Full wwPDB X-ray Structure Validation Report (i)

Apr 16, 2025 – 12:08 PM JST

PDB ID	:	9KEF / pdb_00009kef
Title	:	Crystal strucutre of RABV-G in complex with SOJB-Fab complex
Authors	:	Lu, G.; Yang, F.; Lin, S.
Deposited on	:	2024-11-05
Resolution	:	3.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

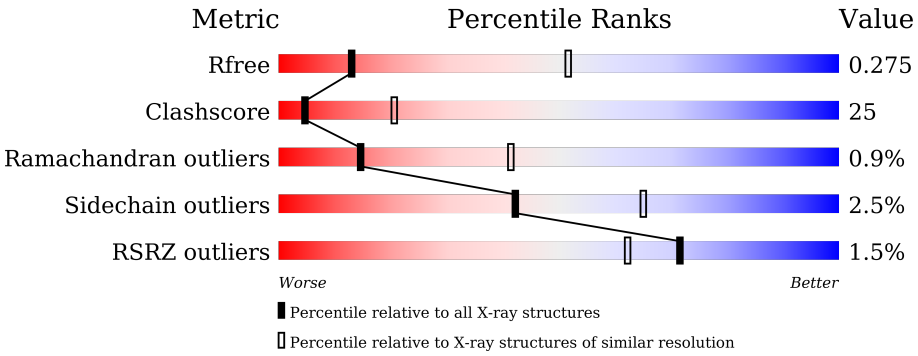
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 3.40 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

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	439	% 52% 27% • 18%
2	H	239	3% 45% 39% 5% 10%
3	L	215	% 48% 46% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6082 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 RABV-G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2833	1797	485	527	24	0	0	0

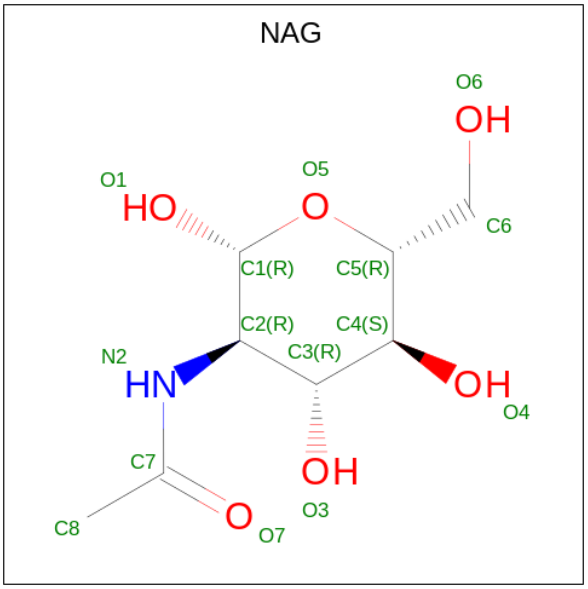
- Molecule 2 is a protein called SOJB-Fab Hchain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	214	1637	1043	271	317	6	0	0	0

- Molecule 3 is a protein called SOJB-Fab Lchian.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	210	1598	995	274	325	4	0	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

