WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 05:21 PM JST

PDB ID	:	5ZXV
Title	:	Structural definition of a unique neutralization epitope on the receptor-binding domain of MERS-CoV spike glycoprotein
Authors	:	Zhang, S.; Wang, X.
Deposited on	:	2018-05-21
Resolution	:	4.48 Å(reported)

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

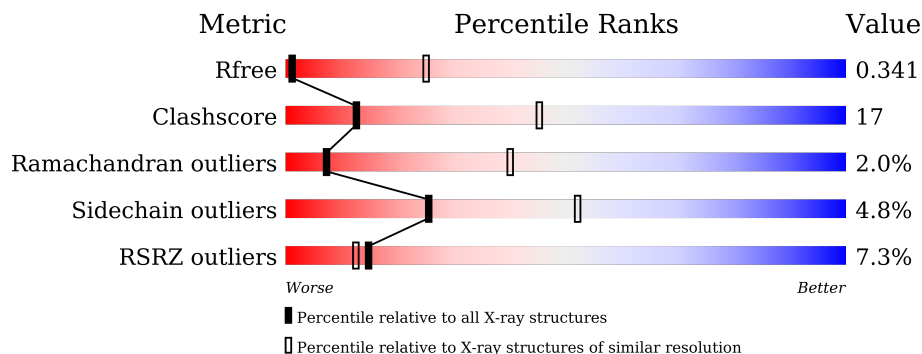|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.48 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	Percentile Ranks	Value
Rfree		0.341
Clashscore		17
Ramachandran outliers		2.0%
Sidechain outliers		4.8%
RSRZ outliers		7.3%

Worse ——— Better

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1051 (5.12-3.80)
Clashscore	141614	1119 (5.12-3.80)
Ramachandran outliers	138981	1065 (5.12-3.80)
Sidechain outliers	138945	1047 (5.12-3.80)
RSRZ outliers	127900	1099 (5.20-3.70)

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 <=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	208	.% / 74% 23% •
1	B	208	3% / 77% 21% •
2	C	213	15% / 62% 32% • •
2	H	213	7% / 58% 37% 5%
3	D	215	7% / 69% 27% •
3	L	215	9% / 70% 26% •

2 Entity composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9462 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 MERS-CoV RBD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1608	1026	256	315	11			
1	B	208	Total	C	N	O	S	0	0	0
			1608	1026	256	315	11			

- Molecule 2 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	2	0
			1606	1015	267	318	6			
2	C	213	Total	C	N	O	S	0	2	0
			1606	1015	267	318	6			

- Molecule 3 is a protein called light chain.

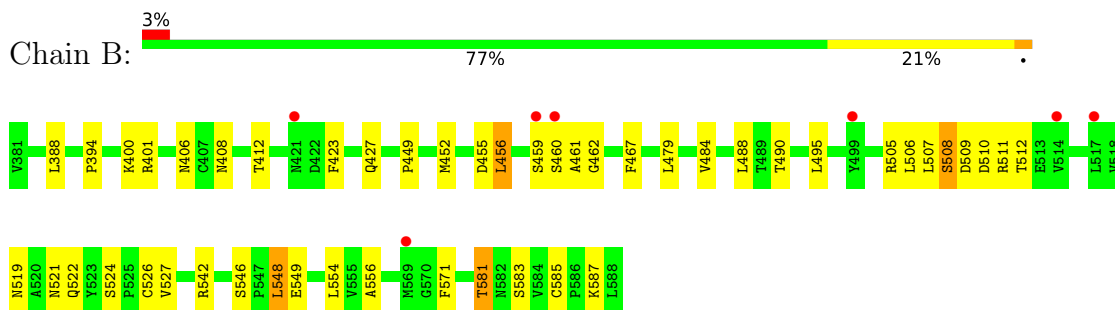| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	206	Total	C	N	O	S	0	0	0
			1517	949	251	313	4			
3	D	206	Total	C	N	O	S	0	0	0
			1517	949	251	313	4			

