



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:53 PM UTC

PDB ID : 7YLB / pdb_00007ylb
Title : Two monobodies recognizing the conserved epitopes of SARS-CoV-2 N antigen applicable to the broad COVID-19 diagnosis
Authors : Hu, M.; Du, Y.; Sun, R.; Hao, Q.
Deposited on : 2022-07-26
Resolution : 2.41 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

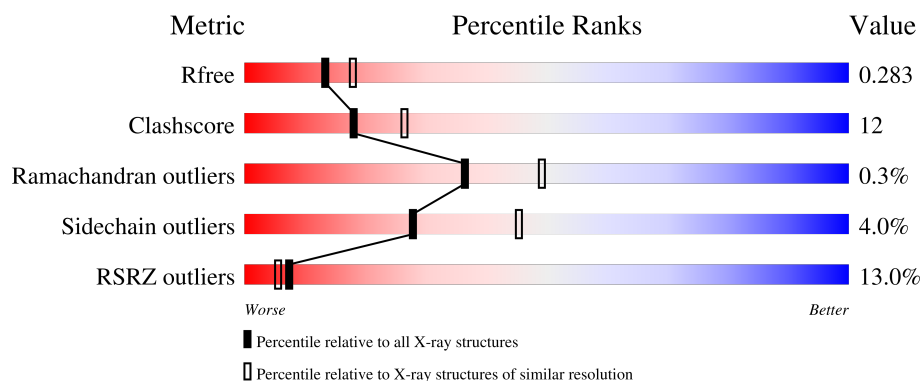
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	122	14% 70% 19% • 10%
1	B	122	3% 73% 16% • 9%
1	C	122	3% 74% 13% • 11%
1	D	122	5% 81% 11% • 7%
1	G	122	4% 70% 20% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	122	7% 74% 16% • 7%
1	J	122	25% 64% 25% • 10%
1	K	122	4% 74% 16% 10%
2	E	94	14% 52% 31% 6% 11%
2	F	94	13% 63% 23% • 11%
2	I	94	24% 62% 26% • 11%
2	L	94	32% 48% 37% • • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9739 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	108	Total	C	N	O	S	0	0	0
			867	551	155	159	2			
1	D	114	Total	C	N	O	S	0	0	0
			904	573	161	168	2			
1	A	110	Total	C	N	O	S	0	0	0
			881	559	157	163	2			
1	B	111	Total	C	N	O	S	0	0	0
			885	562	158	163	2			
1	G	109	Total	C	N	O	S	0	0	0
			873	554	156	161	2			
1	H	113	Total	C	N	O	S	0	0	0
			899	570	160	167	2			
1	J	110	Total	C	N	O	S	0	0	0
			878	557	157	162	2			
1	K	110	Total	C	N	O	S	0	0	0
			880	559	157	162	2			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	243	GLY	-	expression tag	UNP P0DTC9
C	244	SER	-	expression tag	UNP P0DTC9
C	245	GLY	-	expression tag	UNP P0DTC9
C	246	THR	-	expression tag	UNP P0DTC9
D	243	GLY	-	expression tag	UNP P0DTC9
D	244	SER	-	expression tag	UNP P0DTC9
D	245	GLY	-	expression tag	UNP P0DTC9
D	246	THR	-	expression tag	UNP P0DTC9
A	-3	GLY	-	expression tag	UNP P0DTC9
A	-2	SER	-	expression tag	UNP P0DTC9
A	-1	GLY	-	expression tag	UNP P0DTC9
A	0	THR	-	expression tag	UNP P0DTC9
B	-3	GLY	-	expression tag	UNP P0DTC9

Continued on next page...

