



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:36 PM GMT

PDB ID : 1UB5
Title : Crystal structure of Antibody 19G2 with hapten at 100K
Authors : Beuscher, A.B.; Wirsching, P.; Lerner, R.A.; Janda, K.; Stevens, R.C.
Deposited on : 2003-03-30
Resolution : 2.00 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

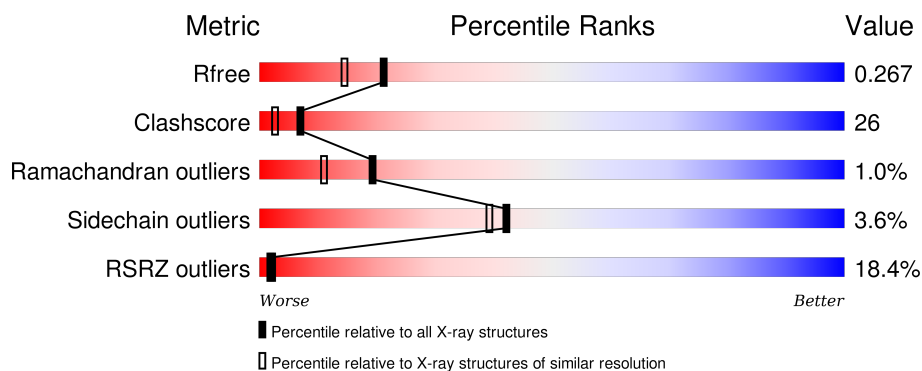
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	209	<div> <div>16%</div> <div>62%</div> <div>35%</div> <div>.</div> </div>
1	H	209	<div> <div>17%</div> <div>66%</div> <div>32%</div> <div>.</div> </div>
2	B	214	<div> <div>22%</div> <div>61%</div> <div>38%</div> <div>.</div> </div>
2	L	214	<div> <div>19%</div> <div>61%</div> <div>36%</div> <div>.</div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7017 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.

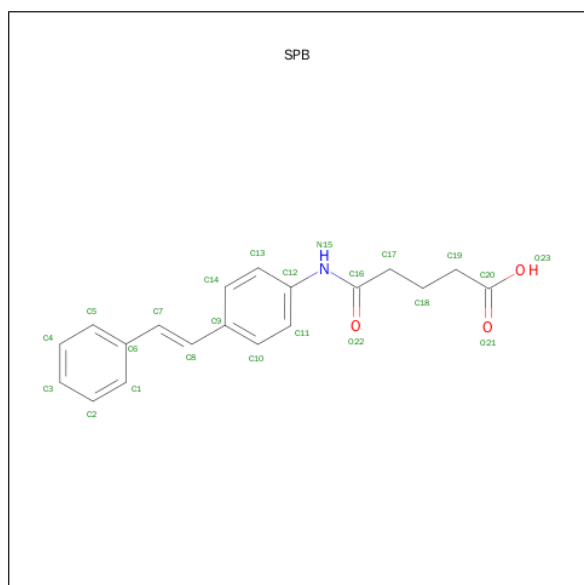
- Molecule 1 is a protein called antibody 19G2, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	209	Total	C	N	O	S	0	0	0
			1560	985	261	306	8			
1	A	209	Total	C	N	O	S	0	0	0
			1560	985	261	306	8			

- Molecule 2 is a protein called antibody 19G2, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total	C	N	O	S	0	0	0
			1647	1032	275	333	7			
2	B	214	Total	C	N	O	S	0	0	0
			1647	1032	275	333	7			

- Molecule 3 is 4-(4-STYRYL-PHENYL-CARBAMOYL)-BUTYRIC ACID (three-letter code: SPB) (formula: C₁₉H₁₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			23	19	1	3		
3	B	1	Total	C	N	O	0	0
			23	19	1	3		

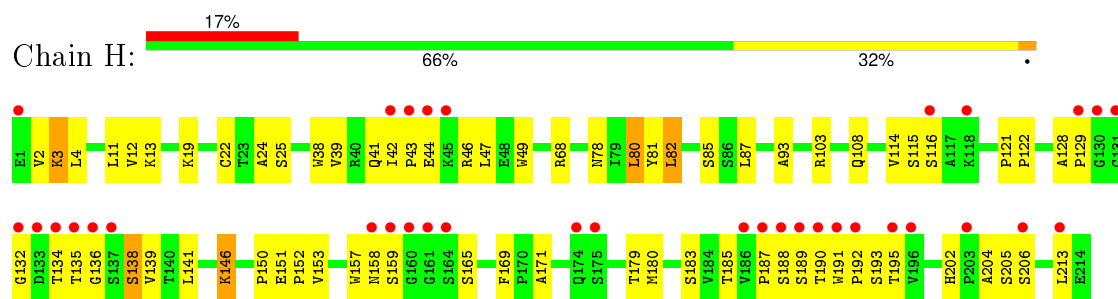
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	145	Total	O	0	0
			145	145		
4	B	157	Total	O	0	0
			157	157		
4	H	92	Total	O	0	0
			92	92		
4	L	163	Total	O	0	0
			163	163		

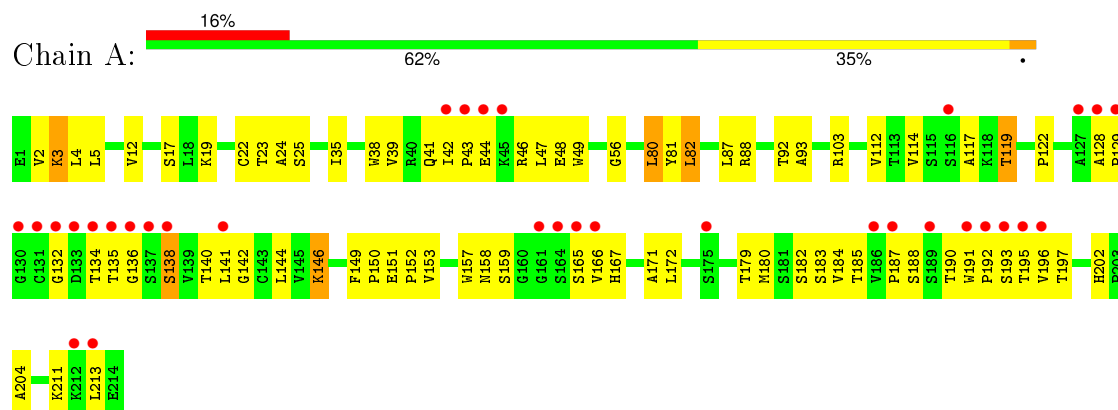
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

