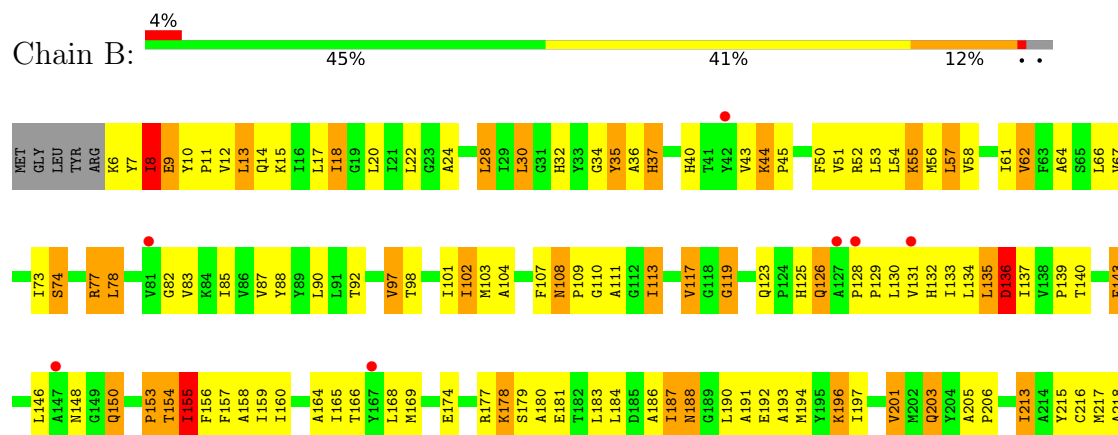
3 Residue-property plots

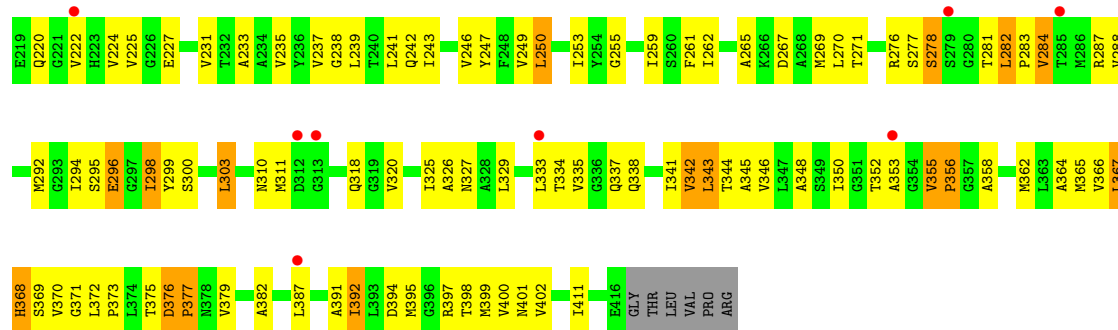
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: sodium-coupled L-aspartate transporter

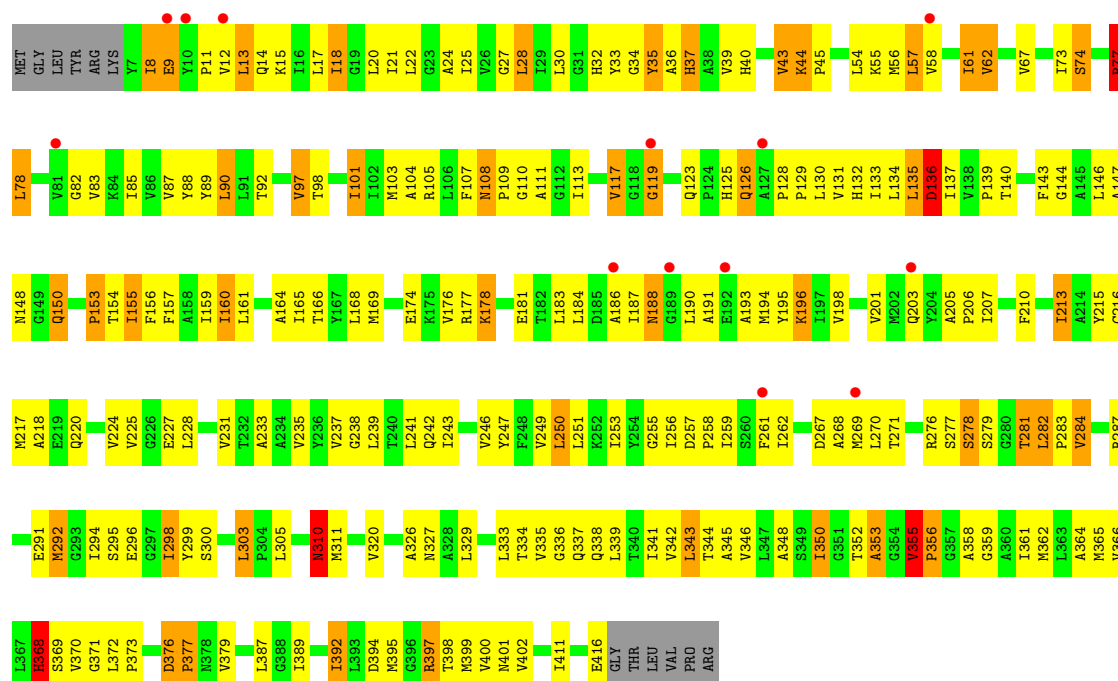
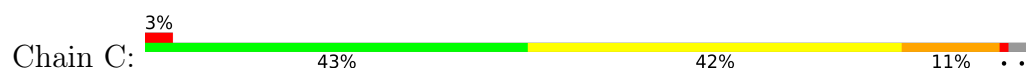


- Molecule 1: sodium-coupled L-aspartate transporter





• Molecule 1: sodium-coupled L-aspartate transporter



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	124.30Å 199.81Å 111.25Å 90.00° 117.08° 90.00°	Depositor
Resolution (Å)	30.00 – 3.80 30.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (30.00-3.80) 99.4 (30.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 3.78Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.243 , 0.255 0.253 , 0.279	Depositor DCC
R_{free} test set	1222 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	152.4	Xtriage
Anisotropy	0.529	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 204.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9155	wwPDB-VP
Average B, all atoms (Å ²)	247.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.76	2/3098 (0.1%)	1.11	6/4227 (0.1%)
1	B	0.91	1/3103 (0.0%)	1.20	15/4234 (0.4%)
1	C	0.94	2/3098 (0.1%)	1.21	14/4227 (0.3%)
All	All	0.87	5/9299 (0.1%)	1.17	35/12688 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	8	ILE	CA-CB	6.70	1.61	1.53
1	A	8	ILE	CA-CB	5.80	1.59	1.53
1	C	310	ASN	N-CA	5.65	1.53	1.46
1	C	355	VAL	CA-C	5.51	1.58	1.52
1	A	97	VAL	CA-CB	5.42	1.61	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ASP	CA-C-N	7.65	129.40	119.84
1	B	376	ASP	C-N-CA	7.65	129.40	119.84
1	B	367	LEU	N-CA-C	-7.60	102.69	110.97
1	B	143	PHE	N-CA-C	-7.33	102.98	110.97
1	B	117	VAL	N-CA-C	6.95	118.54	110.62
1	A	117	VAL	N-CA-C	6.90	118.48	110.62
1	B	155	ILE	N-CA-C	-6.71	104.12	110.42
1	A	376	ASP	CA-C-N	6.68	128.19	119.84
1	A	376	ASP	C-N-CA	6.68	128.19	119.84
1	B	119	GLY	N-CA-C	-6.65	107.17	115.08
1	C	188	ASN	N-CA-C	-6.49	101.93	110.43
1	C	117	VAL	N-CA-C	6.48	118.00	110.62
1	B	113	ILE	N-CA-C	-6.13	106.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ASN	N-CA-C	-6.12	102.41	110.43
1	C	150	GLN	N-CA-C	5.91	119.33	111.30
1	C	77	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	C	376	ASP	CA-C-N	5.84	127.14	119.84
1	C	376	ASP	C-N-CA	5.84	127.14	119.84
1	C	56	MET	CB-CG-SD	-5.82	95.25	112.70
1	C	62	VAL	N-CA-C	-5.79	104.97	110.42
1	B	62	VAL	N-CA-CB	5.74	117.13	110.65
1	A	188	ASN	N-CA-C	-5.70	103.01	110.53
1	C	77	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	C	62	VAL	N-CA-CB	5.46	116.83	110.65
1	C	119	GLY	N-CA-C	-5.40	107.05	114.67
1	B	56	MET	CB-CG-SD	-5.38	96.56	112.70
1	B	150	GLN	N-CA-C	5.32	118.53	111.30
1	B	201	VAL	CB-CA-C	-5.32	105.07	112.04
1	B	158	ALA	N-CA-C	-5.26	105.19	111.03
1	C	353	ALA	N-CA-C	5.21	117.37	111.02
1	C	279	SER	N-CA-C	5.15	116.58	111.07
1	B	62	VAL	CB-CA-C	-5.11	105.28	111.87
1	A	56	MET	CB-CG-SD	-5.07	97.49	112.70
1	A	340	THR	N-CA-C	-5.01	105.71	111.07
1	C	160	ILE	CB-CA-C	5.00	118.90	112.14