3 Residue-property plots ⓘ

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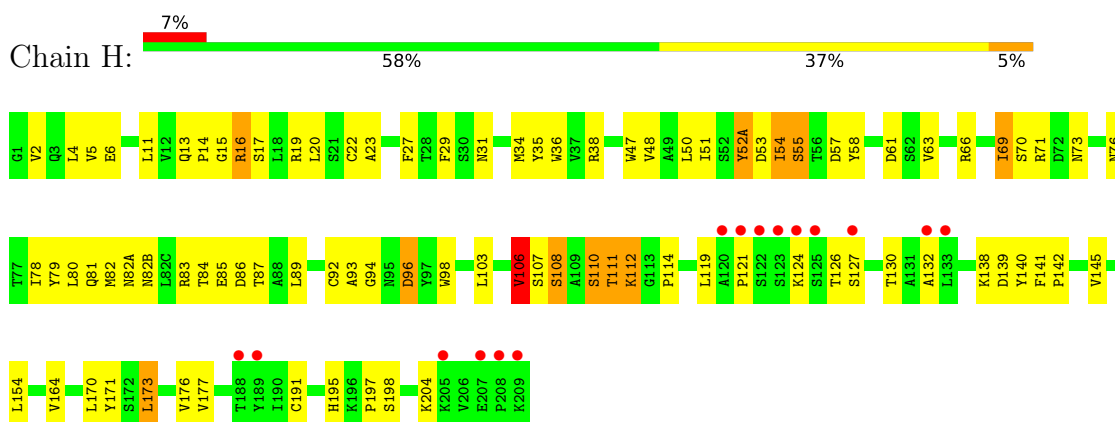
- Molecule 1: MERS-CoV RBD
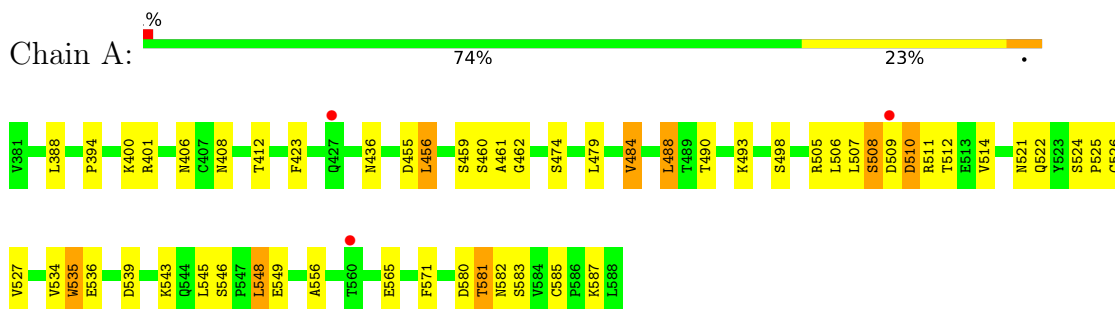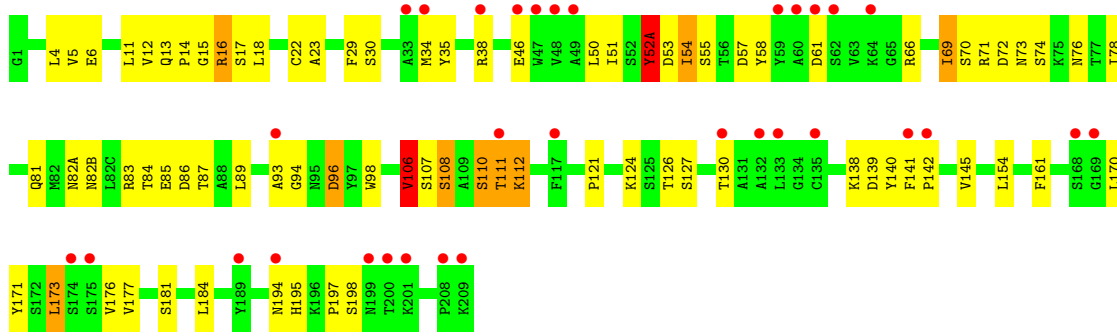

- Molecule 1: MERS-CoV RBD
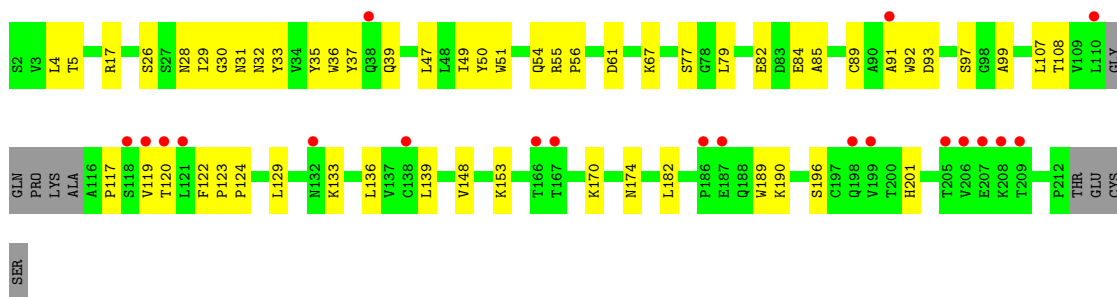

- Molecule 2: heavy chain

- Molecule 2: heavy chain

G1 L4 V5 E6 L11 V12 Q13 P14 G15 R16 S17 L18 C22 A23 F29 S30 A33 M34 Y35 R38 E46 W47 V48 A49 L50 I51 S52 Y52A D53 I54 S55 T56 D57 Y58 Y59 A60 D61 S62 V63 K64 G65 R66 I69 S70 R71 D72 N73 S74 K75 N76 T77 I78

Q81 M82 N82A N82B L82C R83 T84 E85 D86 T87 A88 L89 A93 G94 N95 D96 Y97 W98 V106 S107 S108 A109 S110 T111 K112 F117 P121 K124 S125 T126 S127 T130 A131 A132 L133 G134 C135 K138 D139 Y140 F141 P142 V145 L154 F161 S168 G169 L170

Y171 S172 L173 S174 S175 V176 V177 S181 L184 Y189 N194 H195 K196 P197 S198 N199 T200 K201 P208 K209

- Molecule 3: light chain

Chain L:

9%

70% 26%

S2 V3 L4 T5 R17 S26 S27 N28 I29 G30 N31 N32 Y33 V34 Y35 W36 Y37 Q38 Q39 L47 L48 I49 Y50 W51 Q54 R55 P56 D61 K67 S77 G78 L79 E82 D83 E84 A85 C89 A90 A91 W92 D93 S97 G98 A99 L107 T108 V109 L110 GLY

GLN PRO LYS ALA A116 P117 S118 V119 T120 L121 F122 P123 P124 L129 N132 K133 L136 V137 C138 L139 V148 K153 T166 T167 K170 N174 L182 P186 E187 Q188 W189 K190 S196 C197 Q198 V199 T200 H201 T205 V206 E207 K208 T209 P212 THR GLU CYS

SER

- Molecule 3: light chain

Chain D:

7%

69% 27%

S2 V3 L4 T5 R17 S26 S27 N28 I29 G30 N31 N32 Y33 V34 Y35 W36 Y37 Q38 Q39 L40 L47 L48 I49 Y50 W51 R55 P56 D61 K67 A72 S73 L74 A75 I76 S77 G78 L79 E82 D83 E84 A85 C89 A90 A91 W92 D93 D94 S95 L96 S97

G102 G103 L107 T108 V109 L110 GLY GLN PRO LYS ALA A116 P117 S118 V119 F122 P123 P124 L129 K133 A134 T135 L136 L139 I140 V148 K153 K170 N174 A177 L182 T185 P186 W189 K190 S196 H201 E202 G203 S204 E207 P212 THR