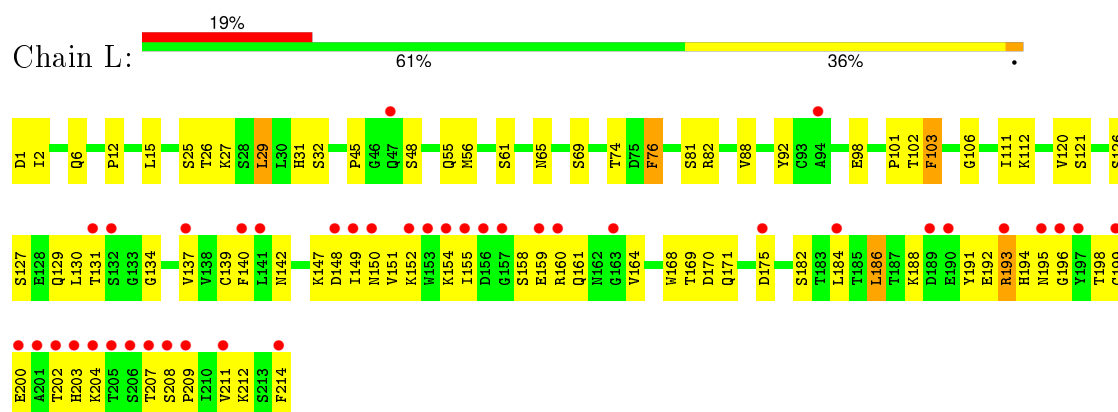
- Molecule 1: antibody 19G2, alpha chain



- Molecule 1: antibody 19G2, alpha chain

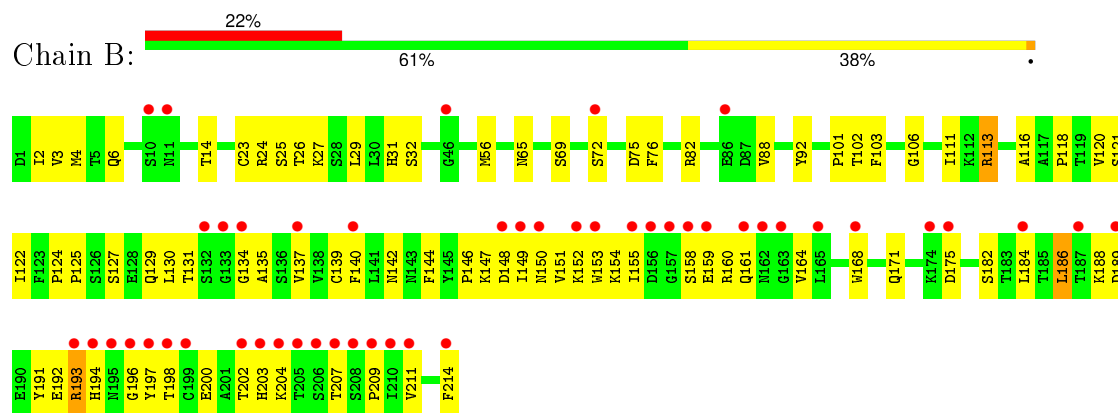


- Molecule 2: antibody 19G2, beta chain



● Molecule 2: antibody 19G2, beta chain

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.93Å 61.06Å 92.59Å 90.00° 117.05° 90.00°	Depositor
Resolution (Å)	19.89 – 2.00 19.88 – 1.89	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.89-2.00) 94.2 (19.88-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.267 0.247 , 0.267	Depositor DCC
R_{free} test set	3207 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.8	EDS
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 76903 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7017	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.31	0/1599	0.63	0/2182
1	H	0.30	0/1599	0.61	0/2182
2	B	0.32	0/1684	0.58	0/2288
2	L	0.33	0/1684	0.59	0/2288
All	All	0.32	0/6566	0.60	0/8940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1560	0	1546	95	0
1	H	1560	0	1546	71	0
2	B	1647	0	1596	95	0
2	L	1647	0	1596	82	1
3	B	23	0	18	1	0
3	H	23	0	18	0	0
4	A	145	0	0	40	0
4	B	157	0	0	42	0
4	H	92	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	163	0	0	31	1
All	All	7017	0	6320	338	1

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 26.