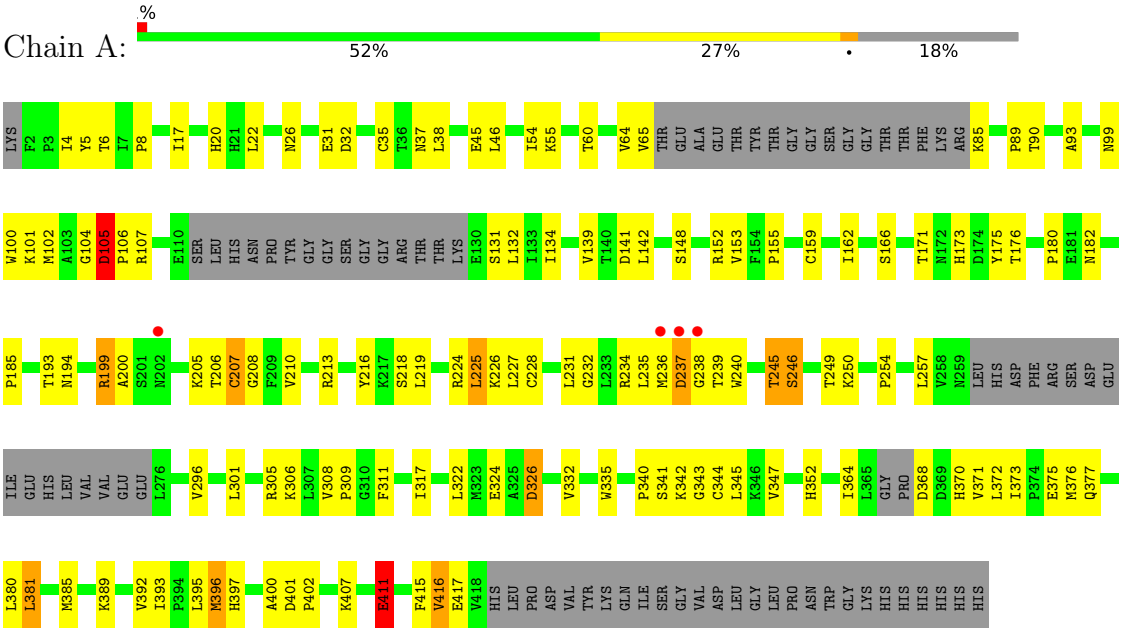


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

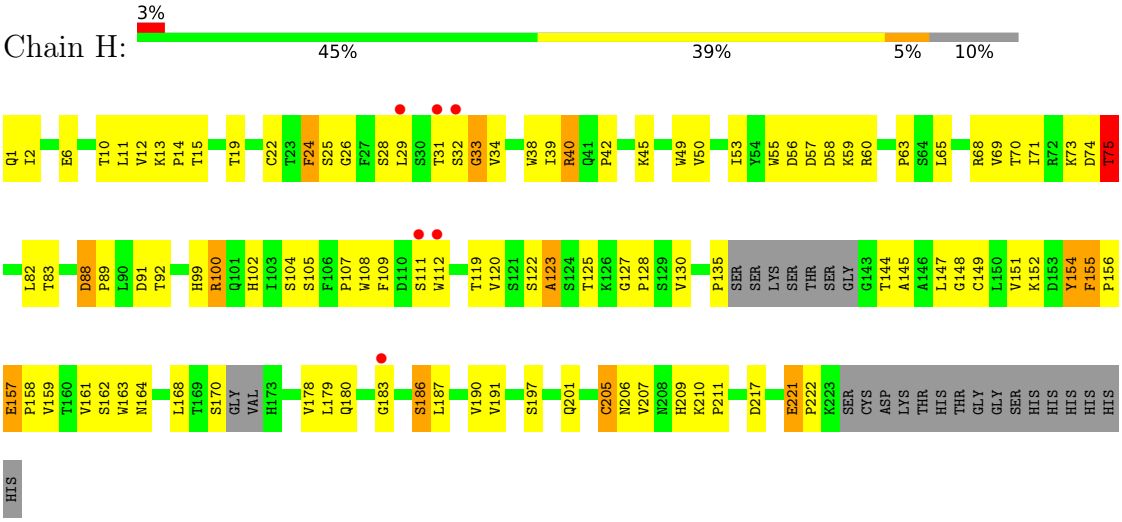
3 Residue-property plots (i)

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: RABV-G

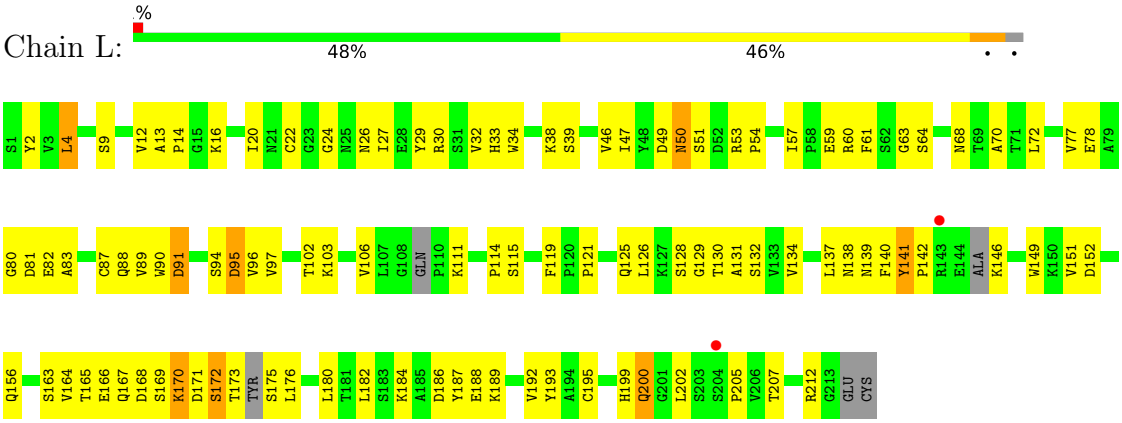


• Molecule 2: SOJB-Fab Hchain



• Molecule 3: SOJB-Fab Lchian

Chain L:


%
48%
46%
S1 Y2 V3 L4 S9 V12 A13 P14 G15 K16 I20 N21 C22 G23 G24 N25 N26 I27 E28 Y29 R30 S31 V32 H33 W34 K38 S39 V46 I47 Y48 D49 N50 S51 D52 R53 P54 I57 P58 E59 R60 F61 S62 G63 S64 N68 T69 A70 T71 L72 V77 E78 A79
G80 D81 E82 A83 C87 Q88 V89 W90 D91 S94 D95 V96 V97 T102 K103 V106 L107 G108 GLN P110 K111 P114 S115 F119 P120 P121 Q125 L126 K127 S128 G129 T130 A131 S132 V133 V134 L137 N138 N139 F140 Y141 P142 R143 E144 ALA K146 W149 K150 V151 D152
Q156 S163 V164 T165 E166 Q167 D168 S169 K170 D171 S172 T173 TYR S175 L176 L180 T181 L182 S183 K184 A185 D186 Y187 E188 K189 V192 Y193 A194 C195 H199 Q200 G201 L202 S203 S204 P205 V206 T207 R212 G213 GLU CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	84.18Å 154.42Å 191.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.84 – 3.40 37.84 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.84-3.40) 95.4 (37.84-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.217 , 0.264 0.240 , 0.275	Depositor DCC
R_{free} test set	907 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	89.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 86.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6082	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

