



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:03 AM UTC

PDB ID : 8EE1 / pdb_00008ee1
Title : KS-AT didomain from module 2 of the 6-deoxyerythronolide B synthase in complex with antibody fragment AA5
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Deposited on : 2022-09-06
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

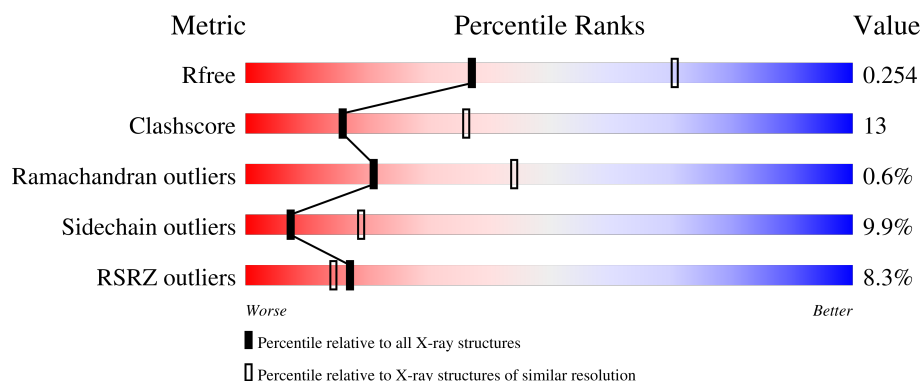
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	932	
1	D	932	
2	B	249	
2	G	249	
3	C	231	

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Mol	Chain	Length	Quality of chain
3	H	231	12% 42% 18% • 38%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 17757 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 6-deoxyerythronolide B synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	0
			6094	3800	1100	1173	21			
1	D	846	Total	C	N	O	S	0	0	0
			6105	3802	1094	1188	21			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q5UNP6
A	2	ALA	-	expression tag	UNP Q5UNP6
A	3	SER	-	expression tag	UNP Q5UNP6
A	4	THR	-	expression tag	UNP Q5UNP6
A	5	ASP	-	expression tag	UNP Q5UNP6
A	6	SER	-	expression tag	UNP Q5UNP6
A	7	GLU	-	expression tag	UNP Q5UNP6
A	8	LYS	-	expression tag	UNP Q5UNP6
A	9	VAL	-	expression tag	UNP Q5UNP6
A	10	ALA	-	expression tag	UNP Q5UNP6
A	11	GLU	-	expression tag	UNP Q5UNP6
A	12	TYR	-	expression tag	UNP Q5UNP6
A	13	LEU	-	expression tag	UNP Q5UNP6
A	14	ARG	-	expression tag	UNP Q5UNP6
A	15	ARG	-	expression tag	UNP Q5UNP6
A	16	ALA	-	expression tag	UNP Q5UNP6
A	17	THR	-	expression tag	UNP Q5UNP6
A	18	LEU	-	expression tag	UNP Q5UNP6
A	19	ASP	-	expression tag	UNP Q5UNP6
A	20	LEU	-	expression tag	UNP Q5UNP6
A	21	ARG	-	expression tag	UNP Q5UNP6
A	22	ALA	-	expression tag	UNP Q5UNP6
A	23	ALA	-	expression tag	UNP Q5UNP6
A	24	ARG	-	expression tag	UNP Q5UNP6
A	25	GLN	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6
A	28	ARG	-	expression tag	UNP Q5UNP6
A	29	GLU	-	expression tag	UNP Q5UNP6
A	30	LEU	-	expression tag	UNP Q5UNP6
A	31	GLU	-	expression tag	UNP Q5UNP6
A	32	SER	-	expression tag	UNP Q5UNP6
A	922	ALA	-	expression tag	UNP Q5UNP6
A	923	ALA	-	expression tag	UNP Q5UNP6
A	924	ALA	-	expression tag	UNP Q5UNP6
A	925	LEU	-	expression tag	UNP Q5UNP6
A	926	GLU	-	expression tag	UNP Q5UNP6
A	927	HIS	-	expression tag	UNP Q5UNP6
A	928	HIS	-	expression tag	UNP Q5UNP6
A	929	HIS	-	expression tag	UNP Q5UNP6
A	930	HIS	-	expression tag	UNP Q5UNP6
A	931	HIS	-	expression tag	UNP Q5UNP6
A	932	HIS	-	expression tag	UNP Q5UNP6
D	1	MET	-	expression tag	UNP Q5UNP6
D	2	ALA	-	expression tag	UNP Q5UNP6
D	3	SER	-	expression tag	UNP Q5UNP6
D	4	THR	-	expression tag	UNP Q5UNP6
D	5	ASP	-	expression tag	UNP Q5UNP6
D	6	SER	-	expression tag	UNP Q5UNP6
D	7	GLU	-	expression tag	UNP Q5UNP6
D	8	LYS	-	expression tag	UNP Q5UNP6
D	9	VAL	-	expression tag	UNP Q5UNP6
D	10	ALA	-	expression tag	UNP Q5UNP6
D	11	GLU	-	expression tag	UNP Q5UNP6
D	12	TYR	-	expression tag	UNP Q5UNP6
D	13	LEU	-	expression tag	UNP Q5UNP6
D	14	ARG	-	expression tag	UNP Q5UNP6
D	15	ARG	-	expression tag	UNP Q5UNP6
D	16	ALA	-	expression tag	UNP Q5UNP6
D	17	THR	-	expression tag	UNP Q5UNP6
D	18	LEU	-	expression tag	UNP Q5UNP6
D	19	ASP	-	expression tag	UNP Q5UNP6
D	20	LEU	-	expression tag	UNP Q5UNP6
D	21	ARG	-	expression tag	UNP Q5UNP6
D	22	ALA	-	expression tag	UNP Q5UNP6
D	23	ALA	-	expression tag	UNP Q5UNP6
D	24	ARG	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	GLN	-	expression tag	UNP Q5UNP6
D	26	ARG	-	expression tag	UNP Q5UNP6
D	27	ILE	-	expression tag	UNP Q5UNP6
D	28	ARG	-	expression tag	UNP Q5UNP6
D	29	GLU	-	expression tag	UNP Q5UNP6
D	30	LEU	-	expression tag	UNP Q5UNP6
D	31	GLU	-	expression tag	UNP Q5UNP6
D	32	SER	-	expression tag	UNP Q5UNP6
D	922	ALA	-	expression tag	UNP Q5UNP6
D	923	ALA	-	expression tag	UNP Q5UNP6
D	924	ALA	-	expression tag	UNP Q5UNP6
D	925	LEU	-	expression tag	UNP Q5UNP6
D	926	GLU	-	expression tag	UNP Q5UNP6
D	927	HIS	-	expression tag	UNP Q5UNP6
D	928	HIS	-	expression tag	UNP Q5UNP6
D	929	HIS	-	expression tag	UNP Q5UNP6
D	930	HIS	-	expression tag	UNP Q5UNP6
D	931	HIS	-	expression tag	UNP Q5UNP6
D	932	HIS	-	expression tag	UNP Q5UNP6

- Molecule 2 is a protein called AA5 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1583	1005	261	312	5			
2	G	165	Total	C	N	O	S	0	0	0
			1260	800	213	244	3			

- Molecule 3 is a protein called AA5 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1562	973	265	319	5			
3	H	144	Total	C	N	O	S	0	0	0
			1079	672	180	223	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total	O	0	0
			40	40		