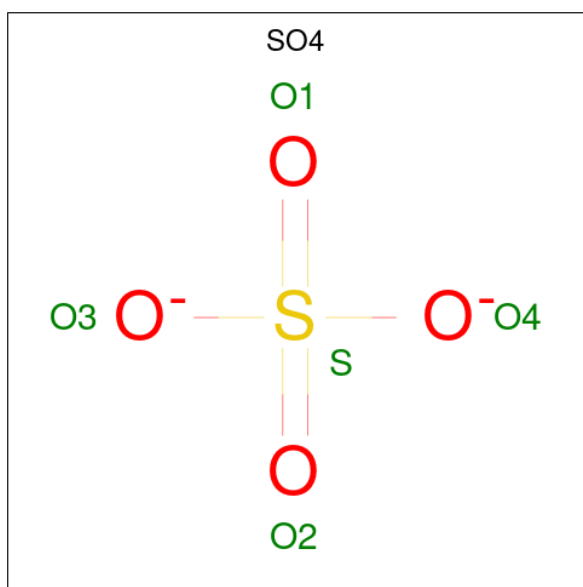
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P0DTC9
B	-1	GLY	-	expression tag	UNP P0DTC9
B	0	THR	-	expression tag	UNP P0DTC9
G	-3	GLY	-	expression tag	UNP P0DTC9
G	-2	SER	-	expression tag	UNP P0DTC9
G	-1	GLY	-	expression tag	UNP P0DTC9
G	0	THR	-	expression tag	UNP P0DTC9
H	-3	GLY	-	expression tag	UNP P0DTC9
H	-2	SER	-	expression tag	UNP P0DTC9
H	-1	GLY	-	expression tag	UNP P0DTC9
H	0	THR	-	expression tag	UNP P0DTC9
J	-3	GLY	-	expression tag	UNP P0DTC9
J	-2	SER	-	expression tag	UNP P0DTC9
J	-1	GLY	-	expression tag	UNP P0DTC9
J	0	THR	-	expression tag	UNP P0DTC9
K	-3	GLY	-	expression tag	UNP P0DTC9
K	-2	SER	-	expression tag	UNP P0DTC9
K	-1	GLY	-	expression tag	UNP P0DTC9
K	0	THR	-	expression tag	UNP P0DTC9

- Molecule 2 is a protein called NC2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	84	Total	C	N	O	0	0	0
			663	430	110	123			
2	E	84	Total	C	N	O	0	0	0
			663	430	110	123			
2	I	84	Total	C	N	O	0	0	0
			663	430	110	123			
2	L	84	Total	C	N	O	0	0	0
			663	430	110	123			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

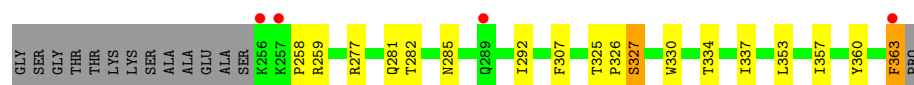
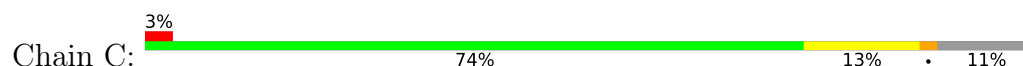


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		

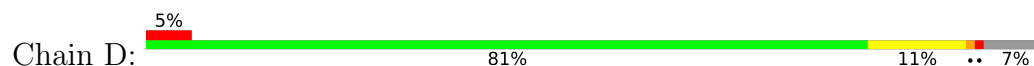
3 Residue-property plots [i](#)

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.

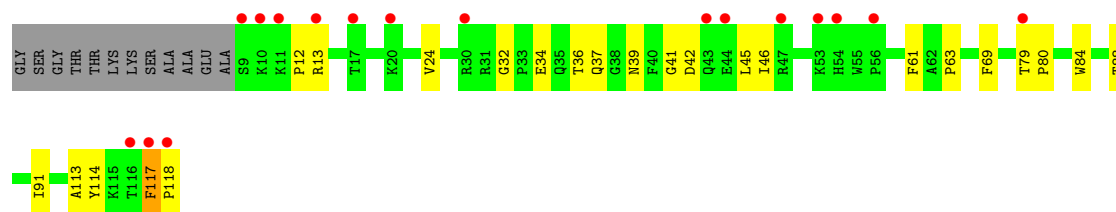
- Molecule 1: Nucleoprotein



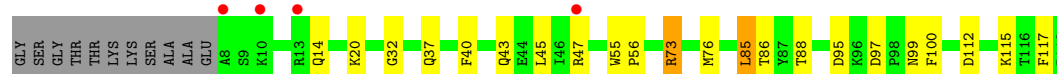
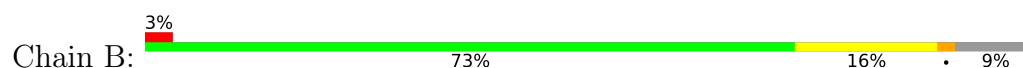
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein