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	3038	0	3204	178	0
1	B	3043	0	3206	186	0
1	C	3038	0	3204	187	0
2	A	9	0	3	2	0
2	B	9	0	3	2	0
2	C	9	0	3	5	0
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
All	All	9155	0	9623	538	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 29.

All (538) 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:335:VAL:HA	1:C:338:GLN:HB2	1.44	0.97
1:A:335:VAL:HA	1:A:338:GLN:HB2	1.48	0.96
1:B:231:VAL:O	1:B:235:VAL:HG23	1.69	0.93
1:C:231:VAL:O	1:C:235:VAL:HG23	1.69	0.92
1:B:335:VAL:HA	1:B:338:GLN:HB2	1.52	0.91
1:B:128:PRO:HB2	1:B:129:PRO:HD2	1.55	0.87
1:A:61:ILE:CG2	1:A:194:MET:HB3	2.05	0.87
1:C:107:PHE:O	1:C:109:PRO:HD3	1.73	0.87
1:C:233:ALA:O	1:C:237:VAL:HG22	1.75	0.85
1:C:139:PRO:HB3	1:C:153:PRO:HB3	1.59	0.85
1:B:233:ALA:O	1:B:237:VAL:HG22	1.78	0.84
1:C:128:PRO:HB2	1:C:129:PRO:HD2	1.58	0.83
1:C:166:THR:HA	1:C:169:MET:HE2	1.59	0.83
1:C:61:ILE:CG2	1:C:194:MET:HB3	2.09	0.82
1:C:334:THR:HG22	1:C:337:GLN:OE1	1.80	0.82
1:C:239:LEU:HD22	1:C:400:VAL:HG21	1.61	0.81
1:A:111:ALA:H	1:A:327:ASN:HB3	1.47	0.80
1:B:61:ILE:CG2	1:B:194:MET:HB3	2.11	0.80
1:A:231:VAL:O	1:A:235:VAL:HG23	1.81	0.80
1:A:107:PHE:O	1:A:109:PRO:HD3	1.82	0.80
1:A:139:PRO:HB3	1:A:153:PRO:HB3	1.62	0.79
1:C:111:ALA:H	1:C:327:ASN:HB3	1.46	0.79
1:A:355:VAL:HG22	1:A:356:PRO:HD2	1.64	0.79
1:C:355:VAL:HG22	1:C:356:PRO:HD2	1.64	0.79
1:A:128:PRO:HB2	1:A:129:PRO:HD2	1.65	0.78
1:B:139:PRO:HB3	1:B:153:PRO:HB3	1.66	0.78
1:B:355:VAL:HG22	1:B:356:PRO:HD2	1.65	0.78
1:C:242:GLN:O	1:C:246:VAL:HB	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:PHE:O	1:B:109:PRO:HD3	1.83	0.77
1:A:55:LYS:O	1:A:58:VAL:HG12	1.84	0.76
1:C:155:ILE:HD11	1:C:365:MET:HG3	1.67	0.76
1:B:55:LYS:O	1:B:58:VAL:HG12	1.85	0.76
1:B:111:ALA:H	1:B:327:ASN:HB3	1.50	0.76
1:A:299:TYR:HB2	1:A:303:LEU:HD23	1.68	0.75
1:A:157:PHE:HA	1:A:160:ILE:HG22	1.67	0.75
1:B:334:THR:HG22	1:B:337:GLN:OE1	1.85	0.75
1:C:203:GLN:HE21	1:C:203:GLN:HA	1.52	0.75
1:A:169:MET:HA	1:A:177:ARG:HG3	1.68	0.75
1:B:128:PRO:CB	1:B:129:PRO:HD2	2.17	0.75
1:A:233:ALA:O	1:A:237:VAL:HG22	1.87	0.74
1:B:157:PHE:HA	1:B:160:ILE:HG22	1.68	0.74
1:A:326:ALA:HB2	1:A:333:LEU:HD13	1.69	0.74
1:A:166:THR:HA	1:A:169:MET:HE2	1.67	0.74
1:C:326:ALA:HB2	1:C:333:LEU:HD13	1.68	0.74
1:B:165:ILE:HG21	1:B:184:LEU:HB2	1.70	0.74
1:C:345:ALA:HA	1:C:348:ALA:HB3	1.69	0.74
1:B:299:TYR:HB2	1:B:303:LEU:HD23	1.70	0.73
1:B:203:GLN:HE21	1:B:203:GLN:HA	1.53	0.73
1:C:299:TYR:HB2	1:C:303:LEU:HD23	1.70	0.73
1:B:166:THR:HA	1:B:169:MET:HE2	1.69	0.73
1:C:128:PRO:CB	1:C:129:PRO:HD2	2.17	0.73
1:C:61:ILE:HG22	1:C:194:MET:HB3	1.70	0.73
1:B:284:VAL:HG13	1:B:287:ARG:HH21	1.53	0.72
1:C:157:PHE:HA	1:C:160:ILE:HG22	1.70	0.72
1:A:334:THR:HG22	1:A:337:GLN:OE1	1.89	0.72
1:B:326:ALA:HB2	1:B:333:LEU:HD13	1.70	0.71
1:C:123:GLN:OE1	1:C:123:GLN:HA	1.89	0.71
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.25	0.71
1:A:61:ILE:HG22	1:A:194:MET:HB3	1.73	0.71
1:A:128:PRO:CB	1:A:129:PRO:HD2	2.21	0.70
1:B:113:ILE:HD11	1:B:224:VAL:HG23	1.73	0.70
1:B:262:ILE:HG23	1:B:269:MET:HE1	1.73	0.70
1:A:203:GLN:HA	1:A:203:GLN:HE21	1.56	0.69
1:C:262:ILE:HG23	1:C:269:MET:HE1	1.74	0.69
1:B:193:ALA:HB2	1:C:168:LEU:HD11	1.74	0.69
1:B:103:MET:HE2	1:B:237:VAL:HG23	1.74	0.69
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.28	0.69
1:A:61:ILE:HG22	1:A:194:MET:CB	2.23	0.69
1:C:15:LYS:O	1:C:18:ILE:HG22	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:GLN:HA	1:B:123:GLN:OE1	1.94	0.68
1:C:113:ILE:HD11	1:C:224:VAL:HG23	1.75	0.68
1:B:15:LYS:O	1:B:18:ILE:HG22	1.92	0.68
1:C:55:LYS:O	1:C:58:VAL:HG12	1.92	0.68
1:B:242:GLN:O	1:B:246:VAL:HB	1.94	0.68
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.29	0.68
1:B:126:GLN:O	1:B:126:GLN:HG2	1.93	0.68
1:A:284:VAL:HG13	1:A:287:ARG:HH21	1.58	0.67
1:C:126:GLN:O	1:C:126:GLN:HG2	1.95	0.67
1:A:15:LYS:O	1:A:18:ILE:HG22	1.95	0.67
1:C:169:MET:HA	1:C:177:ARG:HG3	1.76	0.67
1:A:113:ILE:HD11	1:A:224:VAL:HG23	1.77	0.67
1:C:284:VAL:HG13	1:C:287:ARG:HH21	1.60	0.67
1:A:54:LEU:HD12	1:A:201:VAL:HG11	1.76	0.67
1:C:103:MET:HE2	1:C:237:VAL:HG23	1.76	0.66
1:A:67:VAL:HG11	1:A:187:ILE:HD12	1.78	0.66
1:B:134:LEU:O	1:B:137:ILE:HG12	1.97	0.65
1:A:334:THR:O	1:A:337:GLN:HG2	1.96	0.65
1:B:345:ALA:HA	1:B:348:ALA:HB3	1.77	0.65
1:A:262:ILE:HG23	1:A:269:MET:HE1	1.77	0.65
1:B:13:LEU:HD23	1:B:276:ARG:HD3	1.79	0.65
1:A:35:TYR:N	1:A:35:TYR:CD2	2.65	0.65
1:A:168:LEU:HD11	1:C:193:ALA:HB2	1.79	0.65
1:A:345:ALA:HA	1:A:348:ALA:HB3	1.80	0.64
1:B:344:THR:HB	1:B:366:VAL:HG23	1.80	0.64
1:B:61:ILE:HG22	1:B:194:MET:HB3	1.79	0.64
1:B:371:GLY:O	1:B:373:PRO:HD3	1.98	0.64
1:C:35:TYR:N	1:C:35:TYR:CD2	2.65	0.64
1:C:61:ILE:HG22	1:C:194:MET:CB	2.27	0.64
1:B:205:ALA:N	1:B:206:PRO:HD2	2.13	0.64
1:A:123:GLN:OE1	1:A:123:GLN:HA	1.96	0.64
1:A:111:ALA:N	1:A:327:ASN:HB3	2.12	0.63
1:A:217:MET:SD	1:A:225:VAL:HG22	2.37	0.63
1:A:242:GLN:O	1:A:246:VAL:HB	1.98	0.63
1:B:186:ALA:O	1:B:188:ASN:O	2.17	0.63
1:C:344:THR:HB	1:C:366:VAL:HG23	1.81	0.63
1:B:35:TYR:N	1:B:35:TYR:CD2	2.66	0.63
1:C:111:ALA:N	1:C:327:ASN:HB3	2.11	0.63
1:B:169:MET:HA	1:B:177:ARG:HG3	1.79	0.63
1:C:83:VAL:O	1:C:87:VAL:HG23	1.98	0.63
1:C:334:THR:O	1:C:337:GLN:HG2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD23	1:A:276:ARG:HD3	1.81	0.63
1:A:61:ILE:HG21	1:A:194:MET:HB3	1.79	0.62
1:B:111:ALA:N	1:B:327:ASN:HB3	2.14	0.62
1:C:250:LEU:O	1:C:253:ILE:HG22	1.98	0.62
1:B:217:MET:SD	1:B:225:VAL:HG22	2.39	0.62
1:B:250:LEU:O	1:B:253:ILE:HG22	1.99	0.62
1:B:278:SER:HB2	2:B:901:ASP:O	1.99	0.62
1:A:344:THR:HB	1:A:366:VAL:HG23	1.82	0.62
1:C:13:LEU:HD23	1:C:276:ARG:HD3	1.80	0.62
1:B:129:PRO:CG	1:B:132:HIS:HD2	2.12	0.61
1:C:67:VAL:HG11	1:C:187:ILE:HD12	1.81	0.61
1:A:186:ALA:O	1:A:188:ASN:O	2.19	0.61
1:A:24:ALA:HA	1:A:217:MET:HG3	1.81	0.61
1:B:54:LEU:HD12	1:B:201:VAL:HG11	1.83	0.61
1:A:250:LEU:O	1:A:253:ILE:HG22	2.01	0.60
1:B:364:ALA:O	1:B:368:HIS:HB2	2.01	0.60
1:A:35:TYR:N	1:A:35:TYR:HD2	1.98	0.60
1:C:30:LEU:HD23	1:C:34:GLY:HA3	1.83	0.60