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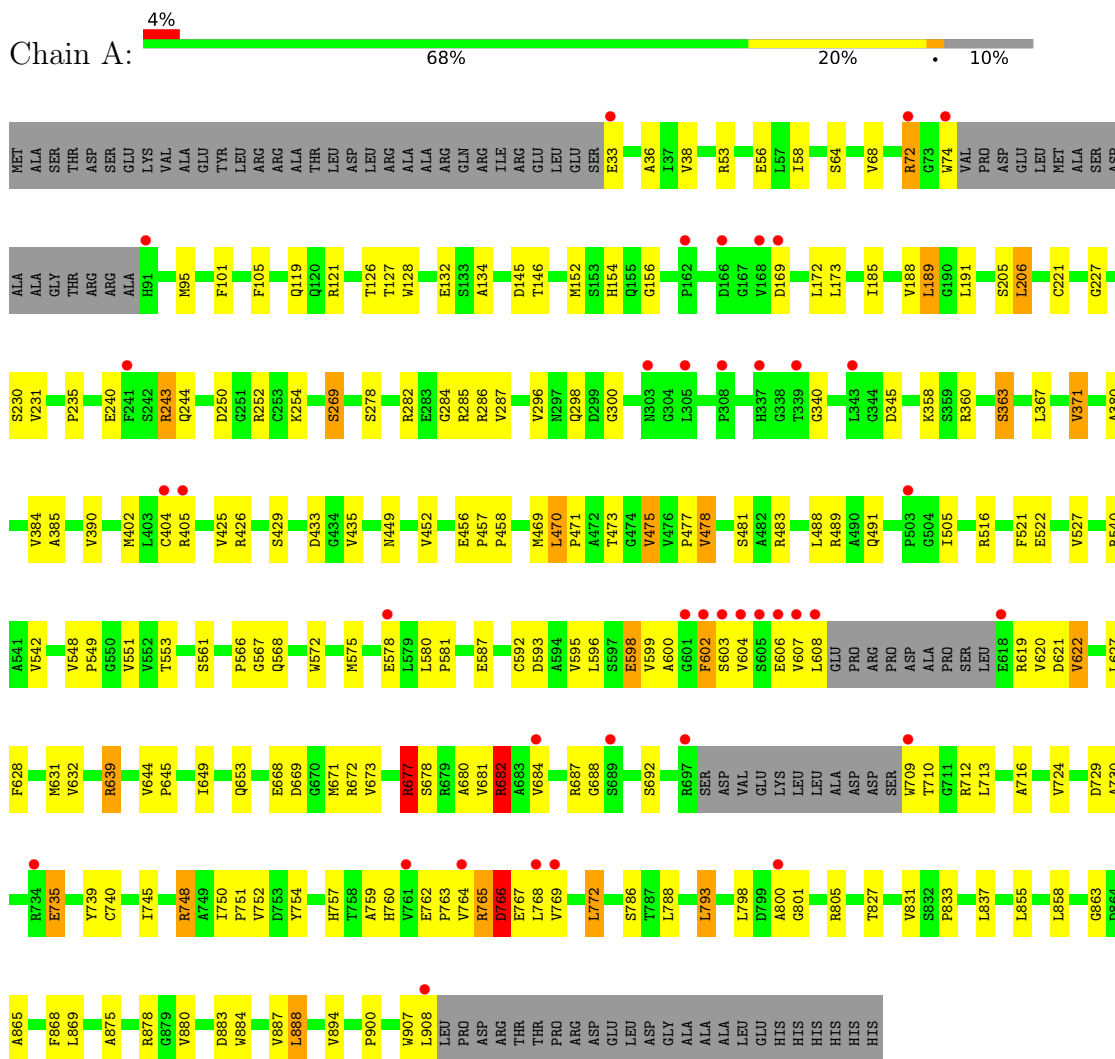
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	O 1	0	0
4	C	4	Total 4	O 4	0	0
4	D	29	Total 29	O 29	0	0

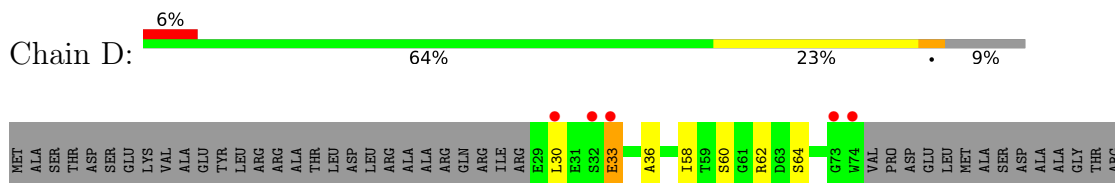
3 Residue-property plots [i](#)

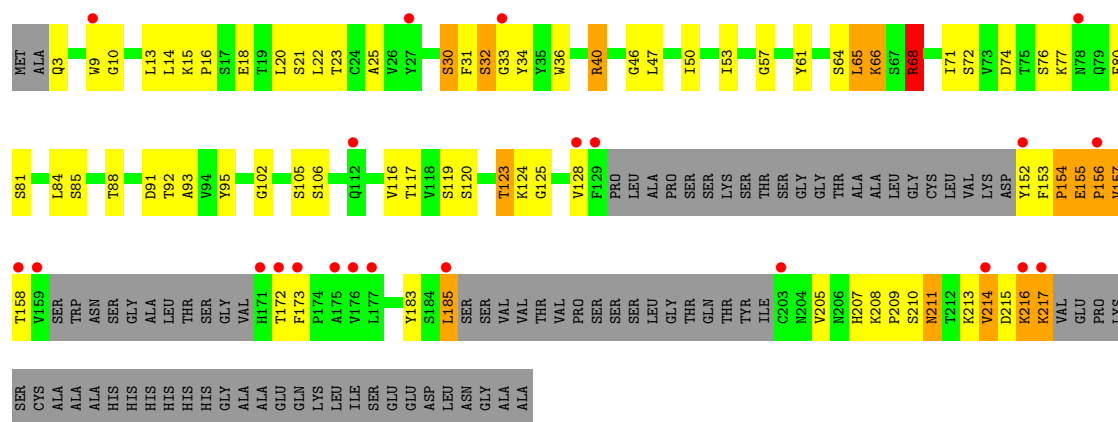
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 6-deoxyerythronolide B synthase

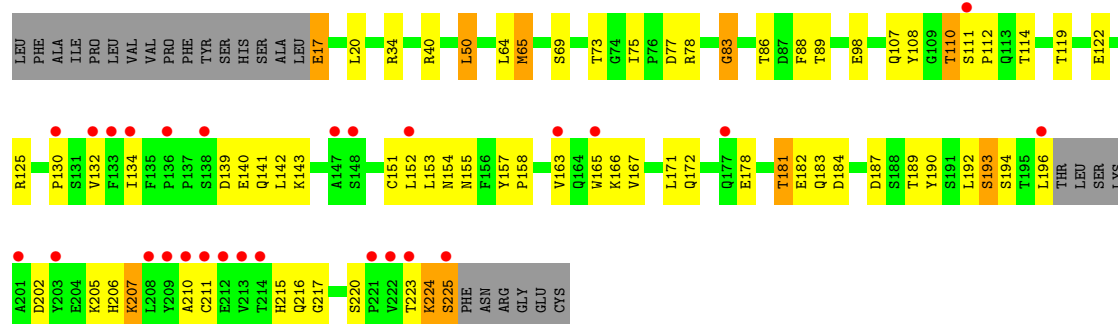


• Molecule 1: 6-deoxyerythronolide B synthase

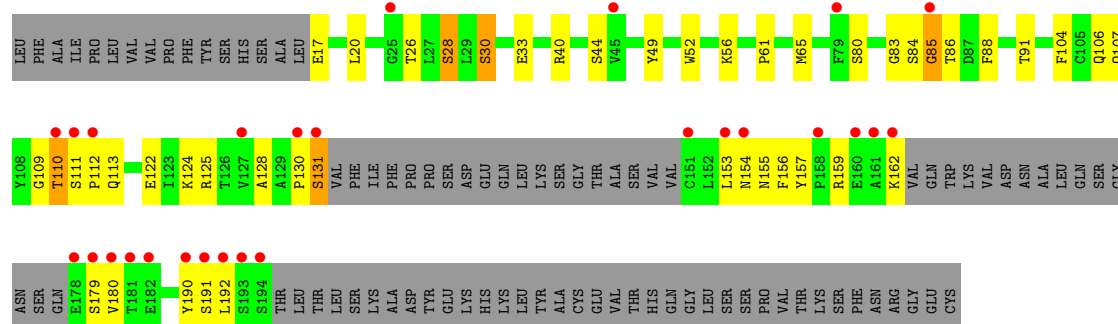




• Molecule 3: AA5 antibody light chain



• Molecule 3: AA5 antibody light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	249.37Å 252.44Å 63.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.62 – 2.70 39.62 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.62-2.70) 92.0 (39.62-2.70)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.225 , 0.254 0.225 , 0.254	Depositor DCC
R_{free} test set	5514 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17757	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.60	0/6215	0.84	1/8470 (0.0%)
1	D	0.59	0/6222	0.79	1/8483 (0.0%)
2	B	0.54	0/1624	0.78	0/2217
2	G	0.58	0/1292	0.81	1/1756 (0.1%)
3	C	0.57	0/1596	0.79	1/2169 (0.0%)
3	H	0.62	0/1101	0.86	0/1496
All	All	0.59	0/18050	0.81	4/24591 (0.0%)

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	5
1	D	0	2
2	B	0	1
2	G	0	1
All	All	0	9

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	102	GLY	CA-C-O	-6.12	118.24	122.22
1	D	741	GLU	N-CA-C	-5.60	106.15	112.87
1	A	768	LEU	N-CA-C	-5.33	105.55	111.36
3	C	83	GLY	CA-C-O	-5.28	118.52	122.37

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	243	ARG	Sidechain
1	A	677	ARG	Sidechain
1	A	682	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	748	ARG	Sidechain
2	B	101	ARG	Sidechain
1	D	360	ARG	Sidechain
1	D	867	ARG	Sidechain
2	G	68	ARG	Sidechain

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	6094	0	5935	123	0
1	D	6105	0	5918	150	0
2	B	1583	0	1540	59	0
2	G	1260	0	1218	55	0
3	C	1562	0	1487	50	0
3	H	1079	0	1007	35	0
4	A	40	0	0	1	0
4	B	1	0	0	0	0
4	C	4	0	0	1	0
4	D	29	0	0	1	0
All	All	17757	0	17105	460	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 13.