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

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	0.58	0/2901	0.99	15/3929 (0.4%)
2	H	0.56	0/1680	1.00	13/2297 (0.6%)
3	L	0.55	0/1630	0.91	10/2211 (0.5%)
All	All	0.57	0/6211	0.97	38/8437 (0.5%)

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
2	H	0	1
3	L	0	1
All	All	0	2

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	411	GLU	N-CA-C	-14.25	72.52	111.00
1	A	411	GLU	N-CA-CB	11.49	131.29	110.60
2	H	25	SER	N-CA-CB	-9.04	96.94	110.50
1	A	246	SER	N-CA-CB	-8.90	97.15	110.50
1	A	381	LEU	CB-CA-C	-8.41	94.22	110.20
2	H	24	PHE	CB-CA-C	-7.76	94.88	110.40
2	H	123	ALA	N-CA-CB	7.71	120.90	110.10
3	L	83	ALA	N-CA-CB	7.45	120.53	110.10
2	H	145	ALA	N-CA-CB	7.41	120.48	110.10
1	A	415	PHE	N-CA-C	-7.06	91.93	111.00
2	H	74	ASP	N-CA-C	-6.60	93.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	392	VAL	CB-CA-C	6.56	123.86	111.40
3	L	82	GLU	N-CA-C	-6.55	93.30	111.00
1	A	245	THR	CB-CA-C	-6.38	94.38	111.60
2	H	40	ARG	CB-CA-C	-6.38	97.64	110.40
3	L	169	SER	CB-CA-C	6.34	122.14	110.10
1	A	411	GLU	CB-CA-C	6.27	122.94	110.40
1	A	381	LEU	CA-CB-CG	6.26	129.70	115.30
2	H	144	THR	CB-CA-C	6.12	128.13	111.60
2	H	74	ASP	CB-CA-C	5.90	122.20	110.40
3	L	200	GLN	CB-CA-C	-5.90	98.60	110.40
1	A	416	VAL	N-CA-C	-5.89	95.09	111.00
2	H	75	THR	N-CA-CB	5.88	121.47	110.30
3	L	51	SER	N-CA-C	5.79	126.65	111.00
3	L	91	ASP	CB-CA-C	5.77	121.95	110.40
1	A	309	PRO	CB-CA-C	-5.72	97.71	112.00
1	A	236	MET	N-CA-CB	5.65	120.76	110.60
3	L	170	LYS	N-CA-CB	-5.54	100.63	110.60
2	H	154	TYR	CB-CA-C	5.52	121.44	110.40
2	H	186	SER	CB-CA-C	5.50	120.55	110.10
1	A	396	MET	CB-CA-C	5.47	121.34	110.40
3	L	51	SER	N-CA-CB	-5.37	102.45	110.50
2	H	25	SER	N-CA-C	5.29	125.28	111.00
1	A	225	LEU	CB-CG-CD2	5.19	119.82	111.00
2	H	221	GLU	N-CA-CB	5.11	119.79	110.60
3	L	170	LYS	CB-CA-C	5.10	120.59	110.40
3	L	64	SER	CB-CA-C	-5.08	100.44	110.10
1	A	393	ILE	N-CA-C	-5.02	97.44	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	157	GLU	Peptide
3	L	141	TYR	Peptide

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	2833	0	2782	120	1
2	H	1637	0	1621	105	0
3	L	1598	0	1543	99	1
4	A	14	0	13	0	0
All	All	6082	0	5959	305	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 25.