1:C:54:LEU:HD12	1:C:201:VAL:HG11	1.82	0.60
1:C:103:MET:HG3	1:C:238:GLY:HA3	1.83	0.60
1:B:61:ILE:HG22	1:B:194:MET:CB	2.32	0.60
1:C:203:GLN:HA	1:C:203:GLN:NE2	2.17	0.60
1:A:83:VAL:O	1:A:87:VAL:HG23	2.02	0.60
1:B:129:PRO:HG2	1:B:132:HIS:HD2	1.67	0.59
1:A:143:PHE:CE2	1:C:146:LEU:HD23	2.38	0.59
1:C:217:MET:SD	1:C:225:VAL:HG22	2.42	0.59
1:B:24:ALA:HA	1:B:217:MET:HG3	1.85	0.59
1:C:165:ILE:HG21	1:C:184:LEU:HB2	1.84	0.59
1:A:103:MET:HG3	1:A:238:GLY:HA3	1.84	0.59
1:A:239:LEU:HD22	1:A:400:VAL:HG21	1.84	0.59
1:B:37:HIS:HA	1:B:40:HIS:HB3	1.85	0.59
1:C:37:HIS:HA	1:C:40:HIS:HB3	1.83	0.59
1:C:165:ILE:HG21	1:C:184:LEU:HD13	1.84	0.59
1:A:103:MET:HE2	1:A:237:VAL:HG23	1.84	0.59
1:B:54:LEU:CD1	1:B:201:VAL:HG11	2.33	0.59
1:A:165:ILE:HG21	1:A:184:LEU:HB2	1.84	0.58
1:B:155:ILE:HD11	1:B:365:MET:HG3	1.84	0.58
1:C:61:ILE:HG21	1:C:194:MET:HB3	1.85	0.58
1:B:35:TYR:N	1:B:35:TYR:HD2	2.00	0.58
1:B:261:PHE:HD1	1:B:292:MET:HE1	1.67	0.58
1:B:129:PRO:HG2	1:B:132:HIS:CD2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:SER:N	1:B:398:THR:HG21	2.19	0.58
1:C:24:ALA:HA	1:C:217:MET:HG3	1.86	0.58
1:B:146:LEU:HD23	1:C:143:PHE:CE2	2.39	0.58
1:C:54:LEU:CD1	1:C:201:VAL:HG11	2.34	0.58
1:C:371:GLY:O	1:C:373:PRO:HD3	2.03	0.58
1:B:130:LEU:HA	1:B:133:ILE:HG22	1.86	0.57
1:B:334:THR:O	1:B:337:GLN:HG2	2.05	0.57
1:C:130:LEU:HA	1:C:133:ILE:CG2	2.34	0.57
1:C:335:VAL:HA	1:C:338:GLN:CB	2.29	0.57
1:A:82:GLY:HA2	1:A:85:ILE:HG22	1.86	0.57
1:B:334:THR:HG23	1:B:335:VAL:O	2.05	0.57
1:C:261:PHE:HD1	1:C:292:MET:HE1	1.69	0.57
1:B:6:LYS:C	1:B:8:ILE:H	2.13	0.57
1:C:73:ILE:O	1:C:78:LEU:HD22	2.05	0.57
1:C:343:LEU:HD13	1:C:343:LEU:C	2.30	0.57
1:A:58:VAL:O	1:A:62:VAL:HG23	2.05	0.57
1:A:155:ILE:HD11	1:A:365:MET:HG3	1.87	0.57
1:B:183:LEU:HD21	1:B:187:ILE:HD11	1.87	0.57
1:B:82:GLY:HA2	1:B:85:ILE:HG22	1.86	0.56
1:C:35:TYR:N	1:C:35:TYR:HD2	2.01	0.56
1:B:83:VAL:O	1:B:87:VAL:HG23	2.05	0.56
1:C:183:LEU:HD21	1:C:187:ILE:HD11	1.87	0.56
1:C:271:THR:HG21	1:C:284:VAL:HG21	1.86	0.56
1:A:37:HIS:HA	1:A:40:HIS:HB3	1.87	0.56
1:B:183:LEU:HD23	1:B:187:ILE:HG13	1.87	0.56
1:B:311:MET:HE2	1:B:401:ASN:ND2	2.21	0.56
1:B:341:ILE:HG13	1:B:370:VAL:HG21	1.88	0.56
1:C:130:LEU:HA	1:C:133:ILE:HG22	1.88	0.56
1:A:193:ALA:HB2	1:B:168:LEU:HD11	1.87	0.56
1:A:64:ALA:HB2	1:A:190:LEU:HD23	1.88	0.55
1:B:6:LYS:O	1:B:8:ILE:N	2.40	0.55
1:B:103:MET:HG3	1:B:238:GLY:HA3	1.89	0.55
1:B:227:GLU:O	1:B:231:VAL:HG23	2.06	0.55
1:B:67:VAL:HG11	1:B:187:ILE:HD12	1.88	0.55
1:C:216:CYS:O	1:C:220:GLN:HB2	2.07	0.55
1:A:44:LYS:N	1:A:45:PRO:HD2	2.21	0.55
1:A:261:PHE:HD1	1:A:292:MET:HE1	1.70	0.55
1:A:371:GLY:O	1:A:373:PRO:HD3	2.07	0.55
1:B:343:LEU:HD13	1:B:343:LEU:C	2.32	0.55
1:C:186:ALA:O	1:C:188:ASN:O	2.25	0.55
1:A:54:LEU:CD1	1:A:201:VAL:HG11	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:MET:HE2	1:C:401:ASN:ND2	2.22	0.55
1:A:139:PRO:CB	1:A:153:PRO:HB3	2.36	0.55
1:B:61:ILE:HG21	1:B:194:MET:HB3	1.85	0.55
1:C:178:LYS:O	1:C:178:LYS:HD3	2.06	0.55
1:A:30:LEU:HD23	1:A:34:GLY:HA3	1.89	0.54
1:B:261:PHE:CD1	1:B:292:MET:HE1	2.42	0.54
1:C:73:ILE:O	1:C:74:SER:C	2.51	0.54
1:B:271:THR:HG21	1:B:284:VAL:HG21	1.89	0.54
1:C:397:ARG:NH1	2:C:901:ASP:OD1	2.40	0.54
1:A:278:SER:HB2	2:A:901:ASP:O	2.08	0.54
1:C:341:ILE:HG13	1:C:370:VAL:HG21	1.90	0.53
1:A:126:GLN:O	1:A:126:GLN:HG2	2.08	0.53
1:B:30:LEU:HD23	1:B:34:GLY:HA3	1.89	0.53
1:B:44:LYS:N	1:B:45:PRO:HD2	2.23	0.53
1:A:104:ALA:HB2	1:A:320:VAL:HG13	1.90	0.53
1:B:52:ARG:HH12	1:C:136:ASP:HA	1.73	0.53
1:C:44:LYS:N	1:C:45:PRO:HD2	2.22	0.53
1:C:227:GLU:O	1:C:231:VAL:HG23	2.07	0.53
1:C:237:VAL:O	1:C:241:LEU:HB2	2.09	0.53
1:B:397:ARG:NH1	2:B:901:ASP:OD1	2.42	0.53
1:A:237:VAL:O	1:A:241:LEU:HB2	2.08	0.53
1:B:296:GLU:HA	1:B:299:TYR:CE1	2.44	0.53
1:A:271:THR:HG21	1:A:284:VAL:HG21	1.91	0.53
1:A:343:LEU:C	1:A:343:LEU:HD13	2.34	0.53
1:B:130:LEU:HA	1:B:133:ILE:CG2	2.39	0.52
1:A:129:PRO:HG2	1:A:132:HIS:CD2	2.45	0.52
1:B:353:ALA:HB3	1:B:358:ALA:HB2	1.92	0.52
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.45	0.52
1:C:353:ALA:HB3	1:C:358:ALA:HB2	1.90	0.52
1:A:155:ILE:O	1:A:158:ALA:N	2.39	0.52
1:B:193:ALA:CB	1:C:168:LEU:HD11	2.39	0.52
1:C:277:SER:N	1:C:398:THR:HG21	2.24	0.52
1:A:130:LEU:HA	1:A:133:ILE:CG2	2.40	0.52
1:C:296:GLU:HA	1:C:299:TYR:CE1	2.44	0.52
1:C:334:THR:HG23	1:C:335:VAL:O	2.09	0.52
1:A:397:ARG:NH1	2:A:901:ASP:OD1	2.42	0.52
1:B:311:MET:HB3	1:B:401:ASN:CG	2.35	0.52
1:C:261:PHE:CD1	1:C:292:MET:HE1	2.45	0.52
1:C:364:ALA:O	1:C:368:HIS:HB2	2.10	0.52
1:A:129:PRO:HG2	1:A:132:HIS:HD2	1.75	0.52
1:A:130:LEU:HA	1:A:133:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:HD12	1:B:337:GLN:HE21	1.75	0.52
1:A:183:LEU:HD23	1:A:187:ILE:HG13	1.91	0.51
1:C:77:ARG:HG2	1:C:166:THR:HB	1.92	0.51
1:C:311:MET:HB3	1:C:401:ASN:CG	2.35	0.51
1:A:98:THR:O	1:A:102:ILE:HG13	2.11	0.51
1:B:277:SER:H	1:B:398:THR:HG21	1.73	0.51
1:A:205:ALA:N	1:A:206:PRO:HD2	2.26	0.51
1:C:129:PRO:CG	1:C:132:HIS:HD2	2.24	0.51
1:A:17:LEU:HD22	1:A:392:ILE:HD11	1.92	0.51
1:A:190:LEU:O	1:A:191:ALA:C	2.53	0.51
1:B:24:ALA:O	1:B:28:LEU:HD22	2.11	0.51
1:B:216:CYS:O	1:B:224:VAL:HG11	2.10	0.51
1:A:243:ILE:HA	1:A:247:TYR:CD2	2.46	0.51
1:B:74:SER:O	1:B:77:ARG:CB	2.58	0.51
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.46	0.51
1:B:294:ILE:CG2	1:B:299:TYR:HB3	2.40	0.51
1:C:24:ALA:O	1:C:28:LEU:HD22	2.11	0.51
1:A:129:PRO:CG	1:A:132:HIS:HD2	2.23	0.51
1:B:73:ILE:O	1:B:78:LEU:HD22	2.11	0.51
1:B:243:ILE:HA	1:B:247:TYR:HD2	1.76	0.51
1:C:205:ALA:N	1:C:206:PRO:HD2	2.26	0.51
1:A:77:ARG:HG2	1:A:166:THR:HB	1.91	0.50
1:A:183:LEU:HD21	1:A:187:ILE:HD11	1.93	0.50
1:A:197:ILE:O	1:A:201:VAL:HG23	2.10	0.50
1:A:216:CYS:O	1:A:224:VAL:HG11	2.11	0.50
1:A:334:THR:O	1:A:338:GLN:N	2.43	0.50
1:B:117:VAL:C	1:B:119:GLY:H	2.20	0.50
1:B:104:ALA:HB2	1:B:320:VAL:HG13	1.94	0.50
1:C:243:ILE:HA	1:C:247:TYR:HD2	1.75	0.50
1:A:341:ILE:HG13	1:A:370:VAL:HG21	1.94	0.50
1:A:364:ALA:O	1:A:368:HIS:HB2	2.11	0.50
1:A:179:SER:O	1:A:181:GLU:N	2.45	0.50
1:B:239:LEU:HD22	1:B:400:VAL:HG21	1.93	0.50