GLU CYS SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	138.65Å 138.65Å 228.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.44 – 4.48 35.44 – 4.48	Depositor EDS
% Data completeness (in resolution range)	95.0 (35.44-4.48) 96.3 (35.44-4.48)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 4.44Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.307 , 0.343 0.318 , 0.341	Depositor DCC
R_{free} test set	469 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	184.4	Xtriage
Anisotropy	0.214	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.19 , 174.1	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.066 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9462	wwPDB-VP
Average B, all atoms (Å^2)	308.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 (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	0.38	1/1647 (0.1%)	0.59	1/2249 (0.0%)
1	B	0.33	0/1647	0.52	0/2249
2	C	0.42	1/1650 (0.1%)	0.66	2/2249 (0.1%)
2	H	0.37	0/1650	0.65	2/2249 (0.1%)
3	D	0.28	0/1554	0.50	0/2126
3	L	0.28	0/1554	0.48	0/2126
All	All	0.35	2/9702 (0.0%)	0.57	5/13248 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	52(A)	TYR	CD1-CE1	-7.95	1.27	1.39
1	A	535	TRP	CB-CG	-6.11	1.39	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	535	TRP	CA-CB-CG	-7.71	99.05	113.70
2	H	106	VAL	CA-CB-CG1	5.58	119.26	110.90
2	C	106	VAL	CA-CB-CG1	5.39	118.98	110.90
2	H	106	VAL	CG1-CB-CG2	-5.14	102.68	110.90
2	C	52(A)	TYR	CA-CB-CG	-5.13	103.65	113.40

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	1608	0	1574	38	0
1	B	1608	0	1574	29	0
2	C	1606	0	1577	82	0
2	H	1606	0	1577	102	0
3	D	1517	0	1435	48	0
3	L	1517	0	1435	50	0
All	All	9462	0	9172	311	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 17.