All (305) 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:H:125:THR:HG23	2:H:156:PRO:HG2	1.24	1.13
1:A:245:THR:HG23	1:A:245:THR:O	1.61	0.99
2:H:14:PRO:O	2:H:15:THR:HG22	1.62	0.99
2:H:28:SER:HB2	2:H:31:THR:HG23	1.46	0.98
3:L:167:GLN:NE2	3:L:172:SER:O	1.99	0.95
1:A:90:THR:HG23	1:A:93:ALA:HB3	1.50	0.94
3:L:121:PRO:HB3	3:L:132:SER:H	1.37	0.90
1:A:377:GLN:O	1:A:381:LEU:HG	1.73	0.87
2:H:24:PHE:O	2:H:24:PHE:CD1	2.30	0.84
2:H:10:THR:HG23	2:H:11:LEU:HD12	1.60	0.83
3:L:166:GLU:HG3	3:L:167:GLN:H	1.44	0.82
2:H:155:PHE:HB3	2:H:156:PRO:HD3	1.62	0.81
2:H:161:VAL:HG22	2:H:207:VAL:HG22	1.64	0.79
1:A:228:CYS:HA	2:H:60:ARG:HH22	1.47	0.79
1:A:341:SER:HB3	1:A:344:CYS:HB3	1.65	0.76
2:H:89:PRO:HA	2:H:120:VAL:HG13	1.66	0.75
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.19	0.75
1:A:199:ARG:NH1	1:A:206:THR:HG21	2.02	0.74
1:A:377:GLN:O	1:A:381:LEU:CD2	2.36	0.73
1:A:64:VAL:HG23	1:A:131:SER:HB2	1.69	0.73
2:H:92:THR:HG23	2:H:119:THR:HA	1.70	0.72
1:A:100:TRP:CD2	1:A:106:PRO:HG2	2.25	0.71
1:A:401:ASP:OD1	1:A:402:PRO:HD2	1.91	0.70
1:A:245:THR:O	1:A:245:THR:CG2	2.36	0.70
1:A:381:LEU:O	1:A:385:MET:HG2	1.91	0.70
3:L:54:PRO:HB2	3:L:57:ILE:HD13	1.74	0.70
1:A:234:ARG:HG3	1:A:238:GLY:HA2	1.74	0.69
2:H:34:VAL:HG12	2:H:102:HIS:HB3	1.75	0.68
2:H:40:ARG:O	2:H:40:ARG:HG3	1.91	0.68
2:H:162:SER:HB3	2:H:206:ASN:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:THR:HG23	2:H:156:PRO:CG	2.13	0.66
3:L:125:GLN:HG2	3:L:130:THR:O	1.94	0.66
3:L:90:TRP:HA	3:L:95:ASP:O	1.95	0.66
2:H:42:PRO:HG2	2:H:45:LYS:HB2	1.77	0.66
3:L:121:PRO:HG3	3:L:131:ALA:HB1	1.77	0.65
2:H:156:PRO:HD2	2:H:209:HIS:NE2	2.11	0.65
1:A:224:ARG:HE	1:A:231:LEU:HB3	1.61	0.65
1:A:153:VAL:HG12	1:A:171:THR:HB	1.79	0.65
1:A:254:PRO:HA	1:A:257:LEU:HD22	1.79	0.65
1:A:199:ARG:HH11	1:A:206:THR:HG21	1.61	0.64
2:H:179:LEU:HD13	2:H:180:GLN:O	1.97	0.64
3:L:140:PHE:CZ	3:L:175:SER:HB2	2.32	0.64
2:H:128:PRO:HD3	2:H:209:HIS:CB	2.29	0.63
3:L:188:GLU:O	3:L:212:ARG:NH2	2.32	0.63
2:H:99:HIS:HB3	2:H:111:SER:HB2	1.80	0.62
3:L:142:PRO:HD2	3:L:199:HIS:CE1	2.34	0.62
1:A:105:ASP:OD1	1:A:105:ASP:N	2.33	0.62
3:L:137:LEU:O	3:L:175:SER:N	2.33	0.62
1:A:231:LEU:HB2	2:H:105:SER:HA	1.81	0.62
2:H:63:PRO:HD3	3:L:94:SER:HB2	1.80	0.62
1:A:99:ASN:O	1:A:102:MET:HB2	1.99	0.61
2:H:100:ARG:NH2	2:H:104:SER:O	2.32	0.61
2:H:15:THR:HG23	2:H:15:THR:O	2.01	0.61
1:A:194:ASN:HB3	3:L:29:TYR:CD2	2.36	0.61
3:L:47:ILE:HD12	3:L:50:ASN:O	2.01	0.61
2:H:155:PHE:CB	2:H:156:PRO:HD3	2.31	0.60
3:L:16:LYS:O	3:L:77:VAL:HG23	2.00	0.60
2:H:123:ALA:HB3	2:H:155:PHE:CD1	2.37	0.60
3:L:195:CYS:O	3:L:207:THR:HA	2.01	0.60
1:A:364:ILE:HG13	1:A:372:LEU:HD21	1.83	0.60
3:L:47:ILE:CD1	3:L:63:GLY:HA3	2.31	0.60
1:A:235:LEU:HB2	1:A:239:THR:HB	1.83	0.60
1:A:35:CYS:O	1:A:200:ALA:HB1	2.00	0.59
2:H:210:LYS:N	2:H:211:PRO:HD2	2.17	0.59
1:A:17:ILE:O	1:A:322:LEU:HB3	2.02	0.59
1:A:372:LEU:H	1:A:372:LEU:HD23	1.68	0.59
1:A:90:THR:CG2	1:A:93:ALA:HB3	2.28	0.58
2:H:127:GLY:HA2	2:H:209:HIS:CD2	2.38	0.58
1:A:182:ASN:HD22	1:A:185:PRO:HA	1.68	0.58
1:A:226:LYS:NZ	2:H:58:ASP:OD2	2.36	0.58
2:H:152:LYS:HA	2:H:186:SER:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:O	1:A:381:LEU:HD23	2.04	0.58
2:H:55:TRP:O	2:H:73:LYS:NZ	2.36	0.58
3:L:151:VAL:HB	3:L:156:GLN:NE2	2.18	0.58
2:H:154:TYR:HE1	2:H:157:GLU:HA	1.69	0.58