1:A:155:ILE:CD1	1:A:365:MET:HE3	2.42	0.50
1:A:265:ALA:HA	1:A:288:VAL:HG11	1.94	0.50
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.46	0.50
1:B:269:MET:HB3	1:B:399:MET:HE3	1.94	0.50
1:C:294:ILE:CG2	1:C:299:TYR:HB3	2.41	0.50
1:C:54:LEU:HD12	1:C:54:LEU:N	2.27	0.49
1:C:287:ARG:HG2	1:C:291:GLU:OE2	2.11	0.49
1:C:334:THR:O	1:C:338:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:ASP:O	1:C:398:THR:OG1	2.26	0.49
1:B:8:ILE:HG12	1:B:15:LYS:HE3	1.93	0.49
1:B:77:ARG:HG2	1:B:166:THR:HB	1.94	0.49
1:B:216:CYS:O	1:B:220:GLN:HB2	2.13	0.49
1:C:77:ARG:O	1:C:77:ARG:HD3	2.12	0.49
1:A:243:ILE:HA	1:A:247:TYR:HD2	1.76	0.49
1:B:139:PRO:CB	1:B:153:PRO:HB3	2.39	0.49
1:C:269:MET:HB3	1:C:399:MET:HE3	1.94	0.49
1:A:157:PHE:HA	1:A:160:ILE:CG2	2.38	0.49
1:A:213:ILE:C	1:A:215:TYR:H	2.21	0.49
1:A:227:GLU:O	1:A:231:VAL:HG23	2.11	0.49
1:A:294:ILE:CG2	1:A:299:TYR:HB3	2.43	0.49
1:C:228:LEU:HD22	1:C:389:ILE:CG2	2.42	0.49
1:A:52:ARG:NH1	1:B:136:ASP:HA	2.28	0.49
1:A:185:ASP:O	1:A:188:ASN:O	2.31	0.49
1:B:190:LEU:O	1:B:191:ALA:C	2.55	0.49
1:B:203:GLN:HA	1:B:203:GLN:NE2	2.24	0.49
1:C:278:SER:HB2	2:C:901:ASP:O	2.12	0.49
1:C:376:ASP:O	1:C:379:VAL:N	2.46	0.49
1:A:74:SER:O	1:A:77:ARG:CB	2.60	0.49
1:A:261:PHE:CD1	1:A:292:MET:HE1	2.47	0.49
1:A:269:MET:HB3	1:A:399:MET:HE3	1.95	0.49
1:A:73:ILE:O	1:A:78:LEU:HD22	2.13	0.49
1:C:183:LEU:HD23	1:C:187:ILE:HG13	1.94	0.49
1:A:203:GLN:HA	1:A:203:GLN:NE2	2.24	0.48
1:B:155:ILE:O	1:B:159:ILE:HD12	2.13	0.48
1:C:82:GLY:HA2	1:C:85:ILE:HG22	1.94	0.48
1:A:117:VAL:C	1:A:119:GLY:H	2.22	0.48
1:A:355:VAL:HG13	1:A:356:PRO:N	2.28	0.48
1:B:135:LEU:C	1:B:137:ILE:H	2.21	0.48
1:C:74:SER:OG	1:C:166:THR:HG21	2.13	0.48
1:A:134:LEU:O	1:A:137:ILE:HG12	2.12	0.48
1:C:155:ILE:O	1:C:156:PHE:C	2.57	0.48
1:C:239:LEU:HD22	1:C:400:VAL:CG2	2.39	0.48
1:A:146:LEU:HD12	1:A:146:LEU:H	1.79	0.48
1:B:20:LEU:HA	1:B:213:ILE:HD11	1.95	0.48
1:C:277:SER:H	1:C:398:THR:HG21	1.79	0.48
1:A:334:THR:HG23	1:A:335:VAL:O	2.14	0.48
1:B:107:PHE:C	1:B:109:PRO:HD3	2.39	0.48
1:B:237:VAL:O	1:B:241:LEU:HB2	2.13	0.48
1:C:187:ILE:O	1:C:190:LEU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:LEU:O	1:C:191:ALA:C	2.56	0.48
1:B:325:ILE:HG13	1:B:367:LEU:HD21	1.95	0.48
1:C:213:ILE:C	1:C:215:TYR:H	2.21	0.48
1:C:216:CYS:O	1:C:224:VAL:HG11	2.14	0.48
1:A:216:CYS:O	1:A:220:GLN:HB2	2.14	0.47
1:C:341:ILE:CG1	1:C:370:VAL:HG21	2.44	0.47
1:B:52:ARG:NH1	1:C:136:ASP:HA	2.30	0.47
1:B:98:THR:O	1:B:102:ILE:HG13	2.15	0.47
1:B:131:VAL:O	1:B:135:LEU:HB2	2.14	0.47
1:B:146:LEU:N	1:B:146:LEU:HD12	2.29	0.47
1:C:129:PRO:HG2	1:C:132:HIS:HD2	1.79	0.47
1:A:8:ILE:C	1:A:9:GLU:HG3	2.38	0.47
1:A:107:PHE:C	1:A:109:PRO:HD3	2.38	0.47
1:C:164:ALA:O	1:C:165:ILE:C	2.55	0.47
1:B:8:ILE:C	1:B:9:GLU:HG3	2.39	0.47
1:B:155:ILE:O	1:B:156:PHE:C	2.58	0.47
1:C:343:LEU:HD13	1:C:343:LEU:O	2.14	0.47
1:A:139:PRO:HB3	1:A:153:PRO:CB	2.39	0.47
1:A:165:ILE:HG21	1:A:184:LEU:HD13	1.96	0.47
1:B:344:THR:HG21	1:B:369:SER:OG	2.15	0.47
1:C:74:SER:O	1:C:77:ARG:CB	2.63	0.47
1:A:353:ALA:HB3	1:A:358:ALA:HB2	1.96	0.47
1:B:334:THR:O	1:B:338:GLN:N	2.48	0.47
1:C:196:LYS:HA	1:C:196:LYS:HD3	1.67	0.47
1:A:8:ILE:HG12	1:A:15:LYS:HE3	1.97	0.47
1:A:322:THR:HG21	1:A:341:ILE:HG12	1.95	0.47
1:A:352:THR:HA	1:A:362:MET:HG3	1.97	0.47
1:C:157:PHE:HA	1:C:160:ILE:CG2	2.43	0.47
1:C:276:ARG:HG2	1:C:395:MET:HG2	1.96	0.47
1:A:187:ILE:O	1:A:190:LEU:HB3	2.15	0.47
1:B:97:VAL:HG13	1:B:342:VAL:HG22	1.96	0.47
1:C:107:PHE:C	1:C:109:PRO:HD3	2.37	0.47
1:A:277:SER:N	1:A:398:THR:HG21	2.30	0.46
1:A:311:MET:HE2	1:A:401:ASN:ND2	2.30	0.46
1:B:165:ILE:CG2	1:B:184:LEU:HB2	2.41	0.46
1:A:20:LEU:HA	1:A:213:ILE:HD11	1.98	0.46
1:A:207:ILE:O	1:A:210:PHE:HB3	2.16	0.46
1:B:146:LEU:HD12	1:B:146:LEU:H	1.80	0.46
1:A:152:LEU:O	1:A:153:PRO:C	2.58	0.46
1:A:196:LYS:HD3	1:A:196:LYS:HA	1.70	0.46
1:C:129:PRO:HG2	1:C:132:HIS:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:LEU:HD12	1:C:361:ILE:CD1	2.45	0.46
1:C:58:VAL:O	1:C:62:VAL:HG23	2.15	0.46
1:C:132:HIS:O	1:C:136:ASP:HB2	2.16	0.46
1:C:271:THR:HB	1:C:281:THR:HG23	1.96	0.46
1:A:146:LEU:HD23	1:B:143:PHE:CE2	2.50	0.46
1:B:64:ALA:HB2	1:B:190:LEU:HD23	1.96	0.46
1:A:311:MET:HB3	1:A:401:ASN:CG	2.41	0.46
1:B:355:VAL:HG13	1:B:356:PRO:N	2.29	0.46
1:C:104:ALA:HB2	1:C:320:VAL:HG13	1.97	0.46
1:C:335:VAL:CA	1:C:338:GLN:HB2	2.31	0.46
1:B:110:GLY:O	1:B:111:ALA:C	2.58	0.46
1:B:128:PRO:HB2	1:B:129:PRO:CD	2.36	0.46
1:C:251:LEU:HD22	1:C:256:ILE:CG2	2.46	0.46
1:B:77:ARG:O	1:B:77:ARG:HD3	2.15	0.46
1:B:178:LYS:O	1:B:178:LYS:HD3	2.16	0.46
1:C:139:PRO:CB	1:C:153:PRO:HB3	2.39	0.46
1:A:164:ALA:O	1:A:165:ILE:C	2.57	0.46
1:C:295:SER:HB3	1:C:298:ILE:HD13	1.98	0.46
1:C:352:THR:HA	1:C:362:MET:HG3	1.98	0.46
1:A:73:ILE:O	1:A:74:SER:C	2.58	0.46
1:A:155:ILE:HD11	1:A:365:MET:HE3	1.98	0.46
1:A:24:ALA:O	1:A:28:LEU:HD22	2.17	0.45
1:B:17:LEU:HD22	1:B:392:ILE:HD11	1.98	0.45
1:B:113:ILE:O	1:B:113:ILE:HG23	2.16	0.45
1:C:8:ILE:HG12	1:C:15:LYS:HE3	1.97	0.45
1:C:282:LEU:H	1:C:283:PRO:CD	2.30	0.45
1:B:183:LEU:HD23	1:B:183:LEU:C	2.42	0.45
1:A:341:ILE:CG1	1:A:370:VAL:HG21	2.46	0.45
1:B:376:ASP:O	1:B:379:VAL:N	2.50	0.45
1:C:207:ILE:O	1:C:210:PHE:HB3	2.17	0.45
1:C:359:GLY:H	2:C:901:ASP:CG	2.25	0.45
1:A:74:SER:OG	1:A:166:THR:HG21	2.17	0.45
1:B:73:ILE:O	1:B:74:SER:C	2.59	0.45
1:B:215:TYR:HA	1:B:218:ALA:HB3	1.97	0.45
1:B:341:ILE:CG1	1:B:370:VAL:HG21	2.47	0.45
1:A:295:SER:HB3	1:A:298:ILE:HD13	1.98	0.45
1:A:344:THR:HG21	1:A:369:SER:OG	2.17	0.45
1:C:134:LEU:O	1:C:137:ILE:HG12	2.17	0.45
1:A:179:SER:O	1:A:180:ALA:C	2.60	0.45
1:B:10:TYR:H	1:B:15:LYS:HZ2	1.64	0.45
1:C:113:ILE:HG23	1:C:113:ILE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:CD2	1:C:187:ILE:HD11	2.46	0.45
1:A:110:GLY:O	1:A:111:ALA:C	2.59	0.45
1:A:132:HIS:O	1:A:136:ASP:HB2	2.17	0.45
1:A:333:LEU:HD11	1:A:370:VAL:HG11	1.99	0.45
1:B:265:ALA:HA	1:B:288:VAL:HG11	1.97	0.45
1:A:57:LEU:HD12	1:A:361:ILE:CD1	2.47	0.44
1:B:352:THR:HA	1:B:362:MET:HG3	1.98	0.44
1:C:161:LEU:O	1:C:165:ILE:HG12	2.17	0.44