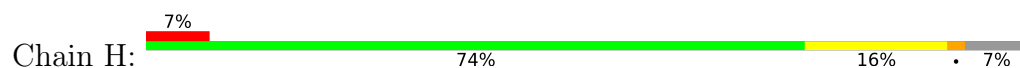


- Molecule 1: Nucleoprotein

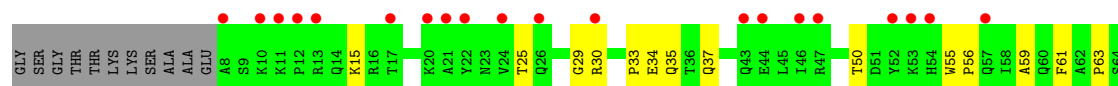




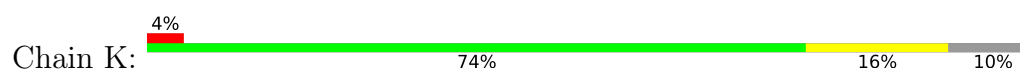
- Molecule 1: Nucleoprotein



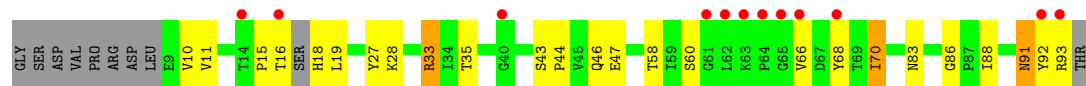
- Molecule 1: Nucleoprotein



- Molecule 1: Nucleoprotein



- Molecule 2: NC2

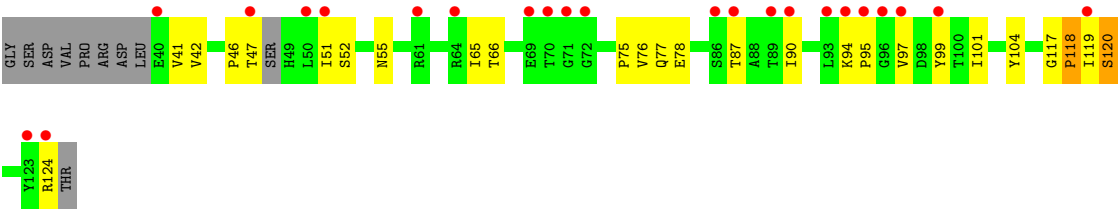


- Molecule 2: NC2

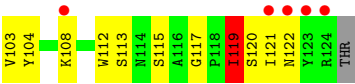
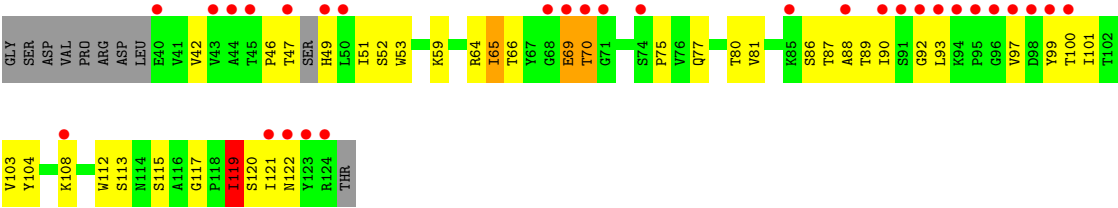