All (311) 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:B:548:LEU:HB2	3:D:92:TRP:HB2	1.37	1.07
2:H:106:VAL:HG12	2:H:107:SER:H	1.26	0.99
2:C:106:VAL:HG12	2:C:107:SER:H	1.26	0.98
2:H:22:CYS:HB3	2:H:78:ILE:HB	1.53	0.90
2:H:14:PRO:HD3	2:H:107:SER:HB2	1.54	0.89
2:C:14:PRO:HD3	2:C:107:SER:HB2	1.56	0.88
2:H:87:THR:OG1	2:H:106:VAL:HG23	1.75	0.87
2:C:22:CYS:HB3	2:C:78:ILE:HB	1.57	0.87
2:H:106:VAL:CG1	2:H:107:SER:H	1.88	0.86
2:C:87:THR:OG1	2:C:106:VAL:HG23	1.75	0.86
2:C:106:VAL:CG1	2:C:107:SER:H	1.88	0.85
2:H:112:LYS:HG2	2:H:141:PHE:H	1.41	0.84
2:C:112:LYS:HG2	2:C:141:PHE:H	1.42	0.84
3:L:50:TYR:HD2	3:L:51:TRP:HD1	1.26	0.83
3:D:50:TYR:HD2	3:D:51:TRP:HD1	1.27	0.81
2:H:13:GLN:HB2	2:H:16:ARG:HD3	1.65	0.79
1:A:546:SER:N	1:A:549:GLU:OE2	2.17	0.78
1:B:548:LEU:HB2	3:D:92:TRP:CB	2.14	0.77
1:B:546:SER:N	1:B:549:GLU:OE2	2.17	0.77
1:B:394:PRO:HG3	1:B:400:LYS:HG3	1.67	0.76
1:B:456:LEU:HG	1:B:479:LEU:HD21	1.68	0.75
2:C:13:GLN:HB2	2:C:16:ARG:HD3	1.67	0.74
1:A:456:LEU:HG	1:A:479:LEU:HD21	1.68	0.73
2:H:112:LYS:HD3	2:H:140:TYR:HB2	1.70	0.72
2:C:112:LYS:HD3	2:C:140:TYR:HB2	1.71	0.71
3:L:17:ARG:HG2	3:L:77:SER:HA	1.73	0.71
1:A:508:SER:HB2	2:H:52(A):TYR:CE1	2.25	0.71
2:H:110:SER:O	2:H:111:THR:OG1	2.08	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:148:VAL:HG12	3:L:201:HIS:HB2	1.73	0.70
1:B:408:ASN:HA	1:B:585:CYS:O	1.90	0.70
2:C:112:LYS:HE2	2:C:195:HIS:CE1	2.27	0.69
1:A:408:ASN:HA	1:A:585:CYS:O	1.92	0.69
2:C:112:LYS:HZ3	2:C:141:PHE:C	1.95	0.69
3:D:28:ASN:HA	3:D:92:TRP:O	1.91	0.69
2:C:111:THR:HG21	2:C:141:PHE:HB3	1.75	0.69
2:C:84:THR:HA	2:C:106:VAL:HG22	1.74	0.68
2:C:53:ASP:HA	2:C:73:ASN:HD21	1.56	0.68
2:H:106:VAL:HG12	2:H:107:SER:N	2.07	0.67
2:C:93:ALA:HB1	2:C:98:TRP:HA	1.76	0.67
2:H:112:LYS:HZ2	2:H:140:TYR:HD2	1.43	0.67
3:L:170:LYS:NZ	3:L:174:ASN:OD1	2.27	0.67
2:H:112:LYS:HZ3	2:H:141:PHE:C	1.98	0.66
1:B:519:ASN:ND2	3:D:50:TYR:OH	2.28	0.66
2:H:13:GLN:HA	2:H:107:SER:HA	1.76	0.66
1:A:535:TRP:HB3	1:A:539:ASP:OD2	1.95	0.66
2:H:195:HIS:CE1	2:H:197:PRO:HB2	2.30	0.66
1:A:505:ARG:NH2	1:A:549:GLU:O	2.29	0.65
2:C:110:SER:O	2:C:111:THR:OG1	2.10	0.65
2:C:106:VAL:HG12	2:C:107:SER:N	2.07	0.65
1:B:509:ASP:N	2:C:52(A):TYR:OH	2.30	0.65
2:C:52(A):TYR:CZ	2:C:53:ASP:HB3	2.32	0.65
2:C:195:HIS:CE1	2:C:197:PRO:HB2	2.32	0.65
1:A:535:TRP:HA	1:A:535:TRP:CE3	2.32	0.65
2:C:112:LYS:HZ2	2:C:140:TYR:HD2	1.44	0.64
3:D:170:LYS:NZ	3:D:174:ASN:OD1	2.30	0.64
2:H:93:ALA:HB1	2:H:98:TRP:HA	1.80	0.64
1:A:509:ASP:O	1:A:511:ARG:N	2.31	0.64
1:B:505:ARG:NH2	1:B:549:GLU:O	2.28	0.64
3:L:50:TYR:CD2	3:L:51:TRP:HD1	2.13	0.64
3:D:35:TYR:O	3:D:89:CYS:HA	1.99	0.63
2:H:84:THR:HA	2:H:106:VAL:CG2	2.28	0.63
2:C:14:PRO:CD	2:C:107:SER:HB2	2.29	0.63
2:H:112:LYS:HE2	2:H:195:HIS:CE1	2.33	0.63
2:H:140:TYR:O	2:H:171:TYR:N	2.24	0.63
3:D:148:VAL:HG12	3:D:201:HIS:HB2	1.80	0.63
1:B:548:LEU:CB	3:D:92:TRP:HB2	2.23	0.63
2:C:52(A):TYR:CE2	2:C:53:ASP:HB3	2.33	0.62
2:H:107:SER:HB3	2:H:108:SER:HA	1.81	0.61
2:H:111:THR:HG21	2:H:141:PHE:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:ASN:HD22	3:D:92:TRP:HB3	1.64	0.61
2:C:4:LEU:HD13	2:C:93:ALA:HA	1.83	0.61
2:C:51:ILE:HG13	2:C:57:ASP:OD1	2.01	0.61
1:B:401:ARG:HH12	1:B:521:ASN:HB3	1.63	0.61
2:H:106:VAL:CG1	2:H:107:SER:N	2.62	0.61
2:H:51:ILE:HB	2:H:69:ILE:HD12	1.83	0.61
3:L:28:ASN:HA	3:L:92:TRP:O	2.00	0.61
2:H:4:LEU:HD13	2:H:93:ALA:HA	1.82	0.60
2:C:13:GLN:HA	2:C:107:SER:HA	1.82	0.60
2:C:84:THR:HA	2:C:106:VAL:CG2	2.31	0.60
3:D:136:LEU:HD12	3:D:182:LEU:HD23	1.82	0.60
2:C:107:SER:HB3	2:C:108:SER:HA	1.83	0.60
3:D:50:TYR:CD2	3:D:51:TRP:HD1	2.15	0.60
1:A:394:PRO:HG3	1:A:400:LYS:HG3	1.84	0.60
1:A:401:ARG:HH12	1:A:521:ASN:HB3	1.66	0.60
2:H:14:PRO:CD	2:H:107:SER:HB2	2.28	0.59
2:H:53:ASP:HA	2:H:73:ASN:HD21	1.66	0.59
1:A:549:GLU:HB3	3:L:51:TRP:CH2	2.38	0.59
2:H:51:ILE:HG13	2:H:57:ASP:OD1	2.02	0.59
1:B:524:SER:HB3	1:B:527:VAL:HG13	1.84	0.59
2:C:51:ILE:HB	2:C:69:ILE:HD12	1.84	0.59
1:B:549:GLU:HB3	3:D:51:TRP:CH2	2.38	0.59
3:D:79:LEU:HD11	3:D:107:LEU:HD21	1.84	0.59
2:C:29:PHE:CD2	2:C:76:ASN:HA	2.38	0.58
2:C:34:MET:HG2	2:C:71:ARG:HH12	1.68	0.58
2:C:52(A):TYR:HA	2:C:71:ARG:NH1	2.17	0.58