2:H:156:PRO:HB2	2:H:211:PRO:CG	2.34	0.58
3:L:114:PRO:HB3	3:L:140:PHE:HD2	1.70	0.57
3:L:2:TYR:HD2	3:L:97:VAL:HG21	1.68	0.57
3:L:34:TRP:CD1	3:L:47:ILE:HD11	2.40	0.57
2:H:128:PRO:HD3	2:H:209:HIS:HB2	1.86	0.57
3:L:49:ASP:O	3:L:50:ASN:HB2	2.04	0.57
3:L:186:ASP:HA	3:L:189:LYS:HG2	1.87	0.56
1:A:208:GLY:HA2	1:A:219:LEU:HD22	1.87	0.56
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.71	0.56
1:A:227:LEU:HD22	1:A:240:TRP:CE2	2.41	0.56
3:L:121:PRO:HB3	3:L:132:SER:N	2.16	0.56
1:A:37:ASN:O	1:A:200:ALA:HA	2.06	0.56
1:A:45:GLU:HB3	1:A:193:THR:HG22	1.87	0.56
2:H:32:SER:HA	2:H:55:TRP:CD1	2.41	0.56
3:L:168:ASP:HB2	3:L:171:ASP:OD1	2.05	0.55
3:L:30:ARG:NH2	3:L:91:ASP:OD1	2.29	0.55
1:A:381:LEU:O	1:A:385:MET:CG	2.55	0.55
3:L:38:LYS:HE2	3:L:80:GLY:O	2.06	0.55
2:H:29:LEU:HD21	2:H:73:LYS:HG3	1.89	0.55
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.88	0.55
1:A:173:HIS:HE1	1:A:175:TYR:HB2	1.72	0.55
3:L:152:ASP:HA	3:L:192:VAL:HB	1.88	0.55
2:H:108:TRP:HB3	3:L:33:HIS:CD2	2.41	0.54
2:H:179:LEU:HD21	2:H:183:GLY:HA2	1.90	0.54
3:L:53:ARG:HD3	3:L:61:PHE:O	2.06	0.54
1:A:104:GLY:HA2	1:A:107:ARG:HB3	1.88	0.54
1:A:199:ARG:HH22	1:A:245:THR:CG2	2.21	0.54
2:H:28:SER:CB	2:H:31:THR:HG23	2.28	0.54
3:L:60:ARG:NH2	3:L:81:ASP:OD2	2.37	0.54
1:A:38:LEU:HA	1:A:199:ARG:O	2.07	0.54
1:A:347:VAL:CG1	1:A:352:HIS:HB2	2.38	0.54
2:H:157:GLU:CD	2:H:157:GLU:H	2.10	0.54
2:H:197:SER:HB2	2:H:201:GLN:HB3	1.89	0.54
3:L:9:SER:HA	3:L:103:LYS:O	2.08	0.54
1:A:208:GLY:HA3	1:A:216:TYR:OH	2.08	0.54
2:H:31:THR:O	2:H:55:TRP:CB	2.56	0.54
1:A:395:LEU:HD22	1:A:396:MET:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ILE:HG13	1:A:166:SER:O	2.08	0.53
3:L:53:ARG:CZ	3:L:59:GLU:HA	2.38	0.53
2:H:156:PRO:HB2	2:H:211:PRO:HG3	1.89	0.53
1:A:306:LYS:HD3	1:A:308:VAL:O	2.08	0.53
1:A:107:ARG:NH2	1:A:134:ILE:H	2.07	0.53
3:L:140:PHE:CZ	3:L:176:LEU:HD23	2.44	0.53
1:A:208:GLY:HA3	1:A:216:TYR:CZ	2.44	0.53
1:A:377:GLN:O	1:A:381:LEU:CG	2.52	0.53
3:L:182:LEU:HB3	3:L:186:ASP:HB2	1.91	0.53
1:A:20:HIS:HB2	1:A:152:ARG:NH2	2.23	0.52
2:H:209:HIS:CE1	2:H:211:PRO:HG2	2.44	0.52
3:L:114:PRO:HB3	3:L:140:PHE:HB3	1.91	0.52
2:H:24:PHE:O	2:H:24:PHE:HD1	1.86	0.52
2:H:33:GLY:HA2	2:H:55:TRP:CZ3	2.45	0.52
2:H:130:VAL:HG22	2:H:151:VAL:HG13	1.92	0.52
3:L:20:ILE:HG12	3:L:102:THR:HG21	1.92	0.52
1:A:224:ARG:HG2	1:A:249:THR:HG23	1.91	0.52
2:H:29:LEU:HB3	2:H:75:THR:HB	1.91	0.52
1:A:199:ARG:HH22	1:A:245:THR:HG21	1.74	0.52
3:L:14:PRO:HG3	3:L:106:VAL:HG12	1.91	0.52
3:L:114:PRO:HB3	3:L:140:PHE:CD2	2.45	0.52
3:L:141:TYR:HA	3:L:142:PRO:O	2.09	0.52
1:A:205:LYS:HE2	1:A:206:THR:O	2.10	0.52
1:A:180:PRO:HG2	1:A:182:ASN:O	2.09	0.52
1:A:194:ASN:HB3	3:L:29:TYR:CE2	2.44	0.52
1:A:216:TYR:HE1	1:A:218:SER:HB2	1.73	0.52
1:A:225:LEU:HD22	1:A:227:LEU:CD1	2.40	0.52
1:A:335:TRP:CZ3	1:A:376:MET:HB2	2.45	0.52
2:H:49:TRP:CG	3:L:96:VAL:HG13	2.45	0.52
3:L:12:VAL:HG21	3:L:77:VAL:HG21	1.91	0.52
3:L:34:TRP:CZ3	3:L:72:LEU:HD22	2.44	0.52
3:L:187:TYR:HA	3:L:193:TYR:OH	2.08	0.52
1:A:60:THR:O	1:A:134:ILE:HA	2.10	0.51
1:A:238:GLY:O	1:A:239:THR:C	2.48	0.51
1:A:342:LYS:HD2	1:A:370:HIS:CE1	2.44	0.51
2:H:148:GLY:HA3	2:H:190:VAL:HG12	1.93	0.51
3:L:171:ASP:O	3:L:172:SER:HB2	2.10	0.51
1:A:235:LEU:N	1:A:239:THR:O	2.30	0.51
2:H:2:ILE:HA	2:H:26:GLY:HA3	1.92	0.51
1:A:347:VAL:HG12	1:A:352:HIS:HB2	1.93	0.51