All (460) 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:D:690:MET:HG3	1:D:752:VAL:HG21	1.57	0.85
1:D:619:ARG:HH22	1:D:682:ARG:HH11	1.25	0.85
1:D:604:VAL:HG13	1:D:606:GLU:HG2	1.57	0.84
1:D:353:LEU:HD22	1:D:419:ILE:HD12	1.62	0.81
1:A:596:LEU:HB2	1:A:671:MET:HE3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLN:HG3	1:A:300:GLY:H	1.48	0.76
1:D:60:SER:HB3	1:D:62:ARG:HG3	1.67	0.76
1:A:887:VAL:HG23	1:A:888:LEU:HD13	1.68	0.76
1:A:516:ARG:HH11	1:A:516:ARG:HG2	1.50	0.76
2:B:61:TYR:HE1	2:B:71:ILE:HG12	1.50	0.76
2:B:61:TYR:CE1	2:B:71:ILE:HG12	2.24	0.73
1:D:298:GLN:HG3	1:D:300:GLY:H	1.52	0.73
1:D:505:ILE:HD11	1:D:894:VAL:HG11	1.70	0.72
3:C:165:TRP:CE2	3:C:196:LEU:HB2	2.24	0.72
3:H:110:THR:HG23	3:H:112:PRO:HD2	1.71	0.72
3:H:83:GLY:HA3	3:H:88:PHE:HA	1.71	0.71
3:C:178:GLU:HG2	3:C:192:LEU:HD21	1.73	0.71
1:A:884:TRP:HA	1:A:887:VAL:HG22	1.73	0.70
1:A:481:SER:HB2	1:A:521:PHE:H	1.56	0.70
1:A:435:VAL:HG13	1:A:456:GLU:HG2	1.74	0.69
1:A:146:THR:HB	1:A:191:LEU:HD22	1.74	0.69
2:B:145:LEU:HD13	2:B:218:VAL:HG11	1.74	0.69
3:C:165:TRP:NE1	3:C:196:LEU:HB2	2.08	0.68
1:A:119:GLN:HB3	1:A:152:MET:HE3	1.76	0.68
2:B:188:VAL:HG11	3:C:152:LEU:HD22	1.76	0.67
1:D:512:TRP:CD1	1:D:891:ALA:H	2.12	0.67
1:A:595:VAL:HG23	1:A:671:MET:HG2	1.77	0.67
1:A:619:ARG:HH12	1:A:682:ARG:HH11	1.42	0.66
2:B:166:LEU:HD21	2:B:189:VAL:HG21	1.77	0.66
1:D:716:ALA:HB1	1:D:757:HIS:HB2	1.76	0.66
1:D:672:ARG:HD3	1:D:676:ARG:HH21	1.61	0.66
1:A:709:TRP:CD1	1:A:712:ARG:HD3	2.31	0.66
1:A:477:PRO:HD3	1:A:869:LEU:HD21	1.78	0.65
2:G:207:HIS:CD2	2:G:209:PRO:HD2	2.31	0.65
1:D:389:LYS:HE3	1:D:400:PRO:HB2	1.77	0.65
2:B:159:VAL:HG22	2:B:205:VAL:HG22	1.77	0.65
3:H:28:SER:HB3	3:H:122:GLU:HG2	1.80	0.64
2:G:20:LEU:HD22	2:G:116:VAL:HG11	1.79	0.64
1:D:619:ARG:NH2	1:D:682:ARG:HH11	1.94	0.64
1:A:58:ILE:HD11	1:A:371:VAL:HG23	1.80	0.64
2:B:13:LEU:HD22	2:B:154:PRO:HG3	1.80	0.64
2:G:92:THR:HG23	2:G:117:THR:HA	1.78	0.64
1:A:712:ARG:HG2	1:A:729:ASP:OD2	1.98	0.64
1:D:119:GLN:OE1	1:D:230:SER:HA	1.97	0.64
3:C:64:LEU:HA	3:C:75:ILE:HG13	1.79	0.63
2:B:71:ILE:HG22	2:B:82:LEU:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:ARG:NH1	1:A:522:GLU:OE2	2.32	0.63
3:H:156:PHE:HE1	3:H:159:ARG:HA	1.63	0.63
1:D:154:HIS:CD2	1:D:156:GLY:H	2.16	0.62
2:B:199:GLN:HE21	2:B:200:THR:N	1.96	0.62
1:D:522:GLU:OE1	1:D:522:GLU:N	2.33	0.62
1:A:631:MET:HG2	1:A:831:VAL:O	1.99	0.62
1:D:408:ARG:HH11	1:D:421:LEU:HG	1.64	0.62
1:D:717:ALA:HB3	1:D:725:VAL:HB	1.82	0.61
2:B:144:ALA:HB2	2:B:190:THR:HG22	1.82	0.61
1:D:621:ASP:HB3	1:D:678:SER:O	2.00	0.61
2:G:31:PHE:HA	2:G:36:TRP:CZ2	2.36	0.61
3:C:202:ASP:HA	3:C:205:LYS:HD2	1.83	0.61
1:D:684:VAL:HG11	1:D:760:HIS:O	2.01	0.60
1:A:527:VAL:HG22	1:A:551:VAL:HG22	1.83	0.60
1:A:250:ASP:OD2	1:A:254:LYS:NZ	2.35	0.60
2:B:23:THR:HG22	2:B:81:SER:HB3	1.84	0.60
1:D:527:VAL:HG22	1:D:551:VAL:HG22	1.84	0.60
1:D:859:GLU:HB3	1:D:862:ALA:HB3	1.82	0.60
1:D:845:LEU:HD22	1:D:852:ALA:HB3	1.83	0.60
1:D:173:LEU:O	1:D:177:THR:HG22	2.02	0.60
1:D:481:SER:HB2	1:D:521:PHE:H	1.65	0.60
1:D:622:VAL:O	1:D:626:VAL:HG23	2.03	0.59
3:C:110:THR:HG23	3:C:112:PRO:HD2	1.84	0.59
1:D:95:MET:HE1	1:D:122:GLN:CD	2.27	0.59
1:A:602:PHE:HD1	1:A:602:PHE:H	1.50	0.59
1:D:858:LEU:HA	1:D:867:ARG:HG2	1.84	0.59
2:B:143:ALA:HB2	2:B:193:SER:HB3	1.85	0.59
1:A:620:VAL:HG21	1:A:754:TYR:CE1	2.37	0.59
3:H:153:LEU:HD22	3:H:192:LEU:HB3	1.85	0.59
1:A:471:PRO:HD2	1:A:865:ALA:HB2	1.85	0.58
2:G:128:VAL:HG21	2:G:205:VAL:HG21	1.85	0.58
2:B:84:LEU:HD21	2:B:91:ASP:OD2	2.03	0.58
2:G:31:PHE:HA	2:G:36:TRP:HZ2	1.68	0.58
1:D:329:ALA:HA	1:D:360:ARG:HH22	1.67	0.58
1:D:205:SER:HB3	1:D:380:ALA:O	2.03	0.58
1:D:418:GLU:OE1	1:D:418:GLU:HA	2.04	0.58
2:B:40:ARG:HB3	2:B:50:ILE:HD11	1.86	0.58
1:D:833:PRO:HA	1:D:858:LEU:HB2	1.85	0.58
1:A:566:PRO:HB3	1:A:837:LEU:HD12	1.84	0.57
1:D:688:GLY:HA2	1:D:728:GLY:O	2.05	0.57
1:A:491:GLN:HB2	1:A:900:PRO:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:ILE:O	1:A:752:VAL:N	2.37	0.57
1:D:565:PHE:CZ	1:D:661:VAL:HG21	2.39	0.57
3:C:125:ARG:HD3	3:C:189:THR:HG22	1.87	0.57
1:D:408:ARG:HH12	1:D:420:GLU:HA	1.69	0.56
2:B:191:VAL:HG21	2:B:201:TYR:OH	2.05	0.56
2:G:216:LYS:HG2	2:G:217:LYS:N	2.21	0.56
1:D:690:MET:HE2	1:D:727:ALA:HB2	1.88	0.56
1:D:817:VAL:HG21	1:D:841:VAL:HG22	1.87	0.56
2:G:74:ASP:CG	2:G:77:LYS:HG3	2.31	0.56
1:A:74:TRP:CD2	1:A:235:PRO:HB3	2.41	0.56
2:B:86:SER:O	2:B:86:SER:OG	2.20	0.56
1:A:95:MET:HE1	1:A:231:VAL:HG22	1.87	0.56
1:A:668:GLU:OE2	1:A:672:ARG:NH2	2.39	0.56
1:D:512:TRP:HB2	1:D:891:ALA:HB3	1.88	0.56
1:A:833:PRO:HA	1:A:858:LEU:HB2	1.87	0.56
3:H:130:PRO:HA	3:H:156:PHE:HB3	1.88	0.56
1:A:68:VAL:HG11	1:A:74:TRP:CE3	2.41	0.55
2:B:8:GLN:HE21	2:B:111:GLY:HA3	1.71	0.55
2:G:53:ILE:HD11	2:G:57:GLY:HA2	1.87	0.55
3:C:83:GLY:HA3	3:C:88:PHE:HA	1.88	0.55
3:H:180:VAL:HG22	3:H:192:LEU:HD12	1.89	0.55
3:C:17:GLU:HA	3:C:112:PRO:HG2	1.89	0.55
1:A:567:GLY:N	1:A:568:GLN:OE1	2.33	0.55
1:A:639:ARG:HD3	1:A:645:PRO:HD3	1.88	0.55
2:B:173:PHE:CD2	3:C:193:SER:HB3	2.41	0.55
1:A:765:ARG:O	1:A:766:ASP:C	2.48	0.55
2:B:220:PRO:O	2:B:221:LYS:HE2	2.06	0.55