1:C:195:TYR:O	1:C:198:VAL:HB	2.17	0.44
1:A:146:LEU:HD12	1:A:146:LEU:N	2.32	0.44
1:A:259:ILE:H	1:A:259:ILE:HG13	1.58	0.44
1:B:213:ILE:C	1:B:215:TYR:H	2.23	0.44
1:C:103:MET:CE	1:C:237:VAL:HG23	2.44	0.44
1:C:376:ASP:HA	1:C:377:PRO:HD2	1.75	0.44
1:B:164:ALA:O	1:B:165:ILE:C	2.59	0.44
1:B:196:LYS:HA	1:B:196:LYS:HD3	1.61	0.44
1:B:318:GLN:HB3	1:B:366:VAL:HG11	1.99	0.44
1:B:157:PHE:HA	1:B:160:ILE:CG2	2.42	0.44
1:A:156:PHE:O	1:A:160:ILE:HG22	2.17	0.44
1:C:183:LEU:HD23	1:C:183:LEU:C	2.43	0.44
1:C:336:GLY:C	1:C:338:GLN:N	2.75	0.44
1:B:282:LEU:HB3	1:B:283:PRO:HD3	1.99	0.44
1:C:117:VAL:C	1:C:119:GLY:H	2.26	0.44
1:C:135:LEU:C	1:C:137:ILE:H	2.26	0.44
1:A:52:ARG:HH12	1:B:136:ASP:HA	1.82	0.44
1:A:127:ALA:HA	1:A:128:PRO:HD3	1.89	0.44
1:C:8:ILE:C	1:C:9:GLU:HG3	2.43	0.44
1:B:295:SER:HB3	1:B:298:ILE:HD13	1.99	0.43
1:C:146:LEU:O	1:C:147:ALA:C	2.60	0.43
1:C:54:LEU:O	1:C:55:LYS:C	2.61	0.43
1:C:110:GLY:O	1:C:111:ALA:C	2.61	0.43
1:A:109:PRO:O	1:A:324:PHE:HA	2.18	0.43
1:A:183:LEU:HD23	1:A:183:LEU:C	2.44	0.43
1:A:272:ALA:HB1	1:A:399:MET:HA	1.99	0.43
1:B:282:LEU:H	1:B:283:PRO:CD	2.31	0.43
1:B:342:VAL:HG12	1:B:343:LEU:N	2.33	0.43
1:C:97:VAL:O	1:C:98:THR:C	2.62	0.43
1:A:246:VAL:O	1:A:250:LEU:HG	2.18	0.43
1:B:74:SER:OG	1:B:166:THR:HG21	2.18	0.43
1:B:153:PRO:O	1:B:154:THR:C	2.61	0.43
1:A:195:TYR:O	1:A:198:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LEU:HD21	1:A:341:ILE:HD11	1.99	0.43
1:B:17:LEU:CD2	1:B:392:ILE:HD11	2.49	0.43
1:C:20:LEU:HA	1:C:213:ILE:HD11	2.00	0.43
1:C:89:TYR:CD1	1:C:310:ASN:CG	2.97	0.43
1:A:168:LEU:HD11	1:C:193:ALA:CB	2.48	0.43
1:B:165:ILE:HG21	1:B:184:LEU:HD13	1.99	0.43
1:C:17:LEU:HD22	1:C:392:ILE:HD11	2.00	0.43
1:C:268:ALA:O	1:C:281:THR:HG21	2.19	0.43
1:A:333:LEU:HD12	1:A:337:GLN:HE21	1.84	0.43
1:B:197:ILE:O	1:B:201:VAL:HG23	2.19	0.43
1:A:135:LEU:C	1:A:137:ILE:H	2.27	0.43
1:A:325:ILE:HG13	1:A:367:LEU:HD21	2.00	0.43
1:A:334:THR:HG22	1:A:337:GLN:CD	2.43	0.43
1:B:44:LYS:HD2	1:B:215:TYR:CZ	2.53	0.43
1:B:179:SER:O	1:B:180:ALA:C	2.61	0.43
1:B:187:ILE:O	1:B:190:LEU:HB3	2.19	0.43
1:B:311:MET:HB3	1:B:401:ASN:OD1	2.19	0.43
1:A:276:ARG:HG2	1:A:395:MET:HG2	2.01	0.42
1:B:246:VAL:O	1:B:250:LEU:HG	2.19	0.42
1:B:294:ILE:HG22	1:B:299:TYR:HB3	2.01	0.42
1:B:373:PRO:C	1:B:375:THR:H	2.27	0.42
1:C:131:VAL:O	1:C:135:LEU:HB2	2.19	0.42
1:C:334:THR:HG22	1:C:337:GLN:CD	2.41	0.42
1:B:54:LEU:HD12	1:B:54:LEU:N	2.33	0.42
1:C:101:ILE:O	1:C:105:ARG:HG2	2.19	0.42
1:A:376:ASP:HA	1:A:377:PRO:HD2	1.72	0.42
1:C:294:ILE:HG22	1:C:299:TYR:HB3	2.00	0.42
1:B:57:LEU:O	1:B:61:ILE:HG12	2.19	0.42
1:B:294:ILE:HG21	1:B:299:TYR:HB3	2.00	0.42
1:A:165:ILE:CG2	1:A:184:LEU:HB2	2.50	0.42
1:B:13:LEU:HB2	1:B:276:ARG:HE	1.85	0.42
1:B:271:THR:HB	1:B:281:THR:HG23	2.01	0.42
1:C:376:ASP:O	1:C:377:PRO:C	2.62	0.42
1:A:103:MET:HG3	1:A:238:GLY:CA	2.48	0.42
1:B:123:GLN:OE1	1:B:123:GLN:CA	2.66	0.42
1:C:397:ARG:HH11	2:C:901:ASP:CG	2.28	0.42
1:B:53:LEU:HD23	1:B:53:LEU:HA	1.90	0.42
1:C:90:LEU:HD11	1:C:350:ILE:HD11	2.02	0.42
1:C:143:PHE:O	1:C:144:GLY:C	2.63	0.42
1:C:401:ASN:ND2	2:C:901:ASP:HA	2.34	0.42
1:B:66:LEU:HD23	1:B:66:LEU:HA	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:LEU:HD21	1:B:341:ILE:HD11	2.02	0.42
1:C:39:VAL:HG13	1:C:43:VAL:HG12	2.01	0.42
1:A:294:ILE:HG22	1:A:299:TYR:HB3	2.01	0.42
1:B:13:LEU:CD2	1:B:276:ARG:HD3	2.47	0.42
1:B:155:ILE:CD1	1:B:365:MET:HE3	2.50	0.42
1:B:334:THR:HG22	1:B:337:GLN:CD	2.45	0.42
1:C:336:GLY:O	1:C:339:LEU:N	2.52	0.42
1:A:20:LEU:HD12	1:A:213:ILE:HG12	2.02	0.42
1:B:50:PHE:O	1:B:51:VAL:C	2.60	0.42
1:B:128:PRO:CB	1:B:129:PRO:CD	2.93	0.41
1:C:352:THR:HG23	1:C:358:ALA:HB1	2.02	0.41
1:A:32:HIS:HB3	1:A:33:TYR:H	1.65	0.41
1:B:58:VAL:O	1:B:62:VAL:HG23	2.20	0.41
1:C:228:LEU:HD22	1:C:389:ILE:HG21	2.01	0.41
1:B:343:LEU:HD13	1:B:343:LEU:O	2.20	0.41
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.83	0.41
1:B:58:VAL:HG21	1:B:364:ALA:HB3	2.03	0.41
1:C:103:MET:HG3	1:C:238:GLY:CA	2.51	0.41
1:A:343:LEU:HD13	1:A:343:LEU:O	2.20	0.41
1:A:27:GLY:O	1:A:28:LEU:C	2.64	0.41
1:A:152:LEU:O	1:A:155:ILE:HB	2.21	0.41
1:A:282:LEU:HB3	1:A:283:PRO:HD3	2.02	0.41
1:C:27:GLY:O	1:C:28:LEU:C	2.63	0.41
1:C:213:ILE:HG22	1:C:216:CYS:HB2	2.03	0.41
1:C:305:LEU:O	1:C:305:LEU:HG	2.20	0.41
1:A:77:ARG:O	1:A:77:ARG:HD3	2.19	0.41
1:A:228:LEU:HD22	1:A:389:ILE:CG2	2.51	0.41
1:C:21:ILE:O	1:C:25:ILE:HD13	2.21	0.41
1:C:130:LEU:HD12	1:C:133:ILE:HG23	2.02	0.41
1:C:294:ILE:HG21	1:C:299:TYR:HB3	2.02	0.41
1:B:192:GLU:HG2	1:C:176:VAL:HG13	2.02	0.41
1:B:376:ASP:O	1:B:377:PRO:C	2.64	0.41
1:A:157:PHE:CA	1:A:160:ILE:HG22	2.44	0.41
1:A:277:SER:H	1:A:398:THR:HG21	1.86	0.41
1:A:318:GLN:HB3	1:A:366:VAL:HG11	2.02	0.41
1:B:391:ALA:O	1:B:395:MET:HG3	2.21	0.41
1:C:156:PHE:C	1:C:156:PHE:CD2	2.99	0.41
1:A:17:LEU:CD2	1:A:392:ILE:HD11	2.50	0.40
1:B:190:LEU:HA	1:B:190:LEU:HD12	1.89	0.40
1:B:362:MET:O	1:B:365:MET:HB3	2.21	0.40
1:C:128:PRO:HB2	1:C:129:PRO:CD	2.39	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:THR:HG21	1:C:369:SER:OG	2.21	0.40
1:A:39:VAL:HG13	1:A:43:VAL:HG12	2.04	0.40
1:A:303:LEU:HD13	1:A:303:LEU:HA	1.94	0.40
1:B:177:ARG:HH11	1:B:177:ARG:HD2	1.77	0.40
1:B:325:ILE:HG23	1:B:382:ALA:HB3	2.03	0.40
1:C:215:TYR:HA	1:C:218:ALA:HB3	2.03	0.40
1:A:131:VAL:O	1:A:135:LEU:HB2	2.22	0.40
1:B:222:VAL:O	1:B:225:VAL:HG23	2.21	0.40
1:A:137:ILE:HA	1:A:153:PRO:HG3	2.04	0.40
1:B:155:ILE:HG23	1:B:159:ILE:CD1	2.52	0.40
1:C:333:LEU:HD12	1:C:337:GLN:HE21	1.86	0.40
1:C:355:VAL:HG13	1:C:356:PRO:N	2.36	0.40
1:A:155:ILE:O	1:A:156:PHE:C	2.64	0.40
1:A:215:TYR:HA	1:A:218:ALA:HB3	2.02	0.40
1:C:24:ALA:O	1:C:28:LEU:CD2	2.69	0.40
1:C:90:LEU:CD1	1:C:350:ILE:HD11	2.51	0.40
1:C:155:ILE:O	1:C:159:ILE:HD12	2.22	0.40
1:C:257:ASP:HA	1:C:258:PRO:HD3	1.82	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	408/422 (97%)	329 (81%)	66 (16%)	13 (3%)	3	24
1	B	409/422 (97%)	328 (80%)	67 (16%)	14 (3%)	3	23
1	C	408/422 (97%)	322 (79%)	70 (17%)	16 (4%)	2	20
All	All	1225/1266 (97%)	979 (80%)	203 (17%)	43 (4%)	3	23