3:L:26:SER:O	3:L:31:ASN:ND2	2.36	0.58
2:C:15:GLY:HA2	2:C:82(B):ASN:HA	1.86	0.58
2:H:112:LYS:HD3	2:H:140:TYR:CB	2.32	0.58
2:H:176:VAL:HG11	3:L:139:LEU:HD13	1.85	0.58
2:H:84:THR:HA	2:H:106:VAL:HG22	1.85	0.57
2:H:112:LYS:HD3	2:H:140:TYR:HA	1.86	0.57
3:L:50:TYR:HD2	3:L:51:TRP:CD1	2.15	0.57
2:C:51:ILE:HD11	2:C:54:ILE:HA	1.86	0.57
1:A:498:SER:HB3	1:A:534:VAL:HG23	1.86	0.57
2:H:11:LEU:HD11	2:H:142:PRO:HD3	1.87	0.57
2:C:35:TYR:CD1	2:C:50:LEU:HD21	2.40	0.57
2:H:96:ASP:HA	3:L:47:LEU:HD22	1.85	0.57
2:C:34:MET:HG2	2:C:71:ARG:NH1	2.19	0.57
3:L:79:LEU:HD11	3:L:107:LEU:HD21	1.86	0.57
2:H:53:ASP:OD2	2:H:55:SER:OG	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:LEU:HB2	3:L:92:TRP:HB2	1.86	0.56
2:H:13:GLN:O	2:H:16:ARG:HB2	2.04	0.56
3:D:17:ARG:HG2	3:D:77:SER:HA	1.86	0.56
3:D:36:TRP:HB2	3:D:49:ILE:HB	1.86	0.56
2:C:140:TYR:OH	2:C:173:LEU:HD23	2.06	0.56
2:H:66:ARG:HB3	2:H:82(A):ASN:O	2.07	0.55
2:H:138:LYS:NZ	3:L:133:LYS:HD3	2.21	0.55
2:H:58:TYR:HB3	3:L:97:SER:O	2.07	0.55
2:C:12:VAL:HG11	2:C:18:LEU:HB2	1.88	0.55
3:D:32:ASN:ND2	3:D:92:TRP:HB3	2.21	0.55
1:B:506:LEU:HD21	1:B:510:ASP:HA	1.89	0.54
2:C:112:LYS:HD3	2:C:140:TYR:HA	1.89	0.54
2:C:112:LYS:HD3	2:C:140:TYR:CB	2.36	0.54
2:C:52(A):TYR:N	2:C:52(A):TYR:CD1	2.74	0.54
1:A:581:THR:O	1:A:583:SER:N	2.41	0.54
2:C:30:SER:O	2:C:52(A):TYR:HD2	1.89	0.54
2:C:140:TYR:O	2:C:171:TYR:N	2.27	0.54
2:H:154:LEU:HD21	2:H:177:VAL:HG21	1.90	0.54
3:L:32:ASN:HD22	3:L:92:TRP:HB3	1.73	0.54
2:H:34:MET:HG2	2:H:71:ARG:HH12	1.74	0.53
2:H:35:TYR:CD1	2:H:50:LEU:HD21	2.43	0.53
2:C:96:ASP:HA	3:D:47:LEU:HD22	1.89	0.53
2:C:11:LEU:HD11	2:C:142:PRO:HD3	1.90	0.53
2:C:138:LYS:NZ	3:D:133:LYS:HD3	2.22	0.53
2:C:176:VAL:HG11	3:D:139:LEU:HD13	1.90	0.53
2:H:51:ILE:HD11	2:H:54:ILE:HA	1.90	0.53
2:H:111:THR:HB	2:H:112:LYS:CG	2.38	0.53
1:A:545:LEU:HD22	3:L:51:TRP:HH2	1.73	0.53
2:H:6:GLU:N	2:H:6:GLU:OE1	2.42	0.53
2:C:181:SER:HA	2:C:184:LEU:HG	1.90	0.53
1:B:507:LEU:HD12	1:B:512:THR:HB	1.90	0.52
2:C:6:GLU:N	2:C:6:GLU:OE1	2.42	0.52
1:A:507:LEU:HD12	1:A:512:THR:HB	1.91	0.52
2:H:84:THR:OG1	2:H:85:GLU:OE2	2.27	0.52
3:D:119:VAL:HA	3:D:139:LEU:O	2.08	0.52
2:H:29:PHE:CD2	2:H:76:ASN:HA	2.45	0.52
2:H:140:TYR:OH	2:H:173:LEU:HD23	2.10	0.52
3:L:28:ASN:OD1	3:L:29:ILE:N	2.34	0.51
3:L:39:GLN:O	3:L:85:ALA:HB1	2.09	0.51
3:D:47:LEU:HD23	3:D:56:PRO:HG3	1.91	0.51
2:H:52(A):TYR:CE2	2:H:53:ASP:HB3	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:30:GLY:H	3:D:67:LYS:HE3	1.75	0.51
3:L:32:ASN:ND2	3:L:92:TRP:HB3	2.26	0.51
2:C:11:LEU:HD21	2:C:142:PRO:HG3	1.93	0.51
2:C:106:VAL:CG1	2:C:107:SER:N	2.63	0.51
2:H:47:TRP:HE1	2:H:50:LEU:HG	1.76	0.50
2:H:195:HIS:CD2	2:H:197:PRO:HD2	2.47	0.50
2:C:111:THR:HB	2:C:112:LYS:CG	2.41	0.50
1:A:507:LEU:HD13	2:H:31:ASN:HB3	1.93	0.50
1:B:526:CYS:SG	1:B:556:ALA:HB2	2.51	0.50
3:D:28:ASN:OD1	3:D:29:ILE:N	2.36	0.50
2:H:140:TYR:N	2:H:170:LEU:HB3	2.27	0.50
2:C:13:GLN:O	2:C:16:ARG:HB2	2.11	0.50
2:H:48:VAL:HG13	2:H:63:VAL:HG11	1.93	0.49
2:H:112:LYS:HD3	2:H:140:TYR:CA	2.42	0.49
2:C:140:TYR:N	2:C:170:LEU:HB3	2.27	0.49
2:H:107:SER:CB	2:H:108:SER:HA	2.41	0.49
1:A:548:LEU:HG	3:L:92:TRP:HB2	1.95	0.49
1:B:459:SER:O	1:B:460:SER:HB3	2.13	0.49
1:A:525:PRO:HA	3:L:54:GLN:HE22	1.76	0.49
3:D:4:LEU:HD11	3:D:91:ALA:HB3	1.93	0.49
3:L:36:TRP:HB2	3:L:49:ILE:HB	1.95	0.48
2:C:112:LYS:CD	2:C:140:TYR:HB2	2.40	0.48
2:H:112:LYS:CD	2:H:140:TYR:HB2	2.39	0.48
3:D:26:SER:O	3:D:31:ASN:ND2	2.46	0.48
2:H:58:TYR:HD2	3:L:92:TRP:HH2	1.61	0.48
2:H:112:LYS:HG3	2:H:141:PHE:O	2.14	0.48
3:L:136:LEU:HD12	3:L:182:LEU:HD23	1.94	0.48
2:C:58:TYR:HB3	3:D:97:SER:O	2.13	0.48
2:C:112:LYS:HD3	2:C:140:TYR:CA	2.44	0.48
3:D:123:PRO:HA	3:D:136:LEU:HD23	1.94	0.48
2:H:20:LEU:O	2:H:79:TYR:HA	2.13	0.48
2:H:13:GLN:HA	2:H:107:SER:CB	2.44	0.48
2:C:84:THR:OG1	2:C:85:GLU:OE2	2.32	0.48
2:H:112:LYS:HE3	2:H:114:PRO:HD3	1.96	0.48
3:L:153:LYS:HB2	3:L:196:SER:HB2	1.96	0.48
2:C:13:GLN:HA	2:C:107:SER:CB	2.44	0.48
1:A:459:SER:O	1:A:460:SER:HB3	2.13	0.47
2:H:112:LYS:CE	2:H:140:TYR:HB2	2.44	0.47
3:L:47:LEU:HD23	3:L:56:PRO:HG3	1.95	0.47
2:C:154:LEU:HD21	2:C:177:VAL:HG21	1.96	0.47
1:A:524:SER:HB3	1:A:527:VAL:HG13	1.97	0.47