1:D:631:MET:HG2	1:D:831:VAL:O	2.06	0.55
1:D:789:THR:HG21	1:D:793:LEU:HD13	1.89	0.55
3:C:151:CYS:HB2	3:C:165:TRP:CH2	2.42	0.54
2:G:123:THR:HB	2:G:154:PRO:HD3	1.89	0.54
3:C:154:ASN:ND2	3:C:155:ASN:OD1	2.40	0.54
1:D:607:VAL:HG11	2:G:30:SER:HB3	1.89	0.54
1:D:750:ILE:HG22	1:D:752:VAL:HG13	1.90	0.54
1:A:145:ASP:O	1:A:221:CYS:HB2	2.07	0.54
3:C:132:VAL:HG22	3:C:153:LEU:HD12	1.88	0.54
1:D:512:TRP:CB	1:D:891:ALA:HB3	2.38	0.54
2:B:126:PRO:HB3	2:B:152:TYR:HB3	1.89	0.54
1:A:677:ARG:HG3	1:A:678:SER:N	2.23	0.53
3:C:122:GLU:OE1	3:C:157:TYR:HE1	1.91	0.53
1:A:227:GLY:HA2	1:A:384:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:VAL:O	1:A:599:VAL:HG23	2.08	0.53
3:C:130:PRO:HD3	3:C:215:HIS:CD2	2.43	0.53
1:D:570:ALA:HB1	1:D:833:PRO:HD2	1.89	0.53
1:D:740:CYS:C	1:D:742:GLY:N	2.63	0.53
3:C:167:VAL:HG23	3:C:172:GLN:HG3	1.89	0.53
1:D:772:LEU:O	1:D:800:ALA:HB2	2.08	0.53
1:D:788:LEU:HD11	1:D:806:ASN:HA	1.90	0.53
1:D:58:ILE:HD11	1:D:371:VAL:HG23	1.89	0.53
1:D:607:VAL:CG1	2:G:30:SER:HB3	2.39	0.53
1:A:205:SER:HB3	1:A:380:ALA:O	2.09	0.53
3:C:17:GLU:HG3	3:C:114:THR:HG21	1.91	0.53
1:D:721:PRO:HG3	1:D:847:ASP:OD2	2.07	0.53
2:B:150:LYS:O	2:B:184:SER:HB2	2.07	0.53
3:H:156:PHE:CE1	3:H:159:ARG:HA	2.43	0.52
1:D:367:LEU:HD23	1:D:399:VAL:HG21	1.91	0.52
3:H:110:THR:CG2	3:H:112:PRO:HD2	2.38	0.52
2:B:32:SER:HA	2:B:55:HIS:HD2	1.75	0.52
1:D:512:TRP:NE1	1:D:890:ARG:HA	2.25	0.52
1:A:540:ARG:HG3	1:A:540:ARG:HH11	1.74	0.52
1:D:477:PRO:HG3	1:D:869:LEU:HD11	1.91	0.52
1:D:750:ILE:O	1:D:752:VAL:HG22	2.10	0.52
2:G:61:TYR:CE2	2:G:71:ILE:HG12	2.45	0.52
1:D:575:MET:HE1	1:D:627:LEU:HD13	1.92	0.52
2:G:20:LEU:HB3	2:G:84:LEU:HB3	1.92	0.52
1:D:298:GLN:HG3	1:D:300:GLY:N	2.24	0.52
2:G:47:LEU:HD12	2:G:47:LEU:H	1.75	0.52
1:A:240:GLU:O	1:A:244:GLN:HG3	2.10	0.51
2:G:172:THR:HG22	2:G:185:LEU:HD21	1.92	0.51
3:C:167:VAL:HG12	3:C:206:HIS:CD2	2.45	0.51
1:D:740:CYS:C	1:D:742:GLY:H	2.18	0.51
3:C:157:TYR:CD1	3:C:158:PRO:HA	2.45	0.51
1:D:684:VAL:HG12	1:D:684:VAL:O	2.10	0.51
2:G:16:PRO:HD3	2:G:119:SER:O	2.11	0.51
2:G:33:GLY:O	2:G:34:TYR:HD1	1.93	0.51
1:A:53:ARG:HD3	1:A:56:GLU:OE1	2.10	0.51
1:A:684:VAL:HG21	1:A:760:HIS:O	2.10	0.51
1:D:566:PRO:HD2	1:D:631:MET:SD	2.50	0.51
1:A:340:GLY:HA2	1:A:345:ASP:OD2	2.11	0.51
2:B:207:HIS:CE1	2:B:209:PRO:HG2	2.45	0.51
1:A:481:SER:CB	1:A:521:PHE:H	2.22	0.51
3:C:134:ILE:HB	3:C:224:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LEU:HD21	1:D:458:PRO:HG2	1.93	0.51
1:D:712:ARG:O	1:D:728:GLY:HA3	2.11	0.51
1:D:490:ALA:O	1:D:494:ARG:HG3	2.10	0.50
1:D:562:VAL:HG11	1:D:820:LEU:HD13	1.91	0.50
1:A:709:TRP:CZ3	1:A:735:GLU:HG2	2.47	0.50
2:B:23:THR:HA	2:B:81:SER:HA	1.92	0.50
2:G:119:SER:OG	2:G:120:SER:N	2.43	0.50
2:G:154:PRO:C	2:G:156:PRO:HD3	2.35	0.50
3:C:98:GLU:OE1	3:C:98:GLU:N	2.27	0.50
1:A:36:ALA:HB1	1:A:287:VAL:HG13	1.92	0.50
2:B:191:VAL:HG21	2:B:201:TYR:CE2	2.47	0.50
3:H:180:VAL:HA	3:H:192:LEU:HA	1.94	0.50
1:D:33:GLU:OE2	1:D:276:ARG:HB3	2.12	0.50
1:A:628:PHE:O	1:A:632:VAL:HG13	2.11	0.50
2:B:14:LEU:O	2:B:118:VAL:HA	2.12	0.50
1:A:119:GLN:CB	1:A:152:MET:HE3	2.41	0.49
1:A:621:ASP:HA	1:A:678:SER:HB2	1.94	0.49
3:C:184:ASP:HB3	3:C:187:ASP:OD1	2.12	0.49
1:D:672:ARG:O	1:D:676:ARG:HG3	2.12	0.49
3:H:30:SER:OG	3:H:33:GLU:OE2	2.30	0.49
1:A:596:LEU:HD21	1:A:602:PHE:CE2	2.47	0.49
1:A:875:ALA:HB1	1:A:880:VAL:HB	1.94	0.49
2:B:42:PRO:HB2	2:B:45:LYS:HB2	1.94	0.49
1:A:74:TRP:CD1	1:A:74:TRP:N	2.80	0.49
1:A:620:VAL:HG21	1:A:754:TYR:HE1	1.78	0.49
1:A:673:VAL:HG22	1:A:772:LEU:HG	1.95	0.49
2:B:126:PRO:HB2	2:B:149:VAL:HG13	1.95	0.49
1:D:146:THR:HB	1:D:191:LEU:HD22	1.94	0.49
3:H:125:ARG:NH2	3:H:128:ALA:HB2	2.28	0.49
3:H:155:ASN:HA	3:H:190:TYR:O	2.12	0.49
1:A:154:HIS:CE1	1:A:156:GLY:H	2.30	0.49
3:C:50:LEU:HD22	3:C:88:PHE:CG	2.48	0.49
2:G:36:TRP:HB3	2:G:80:PHE:CE1	2.48	0.49
3:H:30:SER:O	3:H:33:GLU:HG3	2.12	0.49
2:B:129:PHE:CE2	3:C:141:GLN:HG3	2.48	0.49
1:D:296:VAL:HA	1:D:449:ASN:O	2.12	0.49
3:C:181:THR:HG23	3:C:182:GLU:O	2.13	0.48
3:C:215:HIS:CD2	3:C:217:GLY:H	2.31	0.48
2:G:152:TYR:OH	2:G:185:LEU:HB2	2.13	0.48
1:A:516:ARG:HH11	1:A:516:ARG:CG	2.25	0.48
2:B:130:PRO:O	2:B:131:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:PHE:CD1	1:D:121:ARG:HB3	2.49	0.48
1:A:607:VAL:O	1:A:608:LEU:C	2.56	0.48
1:D:253:CYS:O	1:D:255:PRO:HD3	2.14	0.48
1:D:572:TRP:CD2	1:D:860:ARG:HA	2.49	0.48
3:C:77:ASP:OD1	3:C:77:ASP:N	2.47	0.48
3:C:166:LYS:HD3	3:C:171:LEU:HD22	1.94	0.48
1:D:761:VAL:C	1:D:763:PRO:HD2	2.37	0.48
2:G:40:ARG:HB3	2:G:50:ILE:HD11	1.95	0.48
1:A:580:LEU:N	1:A:581:PRO:CD	2.77	0.48
1:A:709:TRP:HD1	1:A:712:ARG:HD3	1.78	0.48
1:D:697:ARG:NH2	1:D:718:VAL:HG21	2.29	0.48
1:A:38:VAL:O	1:A:134:ALA:HA	2.13	0.48
1:D:481:SER:CB	1:D:521:PHE:H	2.26	0.48
2:G:93:ALA:HB3	2:G:95:TYR:CE1	2.48	0.48
2:G:155:GLU:HG3	2:G:183:TYR:CD2	2.49	0.48
3:H:124:LYS:HA	3:H:157:TYR:OH	2.13	0.48
1:A:250:ASP:OD1	1:A:252:ARG:NH1	2.47	0.48
1:A:402:MET:HE3	1:A:404:CYS:SG	2.54	0.48
1:D:648:VAL:HG21	1:D:662:ALA:HB2	1.96	0.48
1:A:572:TRP:CH2	1:A:575:MET:HA	2.49	0.48
1:A:587:GLU:HG2	2:B:101:ARG:HG3	1.95	0.48
1:D:732:ALA:HA	1:D:735:GLU:HG3	1.96	0.48