All (338) 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:B:24:ARG:HA	4:B:843:HOH:O	1.60	0.99
2:L:175:ASP:HB3	4:L:295:HOH:O	1.63	0.98
2:B:175:ASP:HB3	4:B:752:HOH:O	1.65	0.94
2:B:2:ILE:HG13	4:B:851:HOH:O	1.68	0.94
1:H:11:LEU:HD11	1:H:150:PRO:HG2	1.51	0.90
1:A:144:LEU:HG	4:A:299:HOH:O	1.75	0.86
2:B:139:CYS:HB2	4:B:832:HOH:O	1.75	0.84
2:L:2:ILE:HD11	2:L:25:SER:OG	1.78	0.84
1:A:166:VAL:HG22	4:A:271:HOH:O	1.78	0.83
2:B:2:ILE:HD11	2:B:25:SER:OG	1.80	0.82
2:L:102:THR:HB	4:L:350:HOH:O	1.80	0.81
2:L:98:GLU:HG3	4:L:323:HOH:O	1.81	0.81
1:A:4:LEU:HD23	1:A:24:ALA:HB2	1.63	0.80
2:L:25:SER:HB3	4:L:349:HOH:O	1.82	0.80
2:B:189:ASP:HB3	4:B:829:HOH:O	1.83	0.79
1:H:4:LEU:HD23	1:H:24:ALA:HB2	1.65	0.78
1:H:44:GLU:HG3	1:H:46:ARG:H	1.48	0.78
1:H:41:GLN:HG3	4:H:644:HOH:O	1.82	0.78
2:L:2:ILE:HD13	2:L:27:LYS:HB3	1.67	0.76
2:B:75:ASP:HA	4:B:843:HOH:O	1.84	0.76
2:B:129:GLN:HG3	4:B:824:HOH:O	1.83	0.76
2:L:126:SER:HB3	4:L:348:HOH:O	1.85	0.76
1:A:146:LYS:HD2	4:B:850:HOH:O	1.85	0.76
1:A:44:GLU:HG3	1:A:46:ARG:H	1.49	0.76
2:L:188:LYS:O	2:L:192:GLU:HG2	1.86	0.75
1:A:22:CYS:SG	4:A:331:HOH:O	2.43	0.75
1:H:24:ALA:HB3	4:H:633:HOH:O	1.87	0.75
2:B:2:ILE:HD13	2:B:27:LYS:HB3	1.68	0.74
4:A:334:HOH:O	2:B:124:PRO:HD2	1.86	0.74
2:B:188:LYS:O	2:B:192:GLU:HG2	1.86	0.74
1:A:39:VAL:HG12	1:A:47:LEU:HD12	1.71	0.71
2:B:24:ARG:HD3	4:B:825:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:PRO:HB2	2:L:112:LYS:HB2	1.71	0.71
1:H:11:LEU:HD11	1:H:150:PRO:CG	2.20	0.70
2:B:2:ILE:HG22	4:B:728:HOH:O	1.91	0.70
1:H:39:VAL:HG12	1:H:47:LEU:HD12	1.72	0.70
1:A:144:LEU:HD21	4:B:850:HOH:O	1.91	0.70
2:B:113:ARG:HB2	2:B:113:ARG:NH1	2.07	0.70
1:H:189:SER:HB2	4:H:649:HOH:O	1.91	0.70
2:B:200:GLU:HG3	2:B:211:VAL:HG12	1.74	0.69
2:B:111:ILE:H	2:B:171:GLN:HE22	1.39	0.69
2:B:203:HIS:HB3	4:B:807:HOH:O	1.93	0.69
1:A:136:GLY:O	1:A:188:SER:HB2	1.93	0.69
1:H:136:GLY:O	1:H:188:SER:HB2	1.93	0.69
1:A:41:GLN:HG3	4:A:287:HOH:O	1.93	0.69
1:H:141:LEU:HB3	1:H:213:LEU:HD13	1.76	0.68
1:H:121:PRO:HB3	4:H:678:HOH:O	1.93	0.68
1:H:108:GLN:HB2	4:H:687:HOH:O	1.93	0.68
1:A:141:LEU:HB3	1:A:213:LEU:HD13	1.75	0.68
2:B:186:LEU:HG	4:B:827:HOH:O	1.93	0.67
2:B:111:ILE:HB	4:B:849:HOH:O	1.93	0.67
2:L:200:GLU:HG3	2:L:211:VAL:HG12	1.75	0.67
2:B:135:ALA:HA	4:B:759:HOH:O	1.94	0.67
1:A:157:TRP:HH2	4:A:319:HOH:O	1.77	0.67
2:L:29:LEU:HD13	4:L:375:HOH:O	1.93	0.67
1:H:151:GLU:N	1:H:152:PRO:HD2	2.10	0.66
2:L:154:LYS:HB2	2:L:198:THR:HB	1.78	0.66
2:L:196:GLY:HA2	2:L:214:PHE:O	1.96	0.66
2:L:149:ILE:HG12	4:L:357:HOH:O	1.96	0.66
2:B:154:LYS:HB2	2:B:198:THR:HB	1.78	0.66
1:A:129:PRO:HA	4:A:320:HOH:O	1.94	0.66
2:B:196:GLY:HA2	2:B:214:PHE:O	1.96	0.66
1:A:213:LEU:HB2	4:A:341:HOH:O	1.96	0.66
1:A:213:LEU:HD21	4:A:319:HOH:O	1.95	0.65
1:A:151:GLU:N	1:A:152:PRO:HD2	2.10	0.65
1:A:112:VAL:HA	4:A:258:HOH:O	1.95	0.65
1:H:42:ILE:HB	1:H:43:PRO:HD2	1.78	0.65
2:L:81:SER:HA	4:L:345:HOH:O	1.96	0.65
1:H:4:LEU:HD23	1:H:24:ALA:CB	2.26	0.64
1:A:119:THR:HG22	4:A:337:HOH:O	1.96	0.64
1:A:47:LEU:HD22	4:A:287:HOH:O	1.97	0.64
1:A:196:VAL:HA	4:A:311:HOH:O	1.96	0.64
1:A:42:ILE:HB	1:A:43:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HB	4:A:330:HOH:O	1.98	0.64
1:H:191:TRP:HB3	4:H:668:HOH:O	1.98	0.64
1:A:187:PRO:HG2	1:A:190:THR:HG22	1.79	0.64
1:H:47:LEU:HD23	4:L:245:HOH:O	1.99	0.63
1:H:187:PRO:HG2	1:H:190:THR:HG22	1.79	0.63
1:A:4:LEU:HD23	1:A:24:ALA:CB	2.27	0.63
2:B:207:THR:O	2:B:209:PRO:HD3	1.99	0.63
2:B:72:SER:HB3	4:B:856:HOH:O	1.97	0.63
1:H:150:PRO:HD2	1:H:204:ALA:HB1	1.80	0.63
1:A:196:VAL:HB	4:A:341:HOH:O	1.98	0.63
1:A:3:LYS:HB2	4:A:338:HOH:O	1.98	0.63