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:VAL:HG23	2:H:23:ALA:HB3	1.96	0.47
2:H:69:ILE:HD13	2:H:70:SER:N	2.29	0.47
2:H:34:MET:HG2	2:H:71:ARG:NH1	2.29	0.47
2:C:195:HIS:CD2	2:C:197:PRO:HD2	2.49	0.47
1:A:587:LYS:HB2	1:A:587:LYS:HE3	1.69	0.47
3:D:189:TRP:CD1	3:D:190:LYS:HE2	2.50	0.47
1:A:526:CYS:SG	1:A:556:ALA:HB2	2.55	0.46
3:D:92:TRP:NE1	3:D:94:ASP:HA	2.30	0.46
2:C:17:SER:OG	2:C:81:GLN:NE2	2.48	0.46
3:D:84:GLU:HG3	3:D:108:THR:HA	1.96	0.46
1:A:507:LEU:HD11	1:A:514:VAL:HG23	1.97	0.46
1:A:508:SER:HB2	2:H:52(A):TYR:CZ	2.51	0.45
1:B:388:LEU:HD11	1:B:571:PHE:CE1	2.50	0.45
3:L:84:GLU:HG3	3:L:108:THR:HA	1.97	0.45
1:B:460:SER:OG	1:B:461:ALA:N	2.49	0.45
1:A:460:SER:OG	1:A:461:ALA:N	2.49	0.45
3:L:123:PRO:HA	3:L:136:LEU:HD23	1.98	0.45
3:D:92:TRP:HE1	3:D:94:ASP:HA	1.81	0.45
3:D:93:ASP:HB3	3:D:96:LEU:HB3	1.99	0.45
2:H:111:THR:HB	2:H:112:LYS:HG3	1.97	0.45
2:H:112:LYS:HD2	2:H:112:LYS:C	2.36	0.45
2:H:139:ASP:OD2	3:L:133:LYS:NZ	2.36	0.45
3:L:50:TYR:HD1	3:L:56:PRO:HD3	1.81	0.45
3:L:189:TRP:CD1	3:L:190:LYS:HE2	2.52	0.45
3:D:50:TYR:HD2	3:D:51:TRP:CD1	2.19	0.45
1:B:587:LYS:HB2	1:B:587:LYS:HE3	1.75	0.45
2:H:58:TYR:HD2	3:L:92:TRP:CH2	2.34	0.45
1:A:493:LYS:NZ	1:A:565:GLU:O	2.48	0.44
2:C:112:LYS:CE	2:C:140:TYR:HB2	2.48	0.44
2:H:52(A):TYR:CG	2:H:53:ASP:N	2.86	0.44
3:D:117:PRO:HD3	3:D:201:HIS:CD2	2.51	0.44
2:H:138:LYS:HZ3	3:L:133:LYS:HD3	1.83	0.44
3:L:35:TYR:O	3:L:89:CYS:HA	2.18	0.44
2:H:112:LYS:NZ	2:H:140:TYR:HD2	2.14	0.44
1:A:548:LEU:HD13	3:L:35:TYR:CD2	2.52	0.44
2:C:112:LYS:HG3	2:C:141:PHE:O	2.18	0.44
3:D:118:SER:O	3:D:140:ILE:HA	2.18	0.44
2:H:11:LEU:HD21	2:H:142:PRO:HG3	2.00	0.44
2:H:36:TRP:CE2	2:H:80:LEU:HB2	2.53	0.44
2:H:132:ALA:HB3	3:L:120:THR:HG21	2.00	0.44
3:D:136:LEU:HB2	3:D:182:LEU:HB3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:LYS:HZ3	3:L:33:TYR:HE2	1.65	0.44
2:C:139:ASP:OD2	3:D:133:LYS:NZ	2.46	0.43
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.58	0.43
2:H:13:GLN:HA	2:H:107:SER:CA	2.43	0.43
2:C:69:ILE:HD13	2:C:70:SER:N	2.33	0.43
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.53	0.43
2:C:72:ASP:OD1	2:C:74:SER:OG	2.30	0.43
2:C:111:THR:HB	2:C:112:LYS:HG3	2.00	0.43
3:D:153:LYS:HB2	3:D:196:SER:HB2	2.00	0.43
1:A:525:PRO:CA	3:L:54:GLN:HE22	2.31	0.43
2:C:53:ASP:HA	2:C:73:ASN:ND2	2.30	0.43
2:H:47:TRP:CG	3:L:99:ALA:HB3	2.53	0.43
2:C:195:HIS:ND1	2:C:198:SER:OG	2.42	0.43
3:L:4:LEU:HD11	3:L:91:ALA:HB3	2.00	0.43
3:L:30:GLY:H	3:L:67:LYS:HE3	1.84	0.43
2:H:38:ARG:NH1	2:H:86:ASP:OD1	2.41	0.43
2:C:112:LYS:HD2	2:C:112:LYS:C	2.39	0.43
3:D:93:ASP:O	3:D:97:SER:N	2.52	0.43
1:A:484:VAL:HG23	1:A:488:LEU:HB3	2.01	0.43
2:C:38:ARG:HA	2:C:89:LEU:O	2.19	0.43
2:H:19:ARG:HB2	2:H:81:GLN:OE1	2.19	0.43
3:D:117:PRO:HB2	3:D:140:ILE:HG23	2.01	0.43
2:H:17:SER:OG	2:H:82:MET:O	2.25	0.42
2:H:93:ALA:HB3	2:H:98:TRP:CE3	2.54	0.42
2:H:47:TRP:NE1	2:H:50:LEU:HG	2.33	0.42
2:H:52(A):TYR:CD1	2:H:52(A):TYR:N	2.86	0.42
2:H:89:LEU:HD21	2:H:103:LEU:HG	2.01	0.42
2:H:164:VAL:O	2:H:171:TYR:HA	2.18	0.42
1:B:508:SER:HB3	2:C:52(A):TYR:CE1	2.55	0.42
3:D:36:TRP:CD2	3:D:74:LEU:HB2	2.54	0.42
3:L:93:ASP:O	3:L:97:SER:N	2.52	0.42
3:D:40:LEU:HD23	3:D:85:ALA:HB2	2.00	0.42
1:A:506:LEU:HG	1:A:510:ASP:HA	2.01	0.42
1:A:580:ASP:C	1:A:581:THR:OG1	2.58	0.42
3:L:119:VAL:HA	3:L:139:LEU:O	2.20	0.42
2:H:2:VAL:HG13	2:H:27:PHE:CE1	2.55	0.41
2:H:19:ARG:HA	2:H:80:LEU:O	2.18	0.41
2:H:52(A):TYR:HA	2:H:71:ARG:NH1	2.34	0.41
2:C:14:PRO:HD3	2:C:107:SER:CB	2.38	0.41
1:A:535:TRP:CD1	1:A:536:GLU:HB2	2.55	0.41
2:H:85:GLU:H	2:H:85:GLU:CD	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:119:LEU:HB3	3:L:122:PHE:CG	2.56	0.41
2:C:5:VAL:CG2	2:C:23:ALA:HB3	2.49	0.41
1:A:474:SER:O	1:B:427:GLN:NE2	2.53	0.41
1:A:522:GLN:NE2	3:L:55:ARG:HB2	2.35	0.41
1:B:467:PHE:O	1:B:524:SER:HB2	2.20	0.41
2:H:195:HIS:ND1	2:H:198:SER:OG	2.42	0.41
2:C:38:ARG:NE	2:C:46:GLU:OE1	2.43	0.41
2:C:107:SER:CB	2:C:108:SER:HA	2.44	0.41
3:L:117:PRO:HD3	3:L:201:HIS:CD2	2.55	0.41
2:C:85:GLU:H	2:C:85:GLU:CD	2.23	0.41
3:D:34:VAL:HG21	3:D:72:ALA:HB2	2.01	0.41
2:H:5:VAL:CG2	2:H:23:ALA:HB3	2.51	0.41
2:H:15:GLY:HA2	2:H:82(B):ASN:HA	2.02	0.41
2:H:66:ARG:HD3	2:H:83:ARG:NH2	2.35	0.41
2:C:93:ALA:CB	2:C:98:TRP:HA	2.46	0.41
2:C:83:ARG:N	2:C:86:ASP:OD2	2.47	0.41
2:C:161:PHE:HE2	3:D:177:ALA:HB1	1.85	0.41
1:A:388:LEU:HD11	1:A:571:PHE:CE1	2.55	0.41
2:H:114:PRO:HB3	2:H:140:TYR:HB3	2.03	0.41
1:A:509:ASP:C	1:A:511:ARG:H	2.24	0.41
1:B:449:PRO:HG2	1:B:452:MET:HG3	2.02	0.41
1:B:509:ASP:O	1:B:511:ARG:HG3	2.21	0.41
2:H:17:SER:OG	2:H:81:GLN:NE2	2.54	0.41
2:H:191:CYS:SG	2:H:204:LYS:HB3	2.61	0.41
3:L:35:TYR:CD1	3:L:50:TYR:HA	2.56	0.41
1:B:522:GLN:NE2	3:D:55:ARG:HB2	2.36	0.41
1:B:581:THR:O	1:B:583:SER:N	2.52	0.41
2:H:92:CYS:SG	2:H:92:CYS:O	2.79	0.41
1:B:542:ARG:HA	1:B:554:LEU:O	2.21	0.40
3:D:35:TYR:CD1	3:D:50:TYR:HA	2.57	0.40
1:B:519:ASN:HB2	1:B:522:GLN:CD	2.42	0.40
3:L:37:TYR:CD1	3:L:47:LEU:HA	2.55	0.40
2:C:66:ARG:HB3	2:C:82(A):ASN:O	2.21	0.40
3:L:124:PRO:HD3	3:L:136:LEU:HD23	2.02	0.40
3:D:37:TYR:CD1	3:D:47:LEU:HA	2.57	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	206/208 (99%)	190 (92%)	12 (6%)	4 (2%)	8	41
1	B	206/208 (99%)	192 (93%)	13 (6%)	1 (0%)	29	68
2	C	213/213 (100%)	190 (89%)	13 (6%)	10 (5%)	2	24
2	H	213/213 (100%)	189 (89%)	14 (7%)	10 (5%)	2	24
3	D	202/215 (94%)	193 (96%)	9 (4%)	0	100	100
3	L	202/215 (94%)	193 (96%)	9 (4%)	0	100	100
All	All	1242/1272 (98%)	1147 (92%)	70 (6%)	25 (2%)	7	40

