Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 08:03 PM EDT

PDB ID	:	8EE0
Title	:	KS-AT didomain from module 2 of the 6-deoxyerythronolide B synthase in complex with antibody fragment 1B2
Authors	:	Cogan, D.P.; Brodsky, K.L.; Guzman, K.M.; Mathews, I.I.; Khosla, C.
Deposited on	:	2022-09-06
Resolution	:	2.65 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:

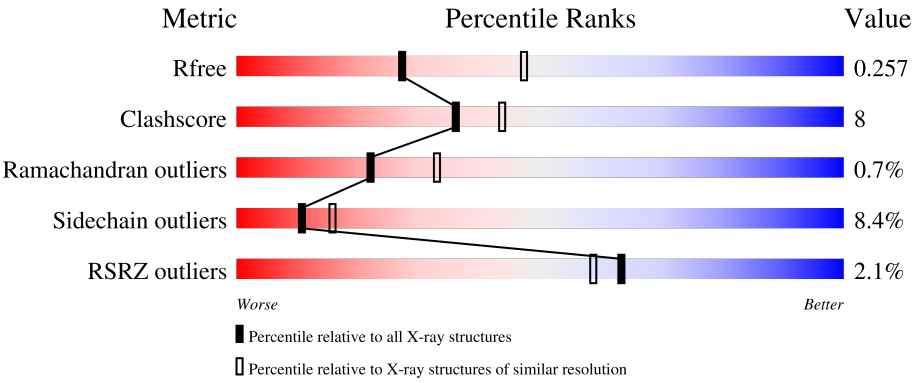
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	2% 73% 18% • 6%
2	L	236	% 71% 18% • 9%
3	H	249	2% 64% 19% • 15%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9704 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	877	Total	C	N	O	S	0	0	0
			6372	3972	1161	1218	21			

There are 43 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
A	26	ARG	-	expression tag	UNP Q5UNP6
A	27	ILE	-	expression tag	UNP Q5UNP6

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called 1B2 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1640	1029	275	330	6			

- Molecule 3 is a protein called 1B2 antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	211	Total	C	N	O	S	0	0	0
			1580	1002	264	308	6			

- Molecule 4 is water.

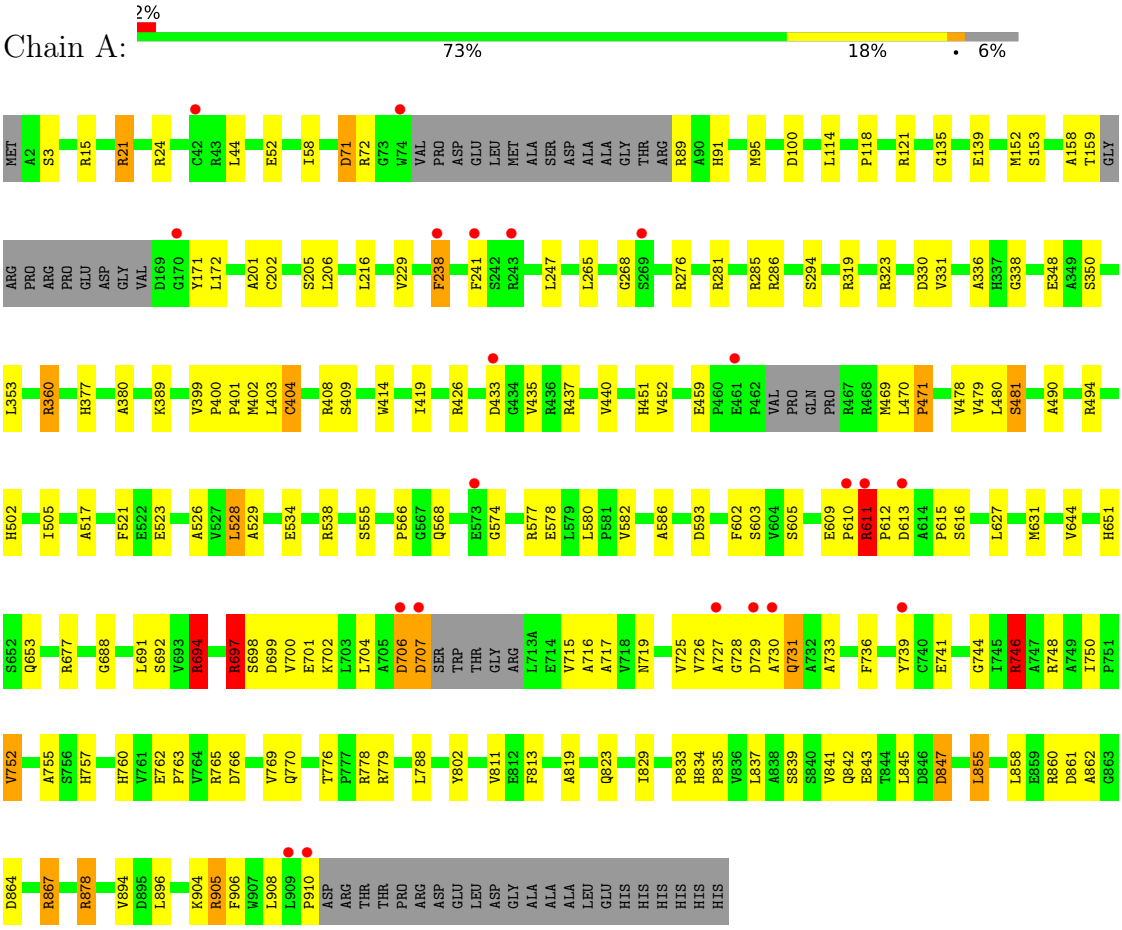
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total	O	0	0
			69	69		
4	L	22	Total	O	0	0
			22	22		
4	H	21	Total	O	0	0
			21	21		