2:L:207:THR:O	2:L:209:PRO:HD3	1.99	0.62
1:A:172:LEU:HD12	4:B:838:HOH:O	1.99	0.62
2:B:6:GLN:NE2	2:B:106:GLY:H	1.97	0.62
1:A:150:PRO:HD2	1:A:204:ALA:HB1	1.80	0.62
2:L:129:GLN:N	4:L:348:HOH:O	2.33	0.61
2:L:6:GLN:NE2	2:L:106:GLY:H	1.97	0.61
1:H:68:ARG:HA	4:H:676:HOH:O	2.00	0.61
1:A:42:ILE:HG22	1:A:93:ALA:HB2	1.83	0.61
2:B:127:SER:O	2:B:131:THR:HG23	2.01	0.61
1:H:42:ILE:HG22	1:H:93:ALA:HB2	1.84	0.60
2:B:120:VAL:HG12	4:B:832:HOH:O	2.02	0.60
1:A:184:VAL:HB	4:A:286:HOH:O	2.00	0.60
1:A:39:VAL:CG1	1:A:47:LEU:HD12	2.32	0.59
2:B:125:PRO:HG3	4:B:815:HOH:O	2.01	0.59
1:A:211:LYS:HE2	4:A:285:HOH:O	2.03	0.59
2:L:127:SER:O	2:L:131:THR:HG23	2.02	0.59
2:L:208:SER:HB3	4:L:312:HOH:O	2.02	0.59
2:B:116:ALA:HB3	4:B:746:HOH:O	2.02	0.59
2:B:182:SER:HB3	4:B:848:HOH:O	2.02	0.58
2:L:76:PHE:HB3	4:L:334:HOH:O	2.02	0.58
1:A:138:SER:H	1:A:187:PRO:HA	1.68	0.58
2:L:137:VAL:CG1	2:L:184:LEU:HB3	2.33	0.58
2:L:111:ILE:H	2:L:171:GLN:HE22	1.51	0.58
1:A:213:LEU:HD11	4:A:319:HOH:O	2.02	0.58
2:L:151:VAL:HG11	2:L:182:SER:OG	2.04	0.58
2:L:193:ARG:HG3	2:L:194:HIS:ND1	2.19	0.57
1:H:42:ILE:HB	1:H:43:PRO:CD	2.34	0.57
2:B:151:VAL:HG11	2:B:182:SER:OG	2.04	0.57
1:H:138:SER:H	1:H:187:PRO:HA	1.69	0.57
2:B:137:VAL:CG1	2:B:184:LEU:HB3	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:187:PRO:O	1:H:190:THR:HG22	2.05	0.56
2:L:74:THR:HG22	4:L:349:HOH:O	2.05	0.56
2:B:193:ARG:HG3	2:B:194:HIS:ND1	2.19	0.56
1:A:42:ILE:HB	1:A:43:PRO:CD	2.35	0.56
1:H:42:ILE:HG13	1:H:44:GLU:HG2	1.88	0.56
1:H:39:VAL:CG1	1:H:47:LEU:HD12	2.35	0.56
2:B:155:ILE:HD12	2:B:160:ARG:HH11	1.71	0.56
4:H:686:HOH:O	2:L:48:SER:HB3	2.06	0.56
2:L:2:ILE:HG22	4:L:279:HOH:O	2.03	0.56
1:A:47:LEU:HD23	4:B:801:HOH:O	2.04	0.56
2:L:186:LEU:CD1	2:L:191:TYR:HB2	2.35	0.56
2:B:182:SER:HB2	4:B:766:HOH:O	2.06	0.56
2:B:186:LEU:CD1	2:B:191:TYR:HB2	2.35	0.56
1:A:187:PRO:O	1:A:190:THR:HG22	2.06	0.56
1:H:3:LYS:HB2	1:H:3:LYS:NZ	2.20	0.56
2:B:149:ILE:HG12	4:B:744:HOH:O	2.05	0.55
2:B:130:LEU:HD12	4:B:831:HOH:O	2.06	0.55
1:H:141:LEU:HB3	1:H:213:LEU:CD1	2.37	0.55
1:A:17:SER:HB3	4:A:354:HOH:O	2.05	0.55
2:B:168:TRP:HB3	4:B:835:HOH:O	2.06	0.55
1:A:153:VAL:HG12	4:A:254:HOH:O	2.07	0.55
2:L:150:ASN:OD1	2:L:202:THR:HB	2.07	0.55
2:L:155:ILE:HD12	2:L:160:ARG:HH11	1.71	0.55
1:A:141:LEU:HB3	1:A:213:LEU:CD1	2.37	0.55
2:B:188:LYS:HE3	4:B:846:HOH:O	2.08	0.54
1:A:213:LEU:HD22	4:A:345:HOH:O	2.07	0.54
2:L:137:VAL:HG12	2:L:184:LEU:HB3	1.89	0.54
1:A:183:SER:HB3	2:B:140:PHE:CE2	2.42	0.54
2:B:137:VAL:HG12	2:B:184:LEU:HB3	1.90	0.54
2:B:125:PRO:HB3	4:B:759:HOH:O	2.08	0.53
1:A:42:ILE:HG13	1:A:44:GLU:HG2	1.89	0.53
2:B:150:ASN:OD1	2:B:202:THR:HB	2.07	0.53
1:A:213:LEU:HD13	4:A:345:HOH:O	2.08	0.53
1:A:150:PRO:HB2	1:A:152:PRO:HD2	1.89	0.53
1:A:150:PRO:HD2	1:A:204:ALA:CB	2.38	0.53
1:H:206:SER:HA	4:H:667:HOH:O	2.08	0.53
1:H:150:PRO:HB2	1:H:152:PRO:HD2	1.91	0.53
1:H:146:LYS:HB3	1:H:179:THR:HG23	1.90	0.53
2:B:23:CYS:O	4:B:843:HOH:O	2.19	0.53
1:H:12:VAL:HG11	1:H:87:LEU:HD12	1.91	0.52
1:A:195:THR:HA	4:A:317:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:183:SER:HB3	2:L:140:PHE:CE2	2.43	0.52
1:A:128:ALA:HB1	1:A:129:PRO:HD2	1.91	0.52
2:L:199:CYS:HB3	4:L:290:HOH:O	2.10	0.52
2:B:113:ARG:HB2	2:B:113:ARG:HH11	1.72	0.52
2:L:152:LYS:HE3	2:L:154:LYS:HE2	1.92	0.52
1:H:150:PRO:HD2	1:H:204:ALA:CB	2.40	0.52
1:A:146:LYS:HB3	1:A:179:THR:HG23	1.90	0.52
2:L:103:PHE:N	4:L:350:HOH:O	2.43	0.52
1:A:3:LYS:HB2	1:A:3:LYS:NZ	2.25	0.52
2:B:186:LEU:HD11	2:B:191:TYR:HB2	1.92	0.51
2:L:160:ARG:HD2	4:L:356:HOH:O	2.09	0.51
2:B:72:SER:HB2	4:B:787:HOH:O	2.09	0.51
2:L:1:ASP:HA	4:L:341:HOH:O	2.10	0.51
1:H:4:LEU:CD2	1:H:24:ALA:HB2	2.38	0.51