3:H:20:LEU:HD11	3:H:107:GLN:H	1.79	0.47
3:C:125:ARG:HG2	3:C:157:TYR:CG	2.49	0.47
3:H:130:PRO:O	3:H:131:SER:C	2.57	0.47
1:A:72:ARG:HG2	1:A:907:TRP:CZ2	2.49	0.47
1:A:595:VAL:O	1:A:598:GLU:HG3	2.14	0.47
3:C:65:MET:HE2	3:C:65:MET:HB2	1.69	0.47
1:A:602:PHE:CE2	1:A:622:VAL:HA	2.49	0.47
2:B:172:THR:HG23	2:B:187:SER:HB2	1.97	0.47
3:H:84:SER:O	3:H:85:GLY:C	2.57	0.47
1:A:250:ASP:HB3	1:A:252:ARG:H	1.78	0.47
1:A:596:LEU:HD21	1:A:602:PHE:CD2	2.50	0.47
1:A:673:VAL:O	1:A:677:ARG:HB3	2.14	0.47
1:A:884:TRP:CE3	1:A:887:VAL:HG21	2.50	0.47
1:D:851:ASP:OD1	1:D:851:ASP:N	2.31	0.47
2:G:20:LEU:HD21	2:G:116:VAL:HG21	1.95	0.47
2:B:53:ILE:HD12	2:B:59:THR:HG22	1.97	0.47
1:D:294:SER:HB2	1:D:452:VAL:HG22	1.95	0.47
1:D:505:ILE:HD11	1:D:894:VAL:CG1	2.42	0.47
1:D:696:GLY:O	1:D:700:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:VAL:HA	1:A:449:ASN:O	2.15	0.47
1:A:858:LEU:HD13	1:A:863:GLY:HA2	1.96	0.47
1:D:625:PRO:HB3	1:D:671:MET:HE2	1.97	0.47
2:G:153:PHE:HA	2:G:154:PRO:O	2.14	0.47
1:D:672:ARG:HD3	1:D:676:ARG:NH2	2.29	0.47
1:D:727:ALA:HB1	1:D:755:ALA:HB1	1.97	0.47
1:D:127:THR:HG23	1:D:225:VAL:HG11	1.96	0.46
1:A:619:ARG:O	1:A:622:VAL:HG22	2.16	0.46
1:A:772:LEU:O	1:A:800:ALA:HB2	2.16	0.46
2:B:104:SER:O	3:C:108:TYR:HB2	2.16	0.46
2:G:208:LYS:HB2	2:G:209:PRO:HD3	1.97	0.46
3:H:111:SER:HB3	3:H:112:PRO:HD3	1.98	0.46
1:A:101:PHE:CD1	1:A:121:ARG:HB3	2.50	0.46
1:A:505:ILE:HD11	1:A:894:VAL:HG11	1.97	0.46
2:B:201:TYR:O	2:B:218:VAL:HG12	2.16	0.46
1:D:139:GLU:CD	1:D:519:GLN:HG3	2.41	0.46
1:D:370:SER:H	1:D:402:MET:HE3	1.80	0.46
1:A:478:VAL:HA	4:A:1005:HOH:O	2.16	0.46
3:C:211:CYS:O	3:C:223:THR:HA	2.15	0.46
1:A:681:VAL:O	1:A:682:ARG:C	2.58	0.46
1:A:855:LEU:HD21	1:A:878:ARG:HG3	1.98	0.46
1:A:712:ARG:O	1:A:713:LEU:HD23	2.16	0.46
1:D:512:TRP:HE1	1:D:890:ARG:HA	1.80	0.46
1:D:572:TRP:CZ3	1:D:861:ASP:N	2.76	0.46
3:H:110:THR:O	3:H:111:SER:C	2.58	0.46
1:D:497:ASP:OD1	1:D:540:ARG:NH2	2.32	0.46
2:G:13:LEU:HD22	2:G:154:PRO:HG3	1.97	0.46
1:A:128:TRP:NE1	1:A:132:GLU:OE2	2.46	0.45
1:A:680:ALA:HB1	1:A:764:VAL:HG11	1.98	0.45
3:C:111:SER:OG	3:C:112:PRO:HD3	2.15	0.45
3:C:153:LEU:HD23	3:C:192:LEU:HB3	1.97	0.45
1:A:206:LEU:HD13	1:A:452:VAL:HG23	1.98	0.45
1:A:358:LYS:HA	1:A:358:LYS:HD3	1.74	0.45
1:A:688:GLY:H	1:A:730:ALA:HB2	1.82	0.45
1:D:270:ALA:HB1	1:D:384:VAL:HG12	1.97	0.45
2:G:124:LYS:HD3	2:G:125:GLY:H	1.80	0.45
3:C:78:ARG:NH1	4:C:301:HOH:O	2.23	0.45
1:D:469:MET:O	1:D:470:LEU:HB2	2.15	0.45
1:D:477:PRO:HD3	1:D:869:LEU:HD21	1.98	0.45
1:D:678:SER:O	1:D:681:VAL:HG12	2.16	0.45
1:A:801:GLY:O	1:A:805:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:VAL:HG11	1:D:908:LEU:HD11	1.98	0.45
2:B:47:LEU:HD12	2:B:47:LEU:H	1.81	0.45
2:B:191:VAL:HG21	2:B:201:TYR:CZ	2.52	0.45
1:D:737:LEU:HD11	1:D:749:ALA:HB2	1.98	0.45
1:D:828:PHE:HB2	1:D:854:VAL:HG13	1.99	0.45
2:G:152:TYR:CE1	2:G:183:TYR:HB2	2.51	0.45
3:C:20:LEU:HD21	3:C:107:GLN:HG2	1.99	0.45
3:C:165:TRP:CG	3:C:196:LEU:HD22	2.51	0.45
1:D:739:TYR:C	1:D:739:TYR:CD1	2.94	0.45
2:B:88:THR:OG1	2:B:89:ALA:N	2.50	0.45
1:D:691:LEU:CD1	1:D:726:VAL:HB	2.47	0.45
1:A:669:ASP:O	1:A:673:VAL:HG23	2.18	0.44
1:D:433:ASP:OD1	1:D:433:ASP:N	2.50	0.44
1:D:572:TRP:CD1	1:D:575:MET:HB3	2.53	0.44
1:D:697:ARG:CZ	1:D:718:VAL:HG21	2.47	0.44
1:A:607:VAL:HG22	1:A:608:LEU:HD23	1.99	0.44
2:B:3:GLN:NE2	2:B:4:VAL:O	2.50	0.44
1:A:119:GLN:OE1	1:A:230:SER:HA	2.17	0.44
2:B:115:LEU:HD12	2:B:116:VAL:H	1.83	0.44
1:D:440:VAL:O	1:D:451:HIS:HA	2.16	0.44
1:D:619:ARG:HG3	1:D:622:VAL:HG12	1.98	0.44
2:G:153:PHE:HA	2:G:154:PRO:C	2.43	0.44
3:H:111:SER:CB	3:H:112:PRO:HD3	2.48	0.44
2:B:91:ASP:N	2:B:91:ASP:OD1	2.50	0.44
3:C:193:SER:O	3:C:193:SER:OG	2.35	0.44
1:D:596:LEU:O	1:D:600:ALA:N	2.51	0.44
2:G:68:ARG:HE	2:G:68:ARG:HB2	1.55	0.44
1:A:548:VAL:HG12	1:A:549:PRO:O	2.17	0.44
3:C:157:TYR:CG	3:C:158:PRO:HA	2.52	0.44
1:D:621:ASP:HA	1:D:678:SER:OG	2.17	0.44
1:D:677:ARG:HH21	1:D:806:ASN:ND2	2.16	0.44
3:H:52:TRP:HB2	3:H:65:MET:HB2	1.98	0.44
1:D:174:THR:O	1:D:180:VAL:HG11	2.17	0.44
1:D:516:ARG:HG3	1:D:516:ARG:HH11	1.82	0.44
1:D:759:ALA:O	1:D:762:GLU:HG3	2.18	0.44
2:G:20:LEU:HD12	2:G:21:SER:H	1.83	0.44
1:D:408:ARG:HD2	1:D:414:TRP:CZ2	2.52	0.44
1:D:678:SER:HA	1:D:681:VAL:HG12	1.99	0.44
1:D:757:HIS:HA	1:D:808:ARG:O	2.18	0.44
2:B:30:SER:C	2:B:32:SER:N	2.75	0.44
1:D:693:VAL:HG13	1:D:745:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:156:PHE:HE2	3:H:192:LEU:H	1.66	0.44
2:B:36:TRP:HB3	2:B:80:PHE:CZ	2.52	0.43
3:C:165:TRP:CZ3	3:C:211:CYS:HB2	2.53	0.43
1:D:389:LYS:NZ	4:D:1005:HOH:O	2.51	0.43
3:C:215:HIS:CG	3:C:216:GLN:N	2.86	0.43
1:A:762:GLU:N	1:A:763:PRO:HD2	2.32	0.43
2:B:7:GLN:HG3	2:B:27:TYR:CE1	2.53	0.43
1:D:540:ARG:HG3	1:D:540:ARG:HH11	1.83	0.43
1:D:736:PHE:O	1:D:739:TYR:HB3	2.19	0.43
2:G:40:ARG:NH2	2:G:91:ASP:HA	2.32	0.43
2:G:157:VAL:HG23	2:G:207:HIS:CD2	2.54	0.43
2:G:105:SER:OG	2:G:106:SER:N	2.51	0.43
1:A:561:SER:OG	1:A:827:THR:HB	2.19	0.43
1:D:509:ASP:HB3	1:D:894:VAL:HG13	2.00	0.43
3:H:153:LEU:O	3:H:156:PHE:HD2	2.02	0.43
1:D:313:GLN:OE1	1:D:348:GLU:HA	2.19	0.43
1:A:469:MET:HE2	1:A:469:MET:HB2	1.80	0.43
1:A:470:LEU:HD21	1:A:868:PHE:HB3	2.01	0.43