- Molecule 2: NC2





● Molecule 2: NC2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	143.08Å 48.46Å 143.25Å 90.00° 105.16° 90.00°	Depositor
Resolution (Å)	138.26 – 2.41 138.26 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.8 (138.26-2.41) 94.1 (138.26-2.41)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.267 , 0.326 0.272 , 0.283	Depositor DCC
R_{free} test set	2003 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.760	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9739	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.57	0/904	1.24	2/1219 (0.2%)
1	B	0.57	0/908	1.23	2/1226 (0.2%)
1	C	0.61	0/889	1.20	1/1199 (0.1%)
1	D	0.60	0/927	1.25	2/1252 (0.2%)
1	G	0.60	0/895	1.23	1/1207 (0.1%)
1	H	0.63	0/922	1.32	5/1245 (0.4%)
1	J	0.53	0/900	1.19	1/1214 (0.1%)
1	K	0.57	0/903	1.18	1/1219 (0.1%)
2	E	0.65	0/683	1.31	4/935 (0.4%)
2	F	0.63	0/683	1.32	4/935 (0.4%)
2	I	0.56	0/683	1.14	4/935 (0.4%)
2	L	0.57	0/683	1.16	3/935 (0.3%)
All	All	0.59	0/9980	1.23	30/13521 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	114	ASN	CB-CA-C	-9.26	95.37	110.74
1	A	117	PHE	CB-CA-C	8.99	123.75	108.91
2	F	83	ASN	CB-CA-C	-8.01	92.24	110.18
1	A	117	PHE	CA-CB-CG	6.86	120.66	113.80
1	C	363	PHE	CA-CB-CG	6.66	120.46	113.80
2	F	91	ASN	CB-CA-C	-6.63	99.15	110.16
2	I	118	PRO	CA-C-N	6.25	131.67	122.99
2	I	118	PRO	C-N-CA	6.25	131.67	122.99
2	F	15	PRO	CA-C-N	5.94	132.39	121.70
2	F	15	PRO	C-N-CA	5.94	132.39	121.70
1	K	83	THR	CA-CB-OG1	-5.92	100.73	109.60
2	E	122	ASN	CB-CA-C	-5.69	100.97	110.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	97	ASP	CA-CB-CG	5.58	118.18	112.60
2	L	119	ILE	CB-CA-C	5.53	117.63	110.12
2	E	106	VAL	CB-CA-C	5.45	117.56	110.96
1	G	95	ASP	CA-CB-CG	5.45	118.05	112.60
1	H	42	ASP	CA-CB-CG	5.42	118.02	112.60
1	D	276	ARG	CB-CA-C	-5.29	100.94	109.72
1	H	86	THR	CB-CA-C	5.29	118.43	109.50
2	I	46	PRO	CA-C-N	5.25	131.14	121.70
2	I	46	PRO	C-N-CA	5.25	131.14	121.70
1	B	73	ARG	CB-CA-C	5.24	119.27	110.88
1	J	97	ASP	CB-CA-C	5.20	116.83	109.08
1	D	334	THR	CB-CA-C	-5.17	98.92	109.94
2	E	95	PRO	N-CA-C	5.07	120.58	113.53
1	H	46	ILE	CA-C-N	5.02	127.01	120.28
1	H	46	ILE	C-N-CA	5.02	127.01	120.28
1	B	97	ASP	CA-CB-CG	5.02	117.62	112.60
2	L	113	SER	CA-C-N	5.01	126.99	120.28
2	L	113	SER	C-N-CA	5.01	126.99	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	881	0	864	22	0
1	B	885	0	869	21	0
1	C	867	0	852	17	0
1	D	904	0	885	11	0
1	G	873	0	857	18	0
1	H	899	0	880	16	0
1	J	878	0	862	22	0
1	K	880	0	864	20	0
2	E	663	0	652	44	0
2	F	663	0	652	34	0
2	I	663	0	652	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	663	0	652	33	0
3	B	5	0	0	0	0
3	D	5	0	0	1	0
3	H	5	0	0	0	0
3	K	5	0	0	1	0
All	All	9739	0	9541	236	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 12.