2:B:3:VAL:C	4:B:851:HOH:O	2.47	0.51
2:B:120:VAL:HG11	4:B:804:HOH:O	2.10	0.51
1:A:12:VAL:HG11	1:A:87:LEU:HD12	1.92	0.51
1:H:165:SER:OG	1:H:185:THR:HB	2.10	0.51
1:A:4:LEU:CD2	1:A:24:ALA:HB2	2.37	0.51
2:L:31:HIS:ND1	2:L:32:SER:N	2.58	0.51
2:B:152:LYS:HE3	2:B:154:LYS:HE2	1.92	0.51
1:A:165:SER:OG	1:A:185:THR:HB	2.10	0.51
2:L:88:VAL:HB	4:L:355:HOH:O	2.10	0.50
1:H:128:ALA:HB1	1:H:129:PRO:HD2	1.92	0.50
2:B:129:GLN:HG2	4:B:759:HOH:O	2.10	0.50
2:L:56:MET:O	2:L:69:SER:HB3	2.11	0.50
1:A:197:THR:HB	4:A:295:HOH:O	2.10	0.50
1:H:12:VAL:O	1:H:114:VAL:HA	2.11	0.50
1:H:153:VAL:HG12	4:H:630:HOH:O	2.11	0.50
1:H:13:LYS:CD	1:H:116:SER:HA	2.41	0.50
2:B:121:SER:O	2:B:139:CYS:HA	2.11	0.50
2:B:111:ILE:H	2:B:171:GLN:NE2	2.09	0.50
2:L:121:SER:O	2:L:139:CYS:HA	2.12	0.50
1:A:141:LEU:HD22	4:A:345:HOH:O	2.12	0.50
2:L:186:LEU:HD11	2:L:191:TYR:HB2	1.93	0.50
2:B:118:PRO:HB3	2:B:144:PHE:HB3	1.93	0.50
2:B:192:GLU:C	2:B:194:HIS:H	2.15	0.49
2:L:212:LYS:HB2	4:L:290:HOH:O	2.09	0.49
2:B:161:GLN:O	2:B:164:VAL:HG12	2.12	0.49
2:L:192:GLU:C	2:L:194:HIS:H	2.15	0.49
1:A:185:THR:HG23	4:A:291:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:2:ILE:HD12	2:L:26:THR:OG1	2.12	0.49
2:B:88:VAL:CG1	2:B:111:ILE:HG12	2.43	0.49
2:L:203:HIS:CD2	2:L:204:LYS:H	2.30	0.49
1:H:44:GLU:OE1	1:H:46:ARG:HB3	2.13	0.49
2:B:2:ILE:HD12	2:B:26:THR:OG1	2.12	0.49
2:L:168:TRP:HB3	4:L:272:HOH:O	2.13	0.49
1:A:35:ILE:HD12	3:B:701:SPB:H192	1.94	0.49
1:A:44:GLU:OE1	1:A:46:ARG:HB3	2.13	0.48
2:L:161:GLN:O	2:L:164:VAL:HG12	2.14	0.48
2:L:12:PRO:HG2	4:L:358:HOH:O	2.12	0.48
2:B:31:HIS:ND1	2:B:32:SER:N	2.61	0.48
1:A:191:TRP:N	1:A:192:PRO:HD2	2.29	0.48
2:B:203:HIS:CD2	2:B:204:LYS:H	2.32	0.48
2:L:2:ILE:CD1	2:L:27:LYS:H	2.26	0.48
2:L:120:VAL:HA	2:L:140:PHE:O	2.14	0.48
2:B:2:ILE:HG23	2:B:102:THR:HG1	1.78	0.48
2:B:154:LYS:HA	2:B:158:SER:O	2.13	0.48
1:A:2:VAL:HA	1:A:25:SER:O	2.14	0.48
1:A:46:ARG:HG2	4:A:343:HOH:O	2.14	0.48
1:A:22:CYS:HB3	1:A:80:LEU:HB3	1.94	0.48
2:B:171:GLN:CD	4:B:849:HOH:O	2.53	0.48
2:B:197:TYR:HD1	4:B:828:HOH:O	1.95	0.47
1:H:44:GLU:HG3	1:H:46:ARG:N	2.24	0.47
1:A:88:ARG:HD2	4:A:281:HOH:O	2.13	0.47
1:H:171:ALA:HA	1:H:180:MET:HB3	1.95	0.47
2:B:204:LYS:HB2	4:B:753:HOH:O	2.14	0.47
1:H:191:TRP:N	1:H:192:PRO:HD2	2.28	0.47
2:L:15:LEU:HD21	2:L:111:ILE:HD13	1.96	0.47
2:B:14:THR:HG23	4:B:748:HOH:O	2.14	0.47
2:B:2:ILE:CD1	2:B:27:LYS:H	2.27	0.47
2:L:154:LYS:HA	2:L:158:SER:O	2.13	0.47
1:A:171:ALA:HA	1:A:180:MET:HB3	1.97	0.47
2:B:82:ARG:HH11	2:B:82:ARG:HG2	1.80	0.47
1:A:49:TRP:CG	2:B:101:PRO:HD2	2.49	0.47
2:B:120:VAL:HA	2:B:140:PHE:O	2.14	0.47
2:L:2:ILE:HD11	2:L:27:LYS:H	1.79	0.47
2:L:195:ASN:HB2	4:L:373:HOH:O	2.14	0.47
2:B:56:MET:O	2:B:69:SER:HB3	2.15	0.47
1:H:22:CYS:HB3	1:H:80:LEU:HB3	1.97	0.47
1:A:39:VAL:HG13	1:A:48:GLU:O	2.16	0.46
2:L:81:SER:CA	4:L:345:HOH:O	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:82:ARG:HH11	2:L:82:ARG:HG2	1.80	0.46
2:B:2:ILE:HD11	2:B:27:LYS:H	1.79	0.46
2:L:45:PRO:HB3	2:L:170:ASP:OD2	2.15	0.46
2:L:25:SER:HB3	4:L:375:HOH:O	2.16	0.46
1:A:3:LYS:NZ	4:A:338:HOH:O	2.49	0.46
1:H:13:LYS:HD3	1:H:115:SER:O	2.15	0.46
1:A:141:LEU:HD13	1:A:213:LEU:HD12	1.98	0.46
2:B:82:ARG:NH1	2:B:82:ARG:HG2	2.30	0.45
2:B:146:PRO:HD3	4:B:762:HOH:O	2.16	0.45
2:L:82:ARG:NH1	2:L:82:ARG:HG2	2.30	0.45
2:L:130:LEU:HD23	2:L:134:GLY:O	2.16	0.45
1:A:193:SER:O	1:A:195:THR:HB	2.17	0.45
1:A:23:THR:N	4:A:331:HOH:O	2.49	0.45
2:L:6:GLN:HE22	2:L:92:TYR:HA	1.81	0.45
1:A:167:HIS:N	4:A:330:HOH:O	2.49	0.45
2:B:4:MET:SD	4:B:851:HOH:O	2.61	0.45
2:B:130:LEU:HD23	2:B:134:GLY:O	2.16	0.45
1:A:140:THR:HA	4:A:291:HOH:O	2.17	0.45