2:B:20:LEU:HD11	2:B:22:LEU:HD21	2.00	0.43
2:B:146:GLY:HA2	2:B:161:TRP:CZ2	2.54	0.43
2:B:159:VAL:HG11	2:B:187:SER:CB	2.48	0.43
1:D:469:MET:HE2	1:D:469:MET:HB2	1.66	0.43
1:D:814:HIS:CE1	1:D:844:THR:HG23	2.53	0.43
2:B:53:ILE:CD1	2:B:73:VAL:HG13	2.48	0.43
1:D:114:LEU:HG	1:D:908:LEU:HG	2.00	0.43
1:D:210:HIS:HD1	1:D:294:SER:HG	1.62	0.43
1:D:630:VAL:O	1:D:634:LEU:HG	2.18	0.43
1:A:908:LEU:HD23	1:A:908:LEU:HA	1.66	0.43
1:D:394:LEU:HD13	1:D:456:GLU:HA	2.00	0.43
1:D:619:ARG:HH22	1:D:682:ARG:NH1	2.04	0.43
2:B:54:ASN:OD1	2:B:58:SER:OG	2.35	0.43
3:H:40:ARG:HA	3:H:86:THR:O	2.18	0.43
1:A:522:GLU:N	1:A:522:GLU:OE1	2.51	0.42
1:A:765:ARG:C	1:A:767:GLU:N	2.76	0.42
3:C:178:GLU:OE1	3:C:192:LEU:HD11	2.18	0.42
1:D:360:ARG:HH21	1:D:363:SER:HB2	1.84	0.42
3:C:40:ARG:HA	3:C:86:THR:O	2.18	0.42
1:D:572:TRP:CE2	1:D:860:ARG:HA	2.54	0.42
2:G:128:VAL:HB	2:G:214:VAL:HG11	2.01	0.42
1:A:653:GLN:HB3	1:A:677:ARG:CZ	2.50	0.42
2:B:208:LYS:HD2	2:B:208:LYS:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:VAL:HG11	1:D:833:PRO:HG3	2.00	0.42
2:G:155:GLU:HG3	2:G:183:TYR:CG	2.54	0.42
1:A:457:PRO:HA	1:A:458:PRO:HD3	1.94	0.42
2:G:10:GLY:HA3	2:G:22:LEU:HD23	2.02	0.42
2:G:65:LEU:O	2:G:66:LYS:C	2.62	0.42
1:A:384:VAL:O	1:A:385:ALA:C	2.61	0.42
1:D:97:GLY:O	1:D:98:ALA:C	2.62	0.42
2:G:9:TRP:CH2	2:G:25:ALA:HB2	2.55	0.42
2:G:46:GLY:HA2	3:H:104:PHE:CE1	2.54	0.42
1:A:786:SER:HB2	1:A:793:LEU:HD22	2.02	0.42
1:D:36:ALA:HB1	1:D:287:VAL:HG13	2.02	0.42
1:D:471:PRO:HD2	1:D:865:ALA:HB2	2.01	0.42
1:D:888:LEU:O	1:D:889:GLY:C	2.62	0.42
3:H:20:LEU:HD11	3:H:107:GLN:N	2.35	0.42
1:D:732:ALA:O	1:D:735:GLU:HB2	2.20	0.42
1:A:884:TRP:O	1:A:888:LEU:HB2	2.19	0.42
1:D:303:ASN:O	1:D:307:ALA:HB2	2.20	0.42
1:D:531:ASP:OD1	1:D:531:ASP:C	2.62	0.42
1:D:691:LEU:HD11	1:D:726:VAL:HB	2.01	0.42
2:G:15:LYS:NZ	2:G:18:GLU:OE2	2.49	0.42
2:G:66:LYS:HB2	2:G:66:LYS:HE2	1.55	0.42
3:H:180:VAL:HA	3:H:191:SER:O	2.19	0.42
1:A:765:ARG:O	1:A:767:GLU:N	2.52	0.42
1:A:883:ASP:O	1:A:884:TRP:HB2	2.20	0.42
2:B:151:ASP:HB3	2:B:182:LEU:HD13	2.02	0.42
1:D:467:ARG:HD3	3:H:49:TYR:CZ	2.54	0.42
2:G:210:SER:O	2:G:211:ASN:C	2.62	0.42
1:A:759:ALA:O	1:A:762:GLU:HG3	2.20	0.42
1:D:733:ALA:O	1:D:734:ARG:C	2.63	0.41
1:A:127:THR:HG21	1:A:185:ILE:HG21	2.02	0.41
2:G:214:VAL:HG13	2:G:216:LYS:HB3	2.02	0.41
1:A:473:THR:C	1:A:475:VAL:H	2.27	0.41
2:B:36:TRP:HB3	2:B:80:PHE:CE1	2.56	0.41
2:B:159:VAL:HG11	2:B:187:SER:HB3	2.02	0.41
1:D:189:LEU:HB2	1:D:191:LEU:HG	2.01	0.41
2:G:14:LEU:HD21	2:G:20:LEU:HA	2.01	0.41
1:A:126:THR:HG21	1:A:269:SER:HB3	2.03	0.41
1:D:467:ARG:HD2	3:H:109:GLY:HA2	2.02	0.41
1:D:408:ARG:NH1	1:D:421:LEU:H	2.19	0.41
1:A:740:CYS:HB3	1:A:745:ILE:O	2.21	0.41
1:A:750:ILE:HG22	1:A:752:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:LEU:HG	1:D:383:GLY:HA3	2.02	0.41
2:G:40:ARG:HH21	2:G:91:ASP:HA	1.86	0.41
2:G:173:PHE:HB3	3:H:179:SER:OG	2.20	0.41
1:A:188:VAL:HG12	1:A:189:LEU:HD13	2.01	0.41
3:C:183:GLN:HB2	3:C:190:TYR:CE1	2.55	0.41
1:D:801:GLY:O	1:D:805:ARG:HG3	2.20	0.41
3:H:106:GLN:HE21	3:H:113:GLN:CD	2.29	0.41
1:A:752:VAL:HB	1:A:754:TYR:CE1	2.56	0.41
3:C:153:LEU:HD21	3:C:163:VAL:HG11	2.03	0.41
1:D:768:LEU:O	1:D:769:VAL:C	2.63	0.41
1:D:769:VAL:HA	1:D:800:ALA:HB1	2.02	0.41
2:G:47:LEU:HD21	3:H:61:PRO:HG2	2.03	0.41
1:A:607:VAL:C	1:A:608:LEU:HG	2.46	0.41
2:B:145:LEU:HD21	2:B:201:TYR:HD2	1.86	0.41
2:B:208:LYS:N	2:B:209:PRO:HD2	2.36	0.41
3:C:125:ARG:CD	3:C:189:THR:HG22	2.50	0.41
1:D:428:TRP:O	1:D:430:PRO:HD3	2.21	0.41
1:D:770:GLN:O	1:D:771:ALA:C	2.63	0.41
2:G:30:SER:C	2:G:32:SER:N	2.78	0.41
3:H:56:LYS:HE2	3:H:56:LYS:HB2	1.89	0.41
1:A:282:ARG:C	1:A:284:GLY:H	2.27	0.41
1:A:425:VAL:O	1:A:426:ARG:HD3	2.20	0.41
1:A:716:ALA:HB1	1:A:757:HIS:HB2	2.03	0.41
3:C:207:LYS:HZ2	3:C:207:LYS:C	2.28	0.41
3:C:210:ALA:HA	3:C:225:SER:HA	2.03	0.41
2:G:154:PRO:HD2	2:G:209:PRO:HB2	2.03	0.41
2:G:71:ILE:HA	2:G:81:SER:O	2.21	0.40
2:G:214:VAL:O	2:G:215:ASP:C	2.63	0.40
1:A:105:PHE:CD1	1:A:483:ARG:HG3	2.57	0.40
2:B:9:TRP:CD1	2:B:23:THR:HG1	2.39	0.40
2:B:201:TYR:HD1	2:B:201:TYR:HA	1.58	0.40
1:D:669:ASP:O	1:D:673:VAL:HG23	2.22	0.40
1:D:714:GLU:CD	1:D:758:THR:HG22	2.46	0.40
1:A:360:ARG:O	1:A:363:SER:OG	2.37	0.40
1:A:489:ARG:HG2	1:A:542:VAL:O	2.22	0.40
1:A:592:CYS:O	1:A:593:ASP:C	2.65	0.40
2:B:146:GLY:HA2	2:B:161:TRP:CH2	2.56	0.40
1:D:359:SER:C	1:D:361:GLY:N	2.78	0.40
3:H:28:SER:HB3	3:H:122:GLU:CG	2.50	0.40
1:A:739:TYR:CD1	1:A:739:TYR:C	2.99	0.40
3:C:139:ASP:O	3:C:140:GLU:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:575:MET:HE3	1:D:630:VAL:HG21	2.04	0.40
1:A:282:ARG:C	1:A:284:GLY:N	2.80	0.40
2:B:30:SER:O	2:B:31:PHE:C	2.63	0.40
1:D:463:VAL:HG22	1:D:464:PRO:HD2	2.04	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	832/932 (89%)	773 (93%)	54 (6%)	5 (1%)	21	44
1	D	836/932 (90%)	772 (92%)	59 (7%)	5 (1%)	21	44
2	B	206/249 (83%)	189 (92%)	17 (8%)	0	100	100
2	G	157/249 (63%)	140 (89%)	15 (10%)	2 (1%)	9	25
3	C	201/231 (87%)	183 (91%)	18 (9%)	0	100	100
3	H	138/231 (60%)	124 (90%)	12 (9%)	2 (1%)	9	23
All	All	2370/2824 (84%)	2181 (92%)	175 (7%)	14 (1%)	21	44