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	PRO
1	B	356	PRO
1	C	356	PRO
1	B	7	TYR
1	B	310	ASN
1	B	377	PRO
1	C	310	ASN
1	A	136	ASP
1	A	180	ALA
1	A	282	LEU
1	A	310	ASN
1	A	377	PRO
1	B	282	LEU
1	B	394	ASP
1	C	108	ASN
1	C	154	THR
1	C	282	LEU
1	C	377	PRO
1	C	397	ARG
1	A	36	ALA
1	A	394	ASP
1	B	36	ALA
1	B	55	LYS
1	B	74	SER
1	C	36	ALA
1	C	292	MET
1	C	368	HIS
1	A	74	SER
1	A	108	ASN
1	B	136	ASP
1	B	154	THR
1	C	11	PRO
1	C	33	TYR
1	C	74	SER
1	C	136	ASP
1	A	11	PRO
1	A	397	ARG
1	B	11	PRO
1	B	108	ASN
1	A	255	GLY
1	B	255	GLY
1	C	255	GLY
1	C	355	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	319/329 (97%)	264 (83%)	55 (17%)	2	13
1	B	319/329 (97%)	258 (81%)	61 (19%)	1	9
1	C	319/329 (97%)	260 (82%)	59 (18%)	1	11
All	All	957/987 (97%)	782 (82%)	175 (18%)	2	11