1:H:193:SER:O	1:H:195:THR:HB	2.17	0.45
1:A:180:MET:HE3	4:A:254:HOH:O	2.17	0.45
2:B:2:ILE:HD13	2:B:27:LYS:CB	2.43	0.44
1:A:5:LEU:N	4:A:331:HOH:O	2.39	0.44
1:H:139:VAL:HA	4:H:639:HOH:O	2.16	0.44
2:L:202:THR:N	4:L:357:HOH:O	2.50	0.44
2:L:61:SER:HA	4:L:280:HOH:O	2.17	0.44
2:B:120:VAL:CG1	4:B:832:HOH:O	2.63	0.44
2:L:154:LYS:HG2	4:L:377:HOH:O	2.18	0.44
1:A:151:GLU:N	1:A:152:PRO:CD	2.81	0.44
2:B:193:ARG:NH2	4:B:829:HOH:O	2.50	0.43
1:A:141:LEU:HD13	1:A:213:LEU:CD1	2.48	0.43
2:L:76:PHE:HZ	4:L:375:HOH:O	2.00	0.43
1:H:202:HIS:NE2	1:H:204:ALA:HB3	2.33	0.43
1:A:38:TRP:CE2	1:A:82:LEU:HB2	2.53	0.43
2:B:154:LYS:HE2	2:B:200:GLU:OE2	2.19	0.43
1:A:142:GLY:C	4:A:319:HOH:O	2.56	0.43
1:A:158:ASN:O	1:A:159:SER:HB2	2.18	0.43
1:A:134:THR:O	1:A:134:THR:HG22	2.18	0.43
2:B:2:ILE:O	2:B:2:ILE:HG23	2.19	0.43
1:H:122:PRO:HD3	1:H:202:HIS:ND1	2.34	0.43
1:A:182:SER:C	4:A:262:HOH:O	2.57	0.43
1:H:158:ASN:O	1:H:159:SER:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ILE:HG23	2:B:102:THR:OG1	2.18	0.43
2:L:25:SER:CB	4:L:375:HOH:O	2.67	0.43
2:B:88:VAL:HG12	2:B:111:ILE:HG12	2.00	0.43
1:H:141:LEU:HD11	1:H:191:TRP:NE1	2.34	0.43
1:H:78:ASN:ND2	4:H:633:HOH:O	2.51	0.42
1:H:141:LEU:HD11	1:H:191:TRP:HE1	1.83	0.42
1:A:128:ALA:HB2	4:A:345:HOH:O	2.19	0.42
1:A:141:LEU:HD11	1:A:191:TRP:HE1	1.85	0.42
1:H:187:PRO:HG2	1:H:190:THR:CG2	2.48	0.42
1:H:85:SER:HB2	4:H:676:HOH:O	2.19	0.42
1:H:134:THR:O	1:H:134:THR:HG22	2.19	0.42
2:L:154:LYS:HE2	2:L:200:GLU:OE2	2.19	0.42
1:A:92:THR:O	1:A:93:ALA:HB2	2.20	0.42
1:H:141:LEU:HD13	1:H:213:LEU:HD12	2.01	0.42
2:L:2:ILE:HD13	2:L:27:LYS:CB	2.43	0.42
1:H:192:PRO:HD3	4:H:668:HOH:O	2.20	0.42
2:B:135:ALA:O	2:B:186:LEU:HD12	2.19	0.42
2:B:75:ASP:CA	4:B:843:HOH:O	2.56	0.42
1:H:136:GLY:C	1:H:188:SER:HB2	2.40	0.42
1:H:2:VAL:HA	1:H:25:SER:O	2.19	0.42
2:B:152:LYS:HD2	2:B:159:GLU:CD	2.40	0.42
2:B:140:PHE:HB3	2:B:142:ASN:ND2	2.35	0.42
1:A:44:GLU:HG3	1:A:46:ARG:N	2.24	0.42
1:H:38:TRP:CE2	1:H:82:LEU:HB2	2.55	0.42
2:L:29:LEU:HD22	4:L:375:HOH:O	2.20	0.41
1:H:205:SER:HB2	4:H:678:HOH:O	2.19	0.41
1:H:157:TRP:C	1:H:159:SER:N	2.73	0.41
2:L:2:ILE:CD1	2:L:27:LYS:N	2.84	0.41
1:A:12:VAL:O	1:A:114:VAL:HA	2.21	0.41
2:L:152:LYS:HD2	2:L:159:GLU:CD	2.39	0.41
2:B:6:GLN:HE22	2:B:92:TYR:HA	1.84	0.41
2:B:151:VAL:HA	2:B:200:GLU:O	2.20	0.41
1:H:169:PHE:CD1	2:L:169:THR:HG23	2.55	0.41
2:B:2:ILE:CD1	2:B:27:LYS:N	2.84	0.41
2:L:2:ILE:HG23	2:L:2:ILE:O	2.21	0.41
1:A:136:GLY:C	1:A:188:SER:HB2	2.41	0.41
1:A:56:GLY:HA3	4:A:251:HOH:O	2.19	0.41
1:A:141:LEU:HD11	1:A:191:TRP:NE1	2.36	0.41
2:L:140:PHE:HB3	2:L:142:ASN:ND2	2.35	0.41
1:H:19:LYS:HE3	1:H:81:TYR:CD2	2.55	0.41
2:B:193:ARG:HG3	2:B:194:HIS:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TRP:C	1:A:159:SER:N	2.73	0.41
1:H:115:SER:HB2	4:H:640:HOH:O	2.20	0.41
1:H:42:ILE:CG1	1:H:44:GLU:HG2	2.51	0.41
1:H:141:LEU:HD13	1:H:213:LEU:CD1	2.51	0.41
1:A:122:PRO:HD3	1:A:202:HIS:ND1	2.35	0.41
1:A:202:HIS:NE2	1:A:204:ALA:HB3	2.36	0.41
2:B:137:VAL:HG13	2:B:153:TRP:CH2	2.56	0.41
1:H:49:TRP:CG	2:L:101:PRO:HD2	2.56	0.41
1:A:19:LYS:HE3	1:A:81:TYR:CD2	2.56	0.40
2:L:151:VAL:HA	2:L:200:GLU:O	2.20	0.40
2:L:207:THR:HG22	2:L:207:THR:O	2.21	0.40
2:B:184:LEU:HD13	2:B:184:LEU:C	2.42	0.40
2:L:2:ILE:HG23	2:L:102:THR:OG1	2.20	0.40
1:A:117:ALA:HB3	1:A:149:PHE:CE2	2.57	0.40
2:B:122:ILE:HG13	2:B:139:CYS:HB3	2.03	0.40
1:A:166:VAL:HG12	4:A:286:HOH:O	2.22	0.40
2:L:193:ARG:HG3	2:L:194:HIS:CE1	2.56	0.40
2:L:55:GLN:O	2:L:56:MET:HB3	2.21	0.40
1:H:157:TRP:O	1:H:159:SER:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:32:SER:OG	4:L:345:HOH:O[4_544]	2.18	0.02