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	156	PRO
3	H	154	ASN
1	A	600	ALA
1	A	603	SER
3	H	85	GLY
1	D	600	ALA
1	D	603	SER
1	A	751	PRO

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Mol	Chain	Res	Type
1	A	765	ARG
1	D	470	LEU
1	A	766	ASP
1	D	566	PRO
1	D	751	PRO
2	G	154	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	605/690 (88%)	556 (92%)	49 (8%)	11	27
1	D	606/690 (88%)	547 (90%)	59 (10%)	8	20
2	B	180/206 (87%)	159 (88%)	21 (12%)	5	13
2	G	141/206 (68%)	118 (84%)	23 (16%)	2	6
3	C	173/199 (87%)	155 (90%)	18 (10%)	7	17
3	H	116/199 (58%)	106 (91%)	10 (9%)	10	25
All	All	1821/2190 (83%)	1641 (90%)	180 (10%)	7	19

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	64	SER
1	A	169	ASP
1	A	172	LEU
1	A	173	LEU
1	A	189	LEU
1	A	206	LEU
1	A	243	ARG
1	A	269	SER
1	A	278	SER
1	A	285	ARG
1	A	286	ARG

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Mol	Chain	Res	Type
1	A	363	SER
1	A	367	LEU
1	A	371	VAL
1	A	390	VAL
1	A	405	ARG
1	A	429	SER
1	A	433	ASP
1	A	470	LEU
1	A	475	VAL
1	A	478	VAL
1	A	488	LEU
1	A	553	THR
1	A	578	GLU
1	A	598	GLU
1	A	602	PHE
1	A	604	VAL
1	A	606	GLU
1	A	622	VAL
1	A	627	LEU
1	A	639	ARG
1	A	644	VAL
1	A	649	ILE
1	A	677	ARG
1	A	682	ARG
1	A	687	ARG
1	A	692	SER
1	A	710	THR
1	A	724	VAL
1	A	735	GLU
1	A	748	ARG
1	A	766	ASP
1	A	769	VAL
1	A	772	LEU
1	A	788	LEU
1	A	793	LEU
1	A	798	LEU
1	A	888	LEU
2	B	8	GLN
2	B	9	TRP
2	B	14	LEU
2	B	22	LEU
2	B	65	LEU

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Mol	Chain	Res	Type
2	B	69	VAL
2	B	75	THR
2	B	81	SER
2	B	86	SER
2	B	87	VAL
2	B	88	THR
2	B	101	ARG
2	B	117	THR
2	B	123	THR
2	B	142	THR
2	B	150	LYS
2	B	168	SER
2	B	179	SER
2	B	184	SER
2	B	186	SER
2	B	198	THR
3	C	17	GLU
3	C	34	ARG
3	C	50	LEU
3	C	65	MET
3	C	69	SER
3	C	73	THR
3	C	89	THR
3	C	110	THR
3	C	119	THR
3	C	142	LEU
3	C	143	LYS
3	C	181	THR
3	C	193	SER
3	C	194	SER
3	C	207	LYS
3	C	220	SER
3	C	224	LYS
3	C	225	SER
1	D	30	LEU
1	D	33	GLU
1	D	64	SER
1	D	145	ASP
1	D	165	GLU
1	D	173	LEU
1	D	174	THR
1	D	177	THR

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Mol	Chain	Res	Type
1	D	196	LEU
1	D	215	SER
1	D	242	SER
1	D	281	ARG
1	D	306	SER
1	D	316	VAL
1	D	333	VAL
1	D	353	LEU
1	D	360	ARG
1	D	363	SER
1	D	367	LEU
1	D	390	VAL
1	D	402	MET
1	D	407	GLU
1	D	408	ARG
1	D	416	SER
1	D	433	ASP
1	D	445	VAL
1	D	448	THR
1	D	468	ARG
1	D	469	MET
1	D	478	VAL
1	D	480	LEU
1	D	481	SER
1	D	527	VAL
1	D	552	VAL
1	D	597	SER
1	D	604	VAL
1	D	607	VAL
1	D	608	LEU
1	D	632	VAL
1	D	649	ILE
1	D	692	SER
1	D	700	VAL
1	D	701	GLU
1	D	710	THR
1	D	714	GLU
1	D	715	VAL
1	D	731	GLN
1	D	741	GLU
1	D	745	ILE
1	D	761	VAL