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.

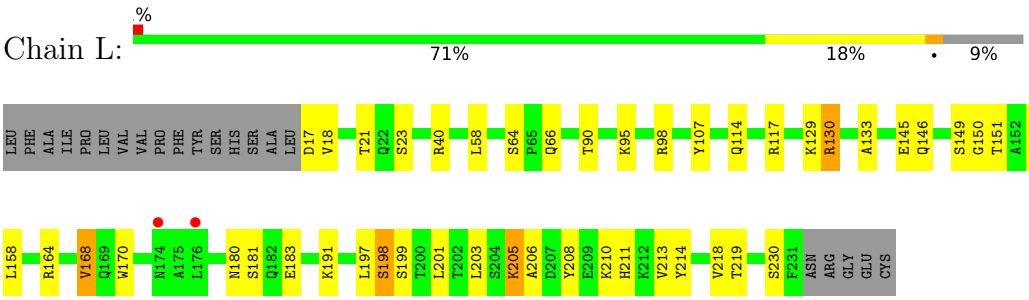
• Molecule 1: 6-deoxyerythronolide B synthase

Chain A:



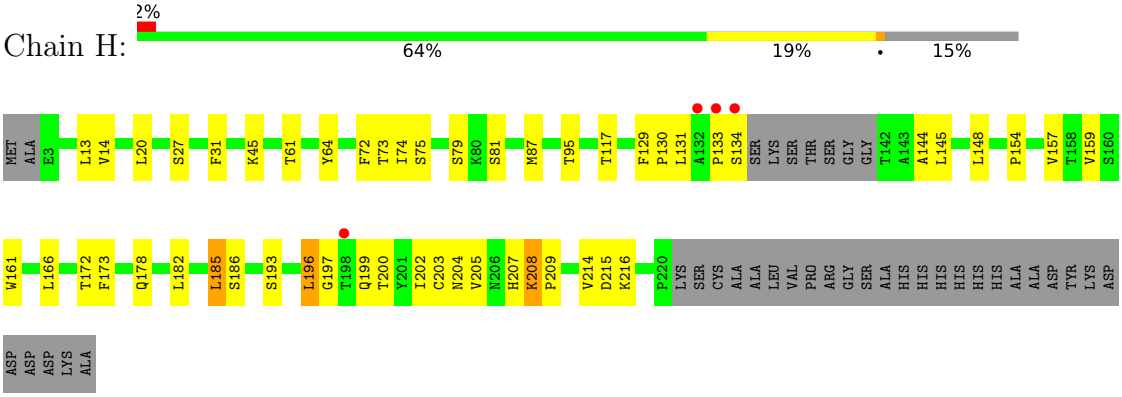
• Molecule 2: 1B2 antibody light chain

Chain L:



• Molecule 3: 1B2 antibody heavy chain

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.85Å 91.85Å 393.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.66 – 2.65 39.66 – 2.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (39.66-2.65) 93.2 (39.66-2.65)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.211 , 0.254 0.215 , 0.257	Depositor DCC
R_{free} test set	2513 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	50.0	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 36.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9704	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.47	0/6491	0.70	0/8838
2	L	0.50	0/1677	0.65	0/2282
3	H	0.50	0/1617	0.65	0/2200
All	All	0.48	0/9785	0.69	0/13320

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	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	611	ARG	Sidechain
1	A	694	ARG	Sidechain
1	A	697	ARG	Sidechain
1	A	72	ARG	Sidechain
1	A	746	ARG	Sidechain
1	A	748	ARG	Sidechain
1	A	860	ARG	Sidechain
1	A	878	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	6372	0	6244	103	0
2	L	1640	0	1596	22	0
3	H	1580	0	1553	28	0
4	A	69	0	0	2	0
4	H	21	0	0	0	0
4	L	22	0	0	0	0
All	All	9704	0	9393	151	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 8.