3:L:129:GLY:HA2	3:L:184:LYS:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:13:LYS:HE2	2:H:122:SER:OG	2.12	0.50
3:L:34:TRP:CZ3	3:L:87:CYS:HB3	2.46	0.50
1:A:381:LEU:O	1:A:385:MET:HB2	2.10	0.50
3:L:77:VAL:HG12	3:L:78:GLU:O	2.12	0.50
3:L:164:VAL:HG22	3:L:176:LEU:HB2	1.93	0.50
1:A:373:ILE:HB	1:A:376:MET:HB3	1.94	0.50
2:H:82:LEU:HD12	2:H:83:THR:N	2.26	0.50
3:L:4:LEU:H	3:L:4:LEU:HD23	1.77	0.50
2:H:12:VAL:O	2:H:120:VAL:HA	2.11	0.50
2:H:69:VAL:HG23	2:H:82:LEU:CD1	2.42	0.49
3:L:34:TRP:HB2	3:L:47:ILE:HG12	1.93	0.49
1:A:5:TYR:HE1	1:A:375:GLU:OE1	1.95	0.49
2:H:109:PHE:HB2	2:H:112:TRP:CZ2	2.47	0.49
1:A:343:GLY:HA2	1:A:371:VAL:HG23	1.95	0.49
2:H:135:PRO:HD3	2:H:147:LEU:HB3	1.95	0.49
2:H:163:TRP:CH2	2:H:205:CYS:HB3	2.48	0.49
3:L:111:LYS:HD2	3:L:200:GLN:HB3	1.95	0.49
1:A:407:LYS:HZ3	1:A:411:GLU:HB2	1.78	0.49
2:H:65:LEU:O	2:H:69:VAL:HG12	2.13	0.48
2:H:31:THR:O	2:H:55:TRP:CG	2.66	0.48
3:L:26:ASN:H	3:L:68:ASN:ND2	2.11	0.48
3:L:47:ILE:HD13	3:L:63:GLY:HA3	1.96	0.48
2:H:40:ARG:O	2:H:40:ARG:CG	2.61	0.48
1:A:54:ILE:HB	1:A:142:LEU:HB3	1.95	0.48
2:H:53:ILE:HB	2:H:71:ILE:HD13	1.96	0.48
2:H:29:LEU:CD2	2:H:73:LYS:HG3	2.44	0.48
1:A:296:VAL:HG21	1:A:301:LEU:HD13	1.95	0.48
2:H:63:PRO:CD	3:L:94:SER:HB2	2.42	0.48
3:L:138:ASN:HA	3:L:175:SER:N	2.29	0.48
3:L:129:GLY:O	3:L:184:LYS:N	2.44	0.48
2:H:107:PRO:HD2	3:L:90:TRP:HB2	1.96	0.47
1:A:4:ILE:HG12	1:A:332:VAL:O	2.13	0.47
1:A:8:PRO:O	1:A:347:VAL:HG23	2.14	0.47
2:H:50:VAL:HG13	2:H:65:LEU:HD13	1.96	0.47
1:A:107:ARG:HH21	1:A:134:ILE:H	1.63	0.47
2:H:70:THR:N	2:H:83:THR:O	2.48	0.47
3:L:46:VAL:HA	3:L:57:ILE:HG12	1.96	0.47
3:L:139:ASN:C	3:L:173:THR:HB	2.34	0.47
2:H:53:ILE:HD13	2:H:73:LYS:HB2	1.96	0.47
2:H:125:THR:CG2	2:H:156:PRO:HG2	2.17	0.47
2:H:206:ASN:HA	2:H:217:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:GLU:OE1	2:H:157:GLU:N	2.41	0.47
3:L:12:VAL:HG22	3:L:13:ALA:N	2.29	0.47
1:A:162:ILE:HD13	1:A:180:PRO:HG3	1.96	0.47
3:L:164:VAL:HG12	3:L:165:THR:O	2.14	0.47
1:A:6:THR:OG1	1:A:305:ARG:NH1	2.48	0.47
1:A:65:VAL:O	1:A:85:LYS:HE3	2.14	0.47
1:A:100:TRP:O	1:A:104:GLY:N	2.41	0.47
1:A:326:ASP:OD1	1:A:326:ASP:N	2.48	0.46
2:H:39:ILE:N	2:H:39:ILE:HD12	2.30	0.46
3:L:49:ASP:O	3:L:50:ASN:CB	2.63	0.46
1:A:173:HIS:CE1	1:A:175:TYR:HD2	2.33	0.46
1:A:207:CYS:C	1:A:219:LEU:HD23	2.35	0.46
1:A:231:LEU:HD22	2:H:100:ARG:NH2	2.31	0.46
3:L:149:TRP:CG	3:L:180:LEU:HD13	2.50	0.46
1:A:26:ASN:HB3	1:A:237:ASP:OD1	2.16	0.46
2:H:159:VAL:HB	2:H:187:LEU:HD21	1.98	0.46
3:L:34:TRP:CH2	3:L:72:LEU:HD22	2.51	0.46
2:H:60:ARG:HG3	3:L:95:ASP:OD2	2.16	0.46
1:A:207:CYS:O	1:A:219:LEU:HD23	2.16	0.45
3:L:188:GLU:O	3:L:212:ARG:CZ	2.64	0.45
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.77	0.45
2:H:38:TRP:CG	2:H:82:LEU:HD22	2.52	0.45
3:L:115:SER:O	3:L:137:LEU:HA	2.17	0.45
2:H:22:CYS:HB2	2:H:38:TRP:CZ2	2.51	0.45
3:L:32:VAL:HA	3:L:89:VAL:HG12	1.98	0.45
1:A:22:LEU:HD21	1:A:322:LEU:HD21	1.99	0.45
2:H:14:PRO:O	2:H:15:THR:CG2	2.50	0.45
3:L:142:PRO:HG2	3:L:200:GLN:OE1	2.16	0.45
1:A:17:ILE:HG21	1:A:324:GLU:CD	2.37	0.45
1:A:173:HIS:HB3	1:A:176:THR:HB	1.98	0.45
2:H:14:PRO:CG	2:H:122:SER:HB2	2.47	0.45
2:H:31:THR:O	2:H:55:TRP:HB2	2.16	0.45
2:H:178:VAL:HG23	3:L:163:SER:HB2	1.98	0.45
1:A:417:GLU:O	1:A:417:GLU:HG2	2.17	0.45
2:H:60:ARG:HD3	2:H:60:ARG:HA	1.58	0.44
2:H:221:GLU:HB2	2:H:222:PRO:HD2	2.00	0.44