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	9	GLU
1	A	12	VAL
1	A	13	LEU
1	A	14	GLN
1	A	18	ILE
1	A	22	LEU
1	A	28	LEU
1	A	30	LEU
1	A	32	HIS
1	A	35	TYR
1	A	37	HIS
1	A	43	VAL
1	A	44	LYS
1	A	77	ARG
1	A	78	LEU
1	A	90	LEU
1	A	97	VAL
1	A	101	ILE
1	A	102	ILE
1	A	108	ASN
1	A	125	HIS
1	A	126	GLN
1	A	135	LEU
1	A	136	ASP
1	A	140	THR

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Mol	Chain	Res	Type
1	A	148	ASN
1	A	153	PRO
1	A	155	ILE
1	A	174	GLU
1	A	178	LYS
1	A	181	GLU
1	A	196	LYS
1	A	213	ILE
1	A	249	VAL
1	A	250	LEU
1	A	259	ILE
1	A	267	ASP
1	A	270	LEU
1	A	278	SER
1	A	284	VAL
1	A	298	ILE
1	A	300	SER
1	A	303	LEU
1	A	329	LEU
1	A	342	VAL
1	A	346	VAL
1	A	350	ILE
1	A	355	VAL
1	A	368	HIS
1	A	372	LEU
1	A	387	LEU
1	A	392	ILE
1	A	402	VAL
1	A	411	ILE
1	B	8	ILE
1	B	9	GLU
1	B	12	VAL
1	B	13	LEU
1	B	14	GLN
1	B	18	ILE
1	B	22	LEU
1	B	28	LEU
1	B	30	LEU
1	B	32	HIS
1	B	35	TYR
1	B	37	HIS
1	B	43	VAL