All (151) 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)
2:L:18:VAL:HG22	2:L:114:GLN:HE22	1.47	0.78
3:H:172:THR:HG22	3:H:185:LEU:HD11	1.69	0.75
1:A:716:ALA:HB1	1:A:757:HIS:HB2	1.69	0.74
1:A:717:ALA:HB3	1:A:725:VAL:HB	1.75	0.67
1:A:691:LEU:HD11	1:A:726:VAL:HB	1.76	0.67
1:A:95:MET:SD	1:A:268:GLY:HA2	2.35	0.67
3:H:95:THR:HG23	3:H:117:THR:HA	1.76	0.66
1:A:688:GLY:HA2	1:A:729:ASP:CB	2.27	0.65
1:A:205:SER:HB3	1:A:380:ALA:O	1.97	0.64
1:A:408:ARG:HB3	1:A:414:TRP:CH2	2.33	0.63
1:A:819:ALA:O	1:A:823:GLN:HG3	1.98	0.62
1:A:862:ALA:HB1	1:A:867:ARG:HB2	1.82	0.61
1:A:389:LYS:HE3	1:A:400:PRO:HB2	1.82	0.61
1:A:730:ALA:O	1:A:733:ALA:N	2.33	0.60
3:H:159:VAL:HG22	3:H:205:VAL:HG12	1.82	0.60
1:A:829:ILE:HG12	1:A:855:LEU:HD12	1.83	0.60
1:A:281:ARG:NH1	1:A:459:GLU:O	2.34	0.59
3:H:185:LEU:HD12	3:H:186:SER:N	2.18	0.59
2:L:154:VAL:HG13	2:L:201:LEU:HB3	1.85	0.58
1:A:121:ARG:NH2	1:A:906:PHE:O	2.35	0.58
1:A:855:LEU:HD21	1:A:878:ARG:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:THR:H	1:A:910:PRO:HG3	1.70	0.57
1:A:114:LEU:HG	1:A:908:LEU:HD13	1.86	0.56
3:H:133:PRO:HA	3:H:144:ALA:O	2.05	0.56
1:A:58:ILE:HG13	1:A:401:PRO:HG2	1.88	0.55
1:A:729:ASP:O	1:A:730:ALA:C	2.45	0.55
2:L:211:HIS:HB2	2:L:214:TYR:OH	2.06	0.54
1:A:294:SER:HB3	1:A:452:VAL:HG22	1.89	0.54
1:A:502:HIS:O	1:A:505:ILE:HG22	2.08	0.54
1:A:766:ASP:O	1:A:770:GLN:HG3	2.08	0.53
1:A:331:VAL:O	1:A:360:ARG:NH2	2.36	0.53
2:L:58:LEU:O	2:L:66:GLN:HG2	2.09	0.53
1:A:691:LEU:CD1	1:A:726:VAL:HB	2.38	0.53
1:A:842:GLN:HA	1:A:845:LEU:HD12	1.91	0.53
1:A:528:LEU:O	1:A:538:ARG:NH1	2.42	0.53
3:H:157:VAL:CG1	3:H:185:LEU:HD23	2.38	0.53
2:L:208:TYR:HA	2:L:214:TYR:OH	2.09	0.53
1:A:21:ARG:NH1	4:A:1004:HOH:O	2.42	0.52
1:A:580:LEU:O	1:A:586:ALA:HB2	2.09	0.52
1:A:158:ALA:HB1	1:A:172:LEU:HD21	1.91	0.52
1:A:610:PRO:O	1:A:612:PRO:HD3	2.09	0.52
2:L:146:GLN:HG3	3:H:129:PHE:CE2	2.45	0.52
1:A:89:ARG:N	4:A:1005:HOH:O	2.43	0.52
1:A:574:GLY:H	1:A:611:ARG:HH22	1.57	0.52
1:A:694:ARG:HH21	1:A:746:ARG:HD2	1.75	0.51
2:L:168:VAL:HG12	2:L:218:VAL:HG22	1.91	0.51
3:H:154:PRO:HD2	3:H:209:PRO:HB2	1.93	0.51
2:L:156:CYS:HB2	2:L:170:TRP:CH2	2.46	0.51
3:H:72:PHE:CZ	3:H:87:MET:HG2	2.45	0.51
1:A:353:LEU:HG	1:A:419:ILE:HD12	1.94	0.50
3:H:72:PHE:CE2	3:H:87:MET:HG2	2.47	0.50