3:L:142:PRO:HD2	3:L:199:HIS:NE2	2.32	0.44
3:L:125:GLN:O	3:L:128:SER:OG	2.34	0.44
1:A:407:LYS:HB2	1:A:411:GLU:OE2	2.18	0.44
1:A:6:THR:OG1	1:A:306:LYS:O	2.33	0.44
1:A:55:LYS:HD3	1:A:141:ASP:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:187:TYR:O	3:L:212:ARG:HD3	2.17	0.44
1:A:148:SER:HB2	1:A:159:CYS:O	2.18	0.43
2:H:6:GLU:H	2:H:6:GLU:CD	2.19	0.43
3:L:199:HIS:O	3:L:202:LEU:HB2	2.18	0.43
1:A:250:LYS:HE3	1:A:250:LYS:HB2	1.85	0.43
2:H:69:VAL:HG23	2:H:82:LEU:HD11	2.00	0.43
3:L:88:GLN:CG	3:L:96:VAL:HG23	2.49	0.43
1:A:210:VAL:O	1:A:210:VAL:HG23	2.17	0.43
1:A:376:MET:O	1:A:380:LEU:HD22	2.18	0.43
2:H:210:LYS:N	2:H:211:PRO:CD	2.81	0.43
2:H:28:SER:HB2	2:H:31:THR:CG2	2.32	0.43
3:L:22:CYS:HB2	3:L:34:TRP:CH2	2.53	0.43
3:L:141:TYR:HA	3:L:142:PRO:C	2.39	0.43
3:L:4:LEU:HD13	3:L:89:VAL:HG22	2.00	0.43
3:L:20:ILE:HB	3:L:72:LEU:CD2	2.49	0.43
3:L:24:GLY:N	3:L:27:ILE:HD12	2.33	0.43
1:A:237:ASP:HB3	1:A:311:PHE:HB3	2.00	0.43
3:L:22:CYS:O	3:L:70:ALA:N	2.52	0.43
1:A:225:LEU:HD12	1:A:234:ARG:HB2	2.00	0.42
3:L:121:PRO:CG	3:L:131:ALA:HB1	2.48	0.42
3:L:170:LYS:HE3	3:L:170:LYS:HB2	1.91	0.42
2:H:68:ARG:HH22	2:H:91:ASP:CG	2.20	0.42
3:L:34:TRP:HD1	3:L:47:ILE:HD11	1.83	0.42
1:A:225:LEU:HD22	1:A:227:LEU:HD13	2.01	0.42
2:H:170:SER:O	2:H:191:VAL:HG23	2.19	0.42
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.74	0.42
1:A:228:CYS:CA	2:H:60:ARG:HH22	2.25	0.42
2:H:49:TRP:CG	3:L:96:VAL:CG1	3.03	0.42
1:A:208:GLY:HA2	1:A:219:LEU:CD2	2.50	0.42
1:A:246:SER:CB	2:H:104:SER:HA	2.49	0.42
3:L:146:LYS:HA	3:L:146:LYS:HD2	1.74	0.42
1:A:55:LYS:HD2	1:A:139:VAL:HG13	2.01	0.42
2:H:56:ASP:O	2:H:57:ASP:C	2.58	0.42
3:L:72:LEU:HD23	3:L:72:LEU:H	1.85	0.42
1:A:100:TRP:CE3	1:A:106:PRO:HG2	2.55	0.42
1:A:397:HIS:HB3	1:A:400:ALA:HB2	2.02	0.42
3:L:90:TRP:CE2	3:L:91:ASP:O	2.72	0.42
2:H:19:THR:HA	2:H:82:LEU:O	2.19	0.41
1:A:155:PRO:HD3	1:A:171:THR:HA	2.02	0.41
2:H:59:LYS:HB3	2:H:71:ILE:CG2	2.50	0.41
1:A:89:PRO:HB3	1:A:132:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:GLY:HA3	1:A:240:TRP:CZ2	2.56	0.41
3:L:16:LYS:HD2	3:L:16:LYS:HA	1.82	0.41
1:A:101:LYS:HE2	1:A:134:ILE:O	2.20	0.41
1:A:381:LEU:O	1:A:385:MET:CB	2.69	0.41
2:H:164:ASN:ND2	2:H:168:LEU:HD22	2.34	0.41
1:A:105:ASP:CG	1:A:106:PRO:HD3	2.41	0.41
1:A:45:GLU:HB3	1:A:193:THR:CG2	2.50	0.41
1:A:395:LEU:HD22	1:A:396:MET:N	2.35	0.41
3:L:91:ASP:O	3:L:94:SER:O	2.38	0.41
1:A:194:ASN:HB3	3:L:29:TYR:CG	2.55	0.41
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.77	0.41
2:H:24:PHE:O	2:H:24:PHE:CG	2.70	0.41
2:H:162:SER:O	2:H:206:ASN:N	2.36	0.41
3:L:166:GLU:HG3	3:L:167:GLN:N	2.23	0.41
1:A:368:ASP:OD2	1:A:370:HIS:HB2	2.21	0.41
1:A:32:ASP:OD2	1:A:216:TYR:OH	2.35	0.40
1:A:246:SER:HB3	2:H:104:SER:HA	2.03	0.40
2:H:1:GLN:OE1	2:H:1:GLN:HA	2.21	0.40
2:H:88:ASP:O	2:H:120:VAL:HG11	2.21	0.40
3:L:119:PHE:HB2	3:L:134:VAL:HB	2.03	0.40
1:A:55:LYS:HD2	1:A:139:VAL:CG1	2.51	0.40
3:L:171:ASP:O	3:L:172:SER:CB	2.69	0.40
1:A:317:ILE:HB	1:A:322:LEU:HD12	2.04	0.40
1:A:389:LYS:HA	1:A:389:LYS:HD3	1.82	0.40
2:H:60:ARG:NH1	3:L:95:ASP:OD1	2.54	0.40
3:L:12:VAL:HG22	3:L:13:ALA:H	1.86	0.40
2:H:34:VAL:HG12	2:H:102:HIS:CB	2.46	0.40
2:H:210:LYS:H	2:H:210:LYS:NZ	2.19	0.40
3:L:126:LEU:O	3:L:184:LYS:HE3	2.22	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)
1:A:182:ASN:OD1	3:L:205:PRO:CD[3_554]	2.05	0.15