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	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	14 6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	207/209 (99%)	191 (92%)	13 (6%)	3 (1%)	14	6
2	B	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	34	26
2	L	212/214 (99%)	202 (95%)	9 (4%)	1 (0%)	34	26
All	All	838/846 (99%)	784 (94%)	46 (6%)	8 (1%)	19	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	135	THR
1	A	135	THR
2	L	193	ARG
2	B	193	ARG
1	H	138	SER
1	A	138	SER
1	H	132	GLY
1	A	132	GLY

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	177/177 (100%)	171 (97%)	6 (3%)	44	41
1	H	177/177 (100%)	172 (97%)	5 (3%)	51	50
2	B	188/188 (100%)	180 (96%)	8 (4%)	35	30
2	L	188/188 (100%)	181 (96%)	7 (4%)	41	38
All	All	730/730 (100%)	704 (96%)	26 (4%)	42	39

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	3	LYS
1	H	80	LEU
1	H	82	LEU

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Mol	Chain	Res	Type
1	H	103	ARG
1	H	146	LYS
2	L	29	LEU
2	L	65	ASN
2	L	76	PHE
2	L	103	PHE
2	L	147	LYS
2	L	148	ASP
2	L	186	LEU
1	A	3	LYS
1	A	80	LEU
1	A	82	LEU
1	A	103	ARG
1	A	119	THR
1	A	146	LYS
2	B	29	LEU
2	B	65	ASN
2	B	76	PHE
2	B	103	PHE
2	B	113	ARG
2	B	147	LYS
2	B	148	ASP
2	B	186	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	174	GLN
2	L	6	GLN
2	L	58	ASN
2	L	65	ASN
2	L	142	ASN
2	L	171	GLN
2	L	203	HIS
2	B	6	GLN
2	B	58	ASN
2	B	65	ASN
2	B	142	ASN
2	B	171	GLN
2	B	203	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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$
3	SPB	B	701	-	21,24,24	1.74	4 (19%)	27,30,30	0.95	1 (3%)
3	SPB	H	601	-	21,24,24	1.68	5 (23%)	27,30,30	0.94	1 (3%)