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	510	ASP
2	H	52(A)	TYR
2	H	54	ILE
2	H	55	SER
2	H	106	VAL
2	H	111	THR
2	C	52(A)	TYR
2	C	54	ILE
2	C	55	SER
2	C	106	VAL
2	C	111	THR
2	H	96	ASP
2	H	126	THR
2	H	127	SER
2	C	96	ASP
2	C	126	THR
2	C	127	SER
1	A	581	THR
1	A	582	ASN
1	B	462	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	94	GLY
2	C	121	PRO
1	A	462	GLY
2	H	121	PRO
2	C	94	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	190/190 (100%)	179 (94%)	11 (6%)	20	47
1	B	190/190 (100%)	178 (94%)	12 (6%)	18	44
2	C	181/179 (101%)	170 (94%)	11 (6%)	18	46
2	H	181/179 (101%)	171 (94%)	10 (6%)	21	49
3	D	168/179 (94%)	164 (98%)	4 (2%)	49	69
3	L	168/179 (94%)	164 (98%)	4 (2%)	49	69
All	All	1078/1096 (98%)	1026 (95%)	52 (5%)	25	52

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	406	ASN
1	A	412	THR
1	A	423	PHE
1	A	436	ASN
1	A	455	ASP
1	A	456	LEU
1	A	484	VAL
1	A	488	LEU
1	A	490	THR
1	A	508	SER
1	A	548	LEU
1	B	406	ASN
1	B	412	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	423	PHE
1	B	455	ASP
1	B	456	LEU
1	B	484	VAL
1	B	488	LEU
1	B	490	THR
1	B	495	LEU
1	B	508	SER
1	B	548	LEU
1	B	581	THR
2	H	16	ARG
2	H	61	ASP
2	H	69	ILE
2	H	108	SER
2	H	110	SER
2	H	112	LYS
2	H	124	LYS
2	H	130	THR
2	H	145	VAL
2	H	173	LEU
3	L	5	THR
3	L	61	ASP
3	L	82	GLU
3	L	129	LEU
2	C	16	ARG
2	C	61	ASP
2	C	69	ILE
2	C	108	SER
2	C	110	SER
2	C	112	LYS
2	C	124	LYS
2	C	130	THR
2	C	145	VAL
2	C	173	LEU
2	C	194	ASN
3	D	5	THR
3	D	61	ASP
3	D	82	GLU
3	D	129	LEU