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Mol	Chain	Res	Type
1	D	764	VAL
1	D	776	THR
1	D	798	LEU
1	D	822	ASP
1	D	854	VAL
1	D	861	ASP
1	D	864	ASP
1	D	867	ARG
1	D	888	LEU
2	G	3	GLN
2	G	23	THR
2	G	30	SER
2	G	32	SER
2	G	40	ARG
2	G	64	SER
2	G	65	LEU
2	G	66	LYS
2	G	68	ARG
2	G	72	SER
2	G	76	SER
2	G	85	SER
2	G	88	THR
2	G	123	THR
2	G	155	GLU
2	G	157	VAL
2	G	158	THR
2	G	185	LEU
2	G	211	ASN
2	G	213	LYS
2	G	214	VAL
2	G	216	LYS
2	G	217	LYS
3	H	17	GLU
3	H	26	THR
3	H	28	SER
3	H	30	SER
3	H	44	SER
3	H	80	SER
3	H	91	THR
3	H	110	THR
3	H	131	SER
3	H	162	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	155	GLN
1	A	298	GLN
1	A	449	ASN
1	A	818	GLN
2	B	3	GLN
2	B	8	GLN
2	B	41	GLN
2	B	55	HIS
2	B	78	ASN
2	B	178	GLN
2	B	199	GLN
3	C	55	GLN
3	C	154	ASN
3	C	172	GLN
3	C	206	HIS
1	D	498	HIS
1	D	624	GLN
1	D	806	ASN
2	G	41	GLN
3	H	55	GLN
3	H	155	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	840/932 (90%)	0.23	39 (4%) 37 34	44, 66, 101, 133	0
1	D	846/932 (90%)	0.32	60 (7%) 22 19	43, 69, 120, 162	0
2	B	212/249 (85%)	0.97	26 (12%) 8 7	64, 95, 119, 154	0
2	G	165/249 (66%)	0.91	22 (13%) 7 6	68, 90, 139, 185	0
3	C	205/231 (88%)	0.86	27 (13%) 7 6	61, 93, 145, 150	0
3	H	144/231 (62%)	1.09	27 (18%) 3 3	70, 98, 141, 170	0
All	All	2412/2824 (85%)	0.48	201 (8%) 17 14	43, 75, 126, 185	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	185	LEU	6.2
3	H	194	SER	6.1
1	A	697	ARG	5.5
1	D	74	TRP	5.4
3	H	180	VAL	5.4
2	G	156	PRO	5.3
1	A	607	VAL	5.2
1	A	337	HIS	5.1
2	G	217	LYS	5.0
1	D	709	TRP	4.9
1	A	608	LEU	4.8
1	D	604	VAL	4.6
3	C	111	SER	4.6
2	B	133	PRO	4.6
1	D	608	LEU	4.5
1	A	168	VAL	4.4
3	H	178	GLU	4.4
1	A	72	ARG	4.4
1	D	32	SER	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	134	SER	4.3
2	G	159	VAL	4.3
3	C	225	SER	4.2
2	B	65	LEU	4.2
1	D	404	CYS	4.2
1	D	605	SER	4.2
3	H	181	THR	4.2
1	D	598	GLU	4.1
1	A	602	PHE	4.1
1	A	604	VAL	4.1
1	D	891	ALA	4.1
3	C	208	LEU	4.1
2	B	29	GLY	4.1
1	A	578	GLU	4.0
2	B	223	CYS	3.9
1	D	888	LEU	3.9
1	D	567	GLY	3.9
3	C	209	TYR	3.9
1	D	363	SER	3.9
1	D	742	GLY	3.8
1	D	470	LEU	3.8
2	G	175	ALA	3.8
3	H	131	SER	3.7
3	C	221	PRO	3.7
1	D	304	GLY	3.7
2	B	31	PHE	3.6
1	D	408	ARG	3.5
1	A	603	SER	3.5
2	B	141	GLY	3.5
1	D	908	LEU	3.5
2	G	214	VAL	3.5
3	H	162	LYS	3.4
2	G	173	PHE	3.4
3	H	151	CYS	3.4
3	H	112	PRO	3.4
1	D	607	VAL	3.4
2	B	63	PRO	3.3
2	G	33	GLY	3.3
3	H	130	PRO	3.3
3	H	85	GLY	3.3
1	D	892	GLY	3.3
2	G	129	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	145	ASP	3.3
1	A	404	CYS	3.2
3	H	179	SER	3.2
1	D	33	GLU	3.2
2	B	155	GLU	3.2
1	A	74	TRP	3.2
1	D	471	PRO	3.2
2	B	9	TRP	3.2
3	H	154	ASN	3.1
3	C	201	ALA	3.1
1	A	601	GLY	3.1
2	B	69	VAL	3.1
3	C	196	LEU	3.1
1	D	862	ALA	3.1
1	A	303	ASN	3.0
3	H	161	ALA	3.0
3	C	163	VAL	3.0
1	D	713	LEU	2.9
2	G	152	TYR	2.9
1	D	73	GLY	2.9
1	D	599	VAL	2.9
2	B	123	THR	2.9
1	D	606	GLU	2.9
2	B	44	GLY	2.9
1	A	305	LEU	2.8
3	H	110	THR	2.8
1	D	306	SER	2.8
1	D	308	PRO	2.8
3	C	132	VAL	2.8
3	C	147	ALA	2.8
3	C	222	VAL	2.8
1	A	162	PRO	2.8
3	H	191	SER	2.8
1	D	730	ALA	2.8
1	D	754	TYR	2.8
3	C	177	GLN	2.7
2	B	30	SER	2.7
2	B	34	TYR	2.7
2	B	28	GLY	2.7
1	D	714	GLU	2.7
1	D	867	ARG	2.7
1	D	162	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	362	SER	2.7
1	A	606	GLU	2.7
1	A	764	VAL	2.7
1	D	305	LEU	2.7
2	G	177	LEU	2.7
1	D	243	ARG	2.7
1	A	605	SER	2.7
1	A	618	GLU	2.6
3	C	212	GLU	2.6
1	D	303	ASN	2.6
2	B	13	LEU	2.6
1	A	761	VAL	2.6
2	G	203	CYS	2.6
1	D	865	ALA	2.6
2	G	9	TRP	2.6
3	H	193	SER	2.6
2	G	216	LYS	2.6
1	A	33	GLU	2.6
1	D	361	GLY	2.6
1	A	308	PRO	2.6
3	H	153	LEU	2.5
2	G	27	TYR	2.5
1	A	689	SER	2.5
1	A	709	TRP	2.5
3	C	136	PRO	2.5
2	B	132	ALA	2.5
2	G	112	GLN	2.5
3	H	111	SER	2.5
3	H	190	TYR	2.5
1	A	769	VAL	2.5
3	C	211	CYS	2.4
1	D	729	ASP	2.4
2	B	149	VAL	2.4
1	D	91	HIS	2.4
1	D	760	HIS	2.4
1	A	339	THR	2.4
1	D	753	ASP	2.4
3	H	182	GLU	2.4
3	C	130	PRO	2.4
1	D	568	GLN	2.4
2	B	112	GLN	2.4
2	G	176	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	737	LEU	2.4
3	C	214	THR	2.4
1	D	601	GLY	2.4
1	D	889	GLY	2.4
2	B	100	GLY	2.4
1	D	715	VAL	2.4
3	C	223	THR	2.3
1	D	809	HIS	2.3
2	G	171	HIS	2.3
1	A	169	ASP	2.3
2	G	128	VAL	2.3
3	C	133	PHE	2.3
3	H	79	PHE	2.3
1	A	800	ALA	2.3
1	D	360	ARG	2.3
3	C	165	TRP	2.3
1	A	684	VAL	2.3
2	B	150	LYS	2.3
3	C	213	VAL	2.3
1	D	755	ALA	2.2
1	A	91	HIS	2.2
1	A	908	LEU	2.2
1	D	752	VAL	2.2
1	D	772	LEU	2.2
3	H	45	VAL	2.2
3	H	192	LEU	2.2
2	G	78	ASN	2.2
1	A	241	PHE	2.2
3	H	158	PRO	2.2
1	A	734	ARG	2.2
1	A	405	ARG	2.1
1	D	302	SER	2.1
2	B	64	SER	2.1
3	C	134	ILE	2.1
3	C	148	SER	2.1
1	D	600	ALA	2.1
3	C	203	TYR	2.1
1	A	166	ASP	2.1
1	D	681	VAL	2.1
3	C	210	ALA	2.1
2	B	20	LEU	2.1
1	D	166	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	222	SER	2.1
3	H	160	GLU	2.1
3	C	152	LEU	2.1
3	H	25	GLY	2.1
3	H	127	VAL	2.1
2	G	172	THR	2.0
1	A	768	LEU	2.0
3	C	138	SER	2.0
1	A	503	PRO	2.0
1	D	710	THR	2.0
2	G	158	THR	2.0
1	A	343	LEU	2.0
1	D	30	LEU	2.0
2	B	71	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.