3:H:133:PRO:HB3	3:H:145:LEU:HB3	1.93	0.50
1:A:471:PRO:HD3	1:A:582:VAL:HG22	1.93	0.50
1:A:904:LYS:HE2	1:A:906:PHE:CZ	2.47	0.50
1:A:609:GLU:O	1:A:610:PRO:C	2.49	0.50
1:A:578:GLU:CB	1:A:864:ASP:HA	2.42	0.49
1:A:730:ALA:O	1:A:731:GLN:C	2.51	0.49
3:H:173:PHE:O	3:H:185:LEU:HD13	2.13	0.48
1:A:100:ASP:OD1	1:A:905:ARG:HG2	2.14	0.48
1:A:21:ARG:HH12	1:A:24:ARG:HH11	1.61	0.48
2:L:40:ARG:HG2	2:L:90:THR:O	2.14	0.48
1:A:602:PHE:CG	1:A:615:PRO:HG2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.74	0.48
1:A:837:LEU:O	1:A:841:VAL:HG23	2.14	0.48
2:L:158:LEU:HB2	2:L:197:LEU:HB3	1.94	0.48
3:H:178:GLN:HG3	3:H:182:LEU:O	2.14	0.47
3:H:64:TYR:CE1	3:H:74:ILE:HD12	2.49	0.47
1:A:706:ASP:O	1:A:707:ASP:C	2.52	0.47
2:L:58:LEU:HD13	2:L:107:TYR:CZ	2.49	0.47
3:H:205:VAL:HG22	3:H:214:VAL:HB	1.97	0.47
1:A:91:HIS:O	1:A:238:PHE:HZ	1.98	0.47
1:A:433:ASP:C	1:A:435:VAL:H	2.18	0.47
2:L:129:LYS:HG3	2:L:130:ARG:N	2.29	0.47
1:A:490:ALA:O	1:A:494:ARG:HG3	2.15	0.47
1:A:729:ASP:CB	1:A:760:HIS:NE2	2.78	0.47
1:A:241:PHE:HB3	1:A:247:LEU:HG	1.97	0.46
1:A:813:PHE:CZ	1:A:837:LEU:HD13	2.50	0.46
1:A:216:LEU:O	1:A:276:ARG:NH1	2.49	0.46
3:H:172:THR:CG2	3:H:185:LEU:HD11	2.41	0.46
1:A:402:MET:HG2	1:A:404:CYS:SG	2.55	0.46
3:H:13:LEU:HD12	3:H:14:VAL:H	1.81	0.46
3:H:157:VAL:HG23	3:H:207:HIS:HB2	1.96	0.46
1:A:478:VAL:O	1:A:526:ALA:HA	2.16	0.46
1:A:727:ALA:O	1:A:729:ASP:N	2.49	0.46
1:A:389:LYS:CE	1:A:400:PRO:HB2	2.46	0.46
1:A:697:ARG:O	1:A:698:SER:C	2.54	0.45
1:A:577:ARG:HA	1:A:580:LEU:HD12	1.98	0.45
1:A:729:ASP:CB	1:A:755:ALA:HB2	2.47	0.45
1:A:750:ILE:O	1:A:752:VAL:N	2.49	0.45
1:A:574:GLY:O	1:A:577:ARG:HB2	2.17	0.45
1:A:727:ALA:C	1:A:729:ASP:H	2.20	0.45
2:L:206:ALA:O	2:L:210:LYS:HG2	2.17	0.45
2:L:145:GLU:H	2:L:145:GLU:HG3	1.47	0.44
1:A:481:SER:OG	1:A:521:PHE:N	2.50	0.44
1:A:330:ASP:HB3	1:A:437:ARG:NH1	2.32	0.44
3:H:185:LEU:HD12	3:H:186:SER:H	1.82	0.44
1:A:21:ARG:NH1	1:A:24:ARG:HH11	2.15	0.44
2:L:180:ASN:N	2:L:180:ASN:OD1	2.51	0.44
3:H:130:PRO:HD3	3:H:216:LYS:HE3	1.99	0.44
1:A:833:PRO:HA	1:A:858:LEU:HB2	2.00	0.44
1:A:736:PHE:O	1:A:739:TYR:HB2	2.18	0.44
2:L:205:LYS:HB2	2:L:205:LYS:HE3	1.65	0.44
2:L:150:GLY:HA2	2:L:205:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:158:LEU:HD21	2:L:218:VAL:HG13	1.99	0.44
1:A:44:LEU:HD23	1:A:268:GLY:HA3	2.00	0.44