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

Mol	Chain	Res	Type
1	B	519	ASN
2	H	194	ASN
3	L	32	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 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, 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(Å²)	Q<0.9
1	A	208/208 (100%)	-0.22	3 (1%)	75	66	180, 222, 287, 379	0
1	B	208/208 (100%)	-0.02	7 (3%)	45	36	229, 302, 392, 455	0
2	C	213/213 (100%)	0.56	32 (15%)	2	3	237, 371, 462, 479	0
2	H	213/213 (100%)	0.20	15 (7%)	16	13	187, 263, 431, 609	0
3	D	206/215 (95%)	0.16	14 (6%)	17	14	236, 327, 417, 449	0
3	L	206/215 (95%)	0.27	20 (9%)	7	7	186, 271, 483, 545	0
All	All	1254/1272 (98%)	0.16	91 (7%)	15	12	180, 299, 446, 609	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	208	PRO	7.8
2	H	208	PRO	7.1
2	H	122	SER	6.7
3	L	207	GLU	6.5
2	C	209	LYS	6.2
2	H	121	PRO	6.2
3	D	102	GLY	6.2
2	H	209	LYS	6.1
2	C	194	ASN	6.0
3	L	206	VAL	5.6
2	H	132	ALA	5.4
2	C	132	ALA	5.0
3	L	205	THR	5.0
2	C	175	SER	4.9
1	B	460	SER	4.5
2	C	200	THR	4.3
2	H	125	SER	4.2
3	L	138	CYS	4.0
2	C	34	MET	4.0

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	205	LYS	3.9
2	H	188	THR	3.9
1	A	427	GLN	3.8
3	D	103	GLY	3.7
1	A	509	ASP	3.7
2	C	38	ARG	3.6
3	L	132	ASN	3.6
2	C	46	GLU	3.5
2	C	48	VAL	3.5
2	C	189	TYR	3.5
2	H	133	LEU	3.5
2	C	111	THR	3.5
2	H	207	GLU	3.4
3	D	202	GLU	3.4
2	C	169	GLY	3.3
2	C	49	ALA	3.2
2	H	120	ALA	3.1
3	L	120	THR	3.1
3	D	185	THR	3.1
2	C	199	ASN	3.1
3	L	38	GLN	3.1
2	C	174[A]	SER	3.0
2	C	47	TRP	3.0
2	C	33	ALA	3.0
3	L	119	VAL	3.0
3	L	186	PRO	3.0
1	B	459	SER	2.8
3	D	204	SER	2.8
3	L	91	ALA	2.8
2	C	142	PRO	2.8
3	D	38	GLN	2.8
3	D	203	GLY	2.8
3	L	121	LEU	2.7
2	H	123	SER	2.7
2	C	64	LYS	2.7
3	L	198	GLN	2.6
2	C	133	LEU	2.6
3	D	133	LYS	2.6
3	L	199	VAL	2.5
3	L	209	THR	2.5
3	L	187	GLU	2.5
2	C	59	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	141	PHE	2.5
1	B	517	LEU	2.5
2	H	127	SER	2.4
3	L	118	SER	2.4
1	B	499	TYR	2.4
3	L	166	THR	2.4
1	A	560	THR	2.4
2	C	130	THR	2.4
2	C	60	ALA	2.4
2	C	201	LYS	2.3
3	D	186	PRO	2.3
3	D	134	ALA	2.3
3	L	110	LEU	2.3
3	L	208	LYS	2.2
2	C	117	PHE	2.1
3	D	76	ILE	2.1
2	H	124	LYS	2.1
3	D	207	GLU	2.1
2	C	135	CYS	2.1
2	C	93	ALA	2.1
3	D	124	PRO	2.1
2	H	189	TYR	2.1
1	B	421	ASN	2.1
2	C	62	SER	2.1
1	B	569	MET	2.1
1	B	514	VAL	2.1
3	L	167	THR	2.1
2	C	61	ASP	2.1
2	C	168	SER	2.1
3	D	122	PHE	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.