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Mol	Chain	Res	Type
1	B	44	LYS
1	B	57	LEU
1	B	77	ARG
1	B	78	LEU
1	B	90	LEU
1	B	97	VAL
1	B	101	ILE
1	B	102	ILE
1	B	108	ASN
1	B	125	HIS
1	B	126	GLN
1	B	135	LEU
1	B	136	ASP
1	B	140	THR
1	B	148	ASN
1	B	150	GLN
1	B	153	PRO
1	B	155	ILE
1	B	174	GLU
1	B	178	LYS
1	B	181	GLU
1	B	187	ILE
1	B	196	LYS
1	B	203	GLN
1	B	213	ILE
1	B	249	VAL
1	B	250	LEU
1	B	259	ILE
1	B	267	ASP
1	B	270	LEU
1	B	278	SER
1	B	284	VAL
1	B	296	GLU
1	B	298	ILE
1	B	300	SER
1	B	303	LEU
1	B	329	LEU
1	B	342	VAL
1	B	343	LEU
1	B	346	VAL
1	B	350	ILE
1	B	355	VAL

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Mol	Chain	Res	Type
1	B	368	HIS
1	B	372	LEU
1	B	387	LEU
1	B	392	ILE
1	B	402	VAL
1	B	411	ILE
1	C	8	ILE
1	C	9	GLU
1	C	12	VAL
1	C	13	LEU
1	C	14	GLN
1	C	18	ILE
1	C	22	LEU
1	C	28	LEU
1	C	32	HIS
1	C	35	TYR
1	C	37	HIS
1	C	43	VAL
1	C	44	LYS
1	C	57	LEU
1	C	61	ILE
1	C	77	ARG
1	C	78	LEU
1	C	90	LEU
1	C	97	VAL
1	C	101	ILE
1	C	108	ASN
1	C	125	HIS
1	C	126	GLN
1	C	135	LEU
1	C	136	ASP
1	C	140	THR
1	C	148	ASN
1	C	150	GLN
1	C	153	PRO
1	C	155	ILE
1	C	174	GLU
1	C	178	LYS
1	C	181	GLU
1	C	196	LYS
1	C	213	ILE
1	C	249	VAL

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Mol	Chain	Res	Type
1	C	250	LEU
1	C	259	ILE
1	C	267	ASP
1	C	270	LEU
1	C	278	SER
1	C	281	THR
1	C	284	VAL
1	C	298	ILE
1	C	300	SER
1	C	303	LEU
1	C	329	LEU
1	C	342	VAL
1	C	343	LEU
1	C	346	VAL
1	C	350	ILE
1	C	355	VAL
1	C	368	HIS
1	C	372	LEU
1	C	387	LEU
1	C	392	ILE
1	C	402	VAL
1	C	411	ILE
1	C	416	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	132	HIS
1	B	108	ASN
1	B	132	HIS
1	C	108	ASN
1	C	132	HIS

5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ASP	A	901	-	7,8,8	1.20	1 (14%)	6,10,10	1.17	0
2	ASP	B	901	-	7,8,8	1.30	1 (14%)	6,10,10	1.45	1 (16%)
2	ASP	C	901	-	7,8,8	1.18	1 (14%)	6,10,10	1.22	1 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	A	901	-	-	4/8/8/8	-
2	ASP	B	901	-	-	5/8/8/8	-
2	ASP	C	901	-	-	5/8/8/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	ASP	OXT-C	-2.55	1.22	1.30
2	A	901	ASP	OXT-C	-2.30	1.23	1.30
2	C	901	ASP	OXT-C	-2.30	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	ASP	OXT-C-O	-2.81	117.70	124.08
2	C	901	ASP	OXT-C-O	-2.12	119.28	124.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	ASP	O-C-CA-N
2	A	901	ASP	OXT-C-CA-N
2	B	901	ASP	OXT-C-CA-N
2	C	901	ASP	OXT-C-CA-N
2	A	901	ASP	CA-CB-CG-OD1
2	A	901	ASP	CA-CB-CG-OD2
2	B	901	ASP	CA-CB-CG-OD1
2	B	901	ASP	CA-CB-CG-OD2
2	C	901	ASP	CA-CB-CG-OD1
2	C	901	ASP	CA-CB-CG-OD2
2	B	901	ASP	N-CA-CB-CG
2	C	901	ASP	N-CA-CB-CG
2	A	901	ASP	O-C-CA-N
2	B	901	ASP	O-C-CA-N

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	ASP	2	0
2	B	901	ASP	2	0
2	C	901	ASP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	410/422 (97%)	0.21	26 (6%)	26 21	164, 286, 403, 467	0
1	B	411/422 (97%)	-0.00	15 (3%)	46 32	135, 215, 334, 372	0
1	C	410/422 (97%)	-0.03	13 (3%)	50 35	132, 219, 316, 424	0
All	All	1231/1266 (97%)	0.06	54 (4%)	39 28	132, 237, 359, 467	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	355	VAL	5.1
1	A	382	ALA	4.7
1	A	407	THR	4.7
1	A	385	CYS	4.2
1	A	147	ALA	4.2
1	A	128	PRO	4.1
1	C	12	VAL	3.9
1	A	150	GLN	3.9
1	B	127	ALA	3.8
1	B	312	ASP	3.8
1	A	148	ASN	3.7
1	A	117	VAL	3.7
1	B	313	GLY	3.6
1	A	389	ILE	3.5
1	A	247	TYR	3.4
1	B	333	LEU	3.4
1	A	206	PRO	3.4
1	A	313	GLY	3.3
1	A	115	LEU	3.2
1	C	119	GLY	3.2
1	A	353	ALA	3.2
1	A	261	PHE	3.1
1	A	381	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	222	VAL	3.1
1	B	42	TYR	3.1
1	C	269	MET	3.0
1	A	29	ILE	2.9
1	C	192	GLU	2.9
1	A	314	THR	2.9
1	C	10	TYR	2.9
1	A	403	THR	2.8
1	A	354	GLY	2.8
1	B	131	VAL	2.8
1	A	199	ASN	2.7
1	B	167	TYR	2.6
1	B	387	LEU	2.6
1	C	261	PHE	2.6
1	B	279	SER	2.6
1	C	58	VAL	2.6
1	C	189	GLY	2.6
1	B	353	ALA	2.5
1	A	149	GLY	2.5
1	C	186	ALA	2.4
1	B	81	VAL	2.4
1	C	9	GLU	2.4
1	C	203	GLN	2.4
1	A	77	ARG	2.4
1	B	128	PRO	2.3
1	B	285	THR	2.2
1	B	147	ALA	2.2
1	A	384	ALA	2.1
1	A	386	ILE	2.1
1	C	81	VAL	2.1
1	C	127	ALA	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](#)

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
3	NA	C	902	1/1	0.88	0.14	183,183,183,183	0
3	NA	C	903	1/1	0.91	0.06	178,178,178,178	0
3	NA	B	902	1/1	0.92	0.14	194,194,194,194	0
3	NA	A	903	1/1	0.94	0.05	258,258,258,258	0
2	ASP	A	901	9/9	0.94	0.04	253,255,264,269	0
2	ASP	C	901	9/9	0.94	0.06	178,184,191,191	0
3	NA	A	902	1/1	0.94	0.04	275,275,275,275	0
4	HG	A	904	1/1	0.94	0.23	312,312,312,312	1
3	NA	B	903	1/1	0.96	0.07	184,184,184,184	0
2	ASP	B	901	9/9	0.97	0.04	173,178,187,190	0
4	HG	B	904	1/1	0.97	0.05	248,248,248,248	1
4	HG	C	904	1/1	0.98	0.08	284,284,284,284	1

6.5 Other polymers [i](#)

There are no such residues in this entry.