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
3	SPB	B	701	-	-	0/13/15/15	0/2/2/2
3	SPB	H	601	-	-	0/13/15/15	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	601	SPB	C13-C12	2.07	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	601	SPB	C1-C6	2.16	1.43	1.39
3	B	701	SPB	C13-C12	2.48	1.43	1.39
3	H	601	SPB	C14-C9	2.51	1.44	1.39
3	B	701	SPB	C14-C9	2.59	1.44	1.39
3	B	701	SPB	C5-C6	2.61	1.44	1.39
3	H	601	SPB	C5-C6	2.67	1.44	1.39
3	B	701	SPB	C11-C12	2.77	1.43	1.39
3	H	601	SPB	C11-C12	2.85	1.43	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	601	SPB	C12-N15-C16	2.75	132.68	127.47
3	B	701	SPB	C12-N15-C16	3.02	133.19	127.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	701	SPB	1	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	209/209 (100%)	0.93	33 (15%) 3 3	16, 42, 83, 96	0
1	H	209/209 (100%)	1.00	35 (16%) 2 3	17, 43, 84, 96	0
2	B	214/214 (100%)	1.19	48 (22%) 1 1	17, 42, 83, 90	0
2	L	214/214 (100%)	0.82	40 (18%) 2 2	15, 36, 83, 90	0
All	All	846/846 (100%)	0.98	156 (18%) 2 2	15, 42, 83, 96	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	134	THR	10.9
1	H	132	GLY	10.6
1	H	191	TRP	10.2
2	B	208	SER	9.6
1	A	131	CYS	9.0
1	H	136	GLY	8.6
1	A	191	TRP	8.4
1	H	135	THR	8.4
1	A	130	GLY	7.9
1	H	131	CYS	7.6
1	A	133	ASP	7.4
1	H	134	THR	7.3
2	B	206	SER	7.2
1	A	137	SER	6.5
1	A	129	PRO	6.4
1	A	138	SER	6.4
2	B	202	THR	6.3
1	A	135	THR	5.9
2	L	193	ARG	5.8
1	A	132	GLY	5.8
2	B	204	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	H	133	ASP	5.8
2	B	207	THR	5.8
1	H	130	GLY	5.8
2	B	189	ASP	5.7
2	L	208	SER	5.6
1	A	127	ALA	5.6
2	B	196	GLY	5.4
1	H	159	SER	5.3
2	B	187	THR	5.2
1	H	43	PRO	5.2
2	B	158	SER	4.9
1	A	43	PRO	4.8
1	A	187	PRO	4.7
2	L	209	PRO	4.7
1	A	164	SER	4.6
2	B	197	TYR	4.6
2	B	205	THR	4.6
2	L	207	THR	4.6
1	A	161	GLY	4.5
2	L	214	PHE	4.4
1	A	186	VAL	4.4
2	B	175	ASP	4.3
1	H	45	LYS	4.3
2	B	210	ILE	4.3
2	L	195	ASN	4.2
1	H	129	PRO	4.2
1	H	42	ILE	4.2
1	H	161	GLY	4.2
1	A	44	GLU	4.2
2	L	205	THR	4.2
2	L	155	ILE	4.2
2	B	133	GLY	4.2
2	B	46	GLY	4.1
2	L	189	ASP	4.1
1	H	164	SER	4.1
2	B	194	HIS	4.1
1	A	189	SER	4.1
1	H	137	SER	4.0
1	A	128	ALA	4.0
1	A	193	SER	4.0
1	A	192	PRO	3.9
1	A	42	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	H	186	VAL	3.8
2	B	157	GLY	3.6
2	L	156	ASP	3.6
2	B	203	HIS	3.6
2	L	157	GLY	3.6
2	B	184	LEU	3.5
2	L	160	ARG	3.5
2	B	214	PHE	3.5
2	B	199	CYS	3.5
2	B	159	GLU	3.4
1	H	160	GLY	3.4
1	H	174	GLN	3.4
1	H	175	SER	3.3
2	B	134	GLY	3.3
2	B	72	SER	3.3
2	B	211	VAL	3.3
1	H	192	PRO	3.2
1	A	136	GLY	3.2
2	L	152	LYS	3.2
2	B	140	PHE	3.2
1	H	213	LEU	3.2
2	L	197	TYR	3.1
2	B	150	ASN	3.1
1	A	195	THR	3.1
2	L	204	LYS	3.1
2	B	161	GLN	3.1
2	B	195	ASN	3.1
2	B	209	PRO	3.1
2	L	201	ALA	3.1
2	B	198	THR	3.1
2	B	148	ASP	3.1
2	L	149	ILE	3.1
1	A	166	VAL	3.0
2	L	206	SER	3.0
2	L	150	ASN	3.0
2	B	162	ASN	3.0
2	B	153	TRP	3.0
2	B	149	ILE	2.9
1	A	116	SER	2.9
1	A	141	LEU	2.9
2	L	154	LYS	2.9
2	L	131	THR	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	211	VAL	2.9
1	H	195	THR	2.9
2	L	202	THR	2.9
2	L	203	HIS	2.8
2	L	159	GLU	2.8
1	A	212	LYS	2.8
2	B	137	VAL	2.8
2	B	168	TRP	2.8
2	B	193	ARG	2.8
1	H	44	GLU	2.8
2	L	196	GLY	2.8
1	A	45	LYS	2.8
2	L	184	LEU	2.7
2	B	156	ASP	2.7
2	B	163	GLY	2.7
1	H	189	SER	2.7
1	H	118	LYS	2.7
1	H	1	GLU	2.6
1	H	203	PRO	2.6
2	B	174	LYS	2.5
2	B	10	SER	2.5
2	L	137	VAL	2.5
1	H	187	PRO	2.5
2	L	148	ASP	2.5
2	L	141	LEU	2.4
1	H	188	SER	2.4
1	A	165	SER	2.4
2	B	132	SER	2.4
1	H	196	VAL	2.3
1	H	190	THR	2.3
2	L	140	PHE	2.3
2	L	153	TRP	2.3
1	A	196	VAL	2.3
2	B	152	LYS	2.3
2	B	165	LEU	2.3
1	A	213	LEU	2.3
2	L	199	CYS	2.2
2	L	163	GLY	2.2
1	A	175	SER	2.2
2	L	200	GLU	2.2
1	H	206	SER	2.2
2	L	47	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	94	ALA	2.1
2	L	190	GLU	2.1
2	B	86	GLU	2.1
1	H	116	SER	2.1
2	L	132	SER	2.1
1	H	158	ASN	2.1
2	B	11	ASN	2.1
2	L	175	ASP	2.1
2	B	155	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	SPB	H	601	23/23	0.91	0.16	0.99	15,22,46,48	0
3	SPB	B	701	23/23	0.94	0.15	0.75	15,21,45,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.