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	351/439 (80%)	327 (93%)	22 (6%)	2 (1%)	22 50
2	H	208/239 (87%)	197 (95%)	8 (4%)	3 (1%)	9 31
3	L	202/215 (94%)	188 (93%)	12 (6%)	2 (1%)	13 39
All	All	761/893 (85%)	712 (94%)	42 (6%)	7 (1%)	14 41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	50	ASN
2	H	155	PHE
3	L	172	SER
2	H	158	PRO
2	H	33	GLY
1	A	105	ASP
1	A	340	PRO

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	321/387 (83%)	312 (97%)	9 (3%)	38 62
2	H	190/211 (90%)	185 (97%)	5 (3%)	41 64
3	L	181/185 (98%)	178 (98%)	3 (2%)	56 74
All	All	692/783 (88%)	675 (98%)	17 (2%)	42 65

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	105	ASP
1	A	199	ARG
1	A	207	CYS
1	A	213	ARG
1	A	237	ASP
1	A	326	ASP
1	A	411	GLU
1	A	416	VAL
2	H	75	THR
2	H	88	ASP
2	H	100	ARG
2	H	149	CYS
2	H	205	CYS
3	L	4	LEU
3	L	39	SER
3	L	95	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	182	ASN
2	H	209	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
4	NAG	A	501	1	14,14,15	0.99	1 (7%)	17,19,21	0.51	0

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
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	C1-C2	2.99	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C4-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	361/439 (82%)	-0.10	4 (1%)	77	70	58, 89, 119, 136	0
2	H	214/239 (89%)	-0.07	6 (2%)	55	47	55, 84, 135, 154	0
3	L	210/215 (97%)	0.01	2 (0%)	79	71	61, 99, 160, 170	0
All	All	785/893 (87%)	-0.06	12 (1%)	71	62	55, 90, 152, 170	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ASP	6.4
2	H	32	SER	3.9
2	H	29	LEU	3.3
2	H	111	SER	3.0
1	A	202	ASN	3.0
1	A	236	MET	3.0
1	A	238	GLY	2.9
2	H	31	THR	2.6
2	H	112	TRP	2.5
2	H	183	GLY	2.4
3	L	204	SER	2.3
3	L	143	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	A	501	14/15	0.56	0.10	117,141,143,144	0

6.5 Other polymers

There are no such residues in this entry.