1:A:691:LEU:HG	1:A:726:VAL:O	2.18	0.44
1:A:904:LYS:HE2	1:A:906:PHE:HZ	1.82	0.43
1:A:593:ASP:OD2	1:A:605:SER:OG	2.31	0.43
3:H:131:LEU:HD21	3:H:148:LEU:HB2	2.00	0.43
1:A:399:VAL:HB	1:A:426:ARG:HB2	2.00	0.43
1:A:765:ARG:O	1:A:769:VAL:HG23	2.19	0.43
3:H:166:LEU:HD12	3:H:166:LEU:HA	1.88	0.43
3:H:161:TRP:CH2	3:H:203:CYS:HB3	2.54	0.43
1:A:778:ARG:NH1	3:H:215:ASP:OD2	2.52	0.43
2:L:130:ARG:NH2	2:L:133:ALA:HB2	2.34	0.42
1:A:336:ALA:HB1	1:A:348:GLU:OE2	2.18	0.42
1:A:602:PHE:CB	1:A:615:PRO:HG2	2.49	0.42
1:A:566:PRO:HB3	1:A:837:LEU:HD12	2.01	0.42
1:A:788:LEU:HD23	1:A:802:TYR:CE2	2.55	0.42
1:A:834:HIS:CG	1:A:835:PRO:HD2	2.55	0.42
1:A:433:ASP:C	1:A:435:VAL:N	2.73	0.42
1:A:479:VAL:O	1:A:480:LEU:HD23	2.19	0.42
3:H:20:LEU:HB3	3:H:87:MET:HE3	2.02	0.42
2:L:146:GLN:HE22	2:L:153:SER:N	2.18	0.41
2:L:183:GLU:HA	2:L:198:SER:O	2.20	0.41
1:A:409:SER:O	1:A:414:TRP:CZ3	2.73	0.41
1:A:651:HIS:CD2	1:A:811:VAL:HG11	2.54	0.41
1:A:15:ARG:HD2	1:A:15:ARG:HA	1.73	0.41
1:A:523:GLU:OE1	1:A:555:SER:HB3	2.20	0.41
1:A:152:MET:HG3	1:A:229:VAL:HG13	2.03	0.41
1:A:894:VAL:HG23	1:A:896:LEU:HG	2.02	0.41
2:L:168:VAL:CG1	2:L:218:VAL:HG22	2.51	0.41
1:A:247:LEU:HD23	1:A:247:LEU:HA	1.90	0.41
1:A:433:ASP:O	1:A:435:VAL:HG23	2.20	0.41
1:A:118:PRO:HA	1:A:121:ARG:HG3	2.02	0.41
1:A:286:ARG:C	1:A:286:ARG:HD2	2.42	0.41
1:A:319:ARG:O	1:A:323:ARG:HG3	2.20	0.41
1:A:577:ARG:HH11	1:A:610:PRO:HD3	1.86	0.41
1:A:904:LYS:H	1:A:904:LYS:HG3	1.64	0.41
1:A:627:LEU:O	1:A:631:MET:HG3	2.21	0.41
3:H:202:ILE:HA	3:H:216:LYS:O	2.21	0.41
1:A:529:ALA:HB1	1:A:534:GLU:HB3	2.04	0.40
1:A:701:GLU:O	1:A:704:LEU:HB2	2.22	0.40
1:A:847:ASP:N	1:A:847:ASP:OD1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:31:PHE:CD2	3:H:81:SER:HA	2.56	0.40
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.77	0.40
3:H:208:LYS:HE2	3:H:208:LYS:H	1.86	0.40
1:A:71:ASP:HB2	1:A:905:ARG:NH1	2.37	0.40
1:A:440:VAL:O	1:A:451:HIS:HA	2.21	0.40
1:A:762:GLU:N	1:A:763:PRO:HD2	2.36	0.40
1:A:135:GLY:HA2	1:A:517:ALA:HB1	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	867/932 (93%)	808 (93%)	52 (6%)	7 (1%)	19 29
2	L	213/236 (90%)	204 (96%)	9 (4%)	0	100 100
3	H	207/249 (83%)	193 (93%)	12 (6%)	2 (1%)	15 23
All	All	1287/1417 (91%)	1205 (94%)	73 (6%)	9 (1%)	22 33

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	471	PRO
3	H	196	LEU
1	A	338	GLY
1	A	728	GLY
1	A	744	GLY
3	H	197	GLY
1	A	201	ALA
1	A	731	GLN
1	A	404	CYS

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	631/690 (91%)	583 (92%)	48 (8%)	13 21
2	L	189/208 (91%)	167 (88%)	22 (12%)	5 7
3	H	175/203 (86%)	161 (92%)	14 (8%)	12 18
All	All	995/1101 (90%)	911 (92%)	84 (8%)	11 16

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	21	ARG
1	A	52	GLU
1	A	71	ASP
1	A	139	GLU
1	A	153	SER
1	A	171	TYR
1	A	202	CYS
1	A	206	LEU
1	A	238	PHE
1	A	285	ARG
1	A	350	SER
1	A	360	ARG
1	A	377	HIS
1	A	403	LEU
1	A	469	MET
1	A	481	SER
1	A	528	LEU
1	A	568	GLN
1	A	603	SER
1	A	611	ARG
1	A	613	ASP
1	A	616	SER
1	A	644	VAL
1	A	653	GLN
1	A	677	ARG

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Mol	Chain	Res	Type
1	A	692	SER
1	A	694	ARG
1	A	697	ARG
1	A	699	ASP
1	A	700	VAL
1	A	702	LYS
1	A	706	ASP
1	A	707	ASP
1	A	715	VAL
1	A	719	ASN
1	A	741	GLU
1	A	746	ARG
1	A	752	VAL
1	A	776	THR
1	A	779	ARG
1	A	839	SER
1	A	843	GLU
1	A	847	ASP
1	A	855	LEU
1	A	861	ASP
1	A	867	ARG
1	A	905	ARG
2	L	17	ASP
2	L	21	THR
2	L	23	SER
2	L	64	SER
2	L	95	LYS
2	L	98	ARG
2	L	117	ARG
2	L	130	ARG
2	L	149	SER
2	L	151	THR
2	L	154	VAL
2	L	164	ARG
2	L	168	VAL
2	L	181	SER
2	L	191	LYS
2	L	198	SER
2	L	199	SER
2	L	203	LEU
2	L	205	LYS
2	L	213	VAL

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Mol	Chain	Res	Type
2	L	219	THR
2	L	230	SER
3	H	27	SER
3	H	45	LYS
3	H	61	THR
3	H	73	THR
3	H	75	SER
3	H	79	SER
3	H	134	SER
3	H	185	LEU
3	H	193	SER
3	H	196	LEU
3	H	199	GLN
3	H	200	THR
3	H	204	ASN
3	H	208	LYS

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	176	ASN
1	A	568	GLN
1	A	814	HIS
2	L	159	ASN
2	L	221	GLN
3	H	171	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	877/932 (94%)	-0.17	21 (2%)	59	54	32, 50, 85, 121	0
2	L	215/236 (91%)	-0.39	2 (0%)	84	83	34, 52, 90, 103	0
3	H	211/249 (84%)	-0.28	4 (1%)	66	63	36, 55, 83, 102	0
All	All	1303/1417 (91%)	-0.22	27 (2%)	63	59	32, 51, 86, 121	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	198	THR	7.2
1	A	910	PRO	4.8
1	A	707	ASP	4.4
3	H	134	SER	4.3
1	A	461	GLU	4.2
1	A	611	ARG	4.0
1	A	729	ASP	4.0
3	H	133	PRO	3.8
1	A	727	ALA	3.5
1	A	42	CYS	3.3
1	A	613	ASP	3.2
1	A	433	ASP	3.0
1	A	243	ARG	3.0
1	A	573	GLU	2.8
1	A	238	PHE	2.6
1	A	706	ASP	2.5
1	A	74	TRP	2.4
1	A	241	PHE	2.3
2	L	174	ASN	2.3
1	A	170	GLY	2.3
2	L	176	LEU	2.2
1	A	739	TYR	2.2
1	A	730	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	909	LEU	2.1
1	A	269	SER	2.0
3	H	132	ALA	2.0
1	A	610	PRO	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 monosaccharides 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.