All (236) 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:E:42:VAL:CG2	2:E:119:ILE:CG2	2.27	1.13
2:L:52:SER:HB3	2:L:87:THR:HG22	1.27	1.12
2:F:11:VAL:CG2	2:F:88:ILE:CG2	2.36	1.04
1:D:355:LYS:NZ	3:D:401:SO4:O2	1.93	1.02
2:F:11:VAL:HG23	2:F:88:ILE:CG2	1.87	1.02
2:E:42:VAL:HG21	2:E:119:ILE:CG2	1.89	1.01
2:I:42:VAL:CG2	2:I:119:ILE:HG22	1.91	0.99
2:L:103:VAL:HB	2:L:119:ILE:HG22	1.49	0.91
2:F:11:VAL:CG2	2:F:88:ILE:HG21	2.00	0.90
2:I:52:SER:CB	2:I:87:THR:HG22	2.02	0.89
2:E:42:VAL:HG21	2:E:119:ILE:HG22	1.53	0.88
2:F:11:VAL:HG23	2:F:88:ILE:HG21	1.56	0.87
2:E:101:ILE:HD11	2:E:123:TYR:CE1	2.10	0.87
2:I:42:VAL:HG23	2:I:119:ILE:CG2	2.06	0.86
1:J:107:LEU:HD13	1:K:85:LEU:HD12	1.58	0.85
2:I:42:VAL:CG2	2:I:119:ILE:CG2	2.55	0.84
1:K:44:GLU:OE1	3:K:201:SO4:O2	1.94	0.84
1:A:32:GLY:HA3	1:A:37:GLN:NE2	1.92	0.84
2:F:11:VAL:CG2	2:F:88:ILE:HG22	2.07	0.84
2:E:42:VAL:CG2	2:E:119:ILE:HG21	2.07	0.84
2:F:11:VAL:HG21	2:F:88:ILE:HG22	1.57	0.83
1:J:79:THR:HB	1:J:80:PRO:HD2	1.61	0.83
2:E:49:HIS:CD2	2:E:123:TYR:HE2	1.97	0.82
2:E:42:VAL:CG2	2:E:119:ILE:HG23	2.11	0.80
2:E:42:VAL:HG23	2:E:119:ILE:HG23	1.63	0.79
2:E:101:ILE:HD11	2:E:123:TYR:CD1	2.18	0.78
1:K:44:GLU:HG3	1:K:47:ARG:NH2	1.98	0.78
2:I:52:SER:HB3	2:I:87:THR:CG2	2.14	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:52:SER:HB3	2:I:87:THR:HG22	1.68	0.76
2:I:51:ILE:HG13	2:I:90:ILE:HD12	1.68	0.75
1:A:88:THR:HG23	1:B:88:THR:HG22	1.70	0.74
1:B:43:GLN:O	1:B:47:ARG:HG2	1.88	0.73
2:F:70:ILE:HD12	2:F:70:ILE:N	2.02	0.73
2:E:49:HIS:CD2	2:E:123:TYR:CE2	2.76	0.73
2:I:42:VAL:HG23	2:I:119:ILE:HG22	1.64	0.73
2:E:101:ILE:HD13	2:E:121:ILE:HG23	1.71	0.72
1:C:325:THR:HB	1:C:326:PRO:HD2	1.71	0.72
1:A:88:THR:HG23	1:B:88:THR:CG2	2.20	0.72
2:F:44:PRO:HD2	2:E:64:ARG:NH1	2.05	0.70
2:F:33:ARG:NH1	2:E:75:PRO:HD2	2.06	0.70
2:I:42:VAL:HG21	2:I:119:ILE:HG22	1.73	0.70
2:F:70:ILE:HD11	2:F:92:TYR:CE1	2.27	0.69
1:J:15:LYS:NZ	1:K:62:ALA:O	2.26	0.68
2:L:101:ILE:HD12	2:L:121:ILE:HG23	1.76	0.68
1:B:85:LEU:HD23	1:B:85:LEU:C	2.19	0.67
2:I:51:ILE:HD11	2:I:101:ILE:HD13	1.77	0.67
1:C:360:TYR:HA	1:C:363:PHE:CZ	2.31	0.66
2:L:53:TRP:O	2:L:86:SER:OG	2.13	0.66
1:A:114:TYR:HA	1:A:117:PHE:CZ	2.30	0.65
1:C:325:THR:HB	1:C:326:PRO:CD	2.26	0.65
2:E:49:HIS:NE2	2:E:123:TYR:HE2	1.94	0.65
1:G:13:ARG:HG3	1:G:13:ARG:HH11	1.61	0.65
2:E:66:THR:HA	2:E:77:GLN:O	1.98	0.64
2:E:101:ILE:HD11	2:E:123:TYR:HE1	1.62	0.64
2:E:46:PRO:O	2:E:47:THR:HB	1.97	0.63
2:E:92:GLY:O	2:E:93:LEU:HB2	1.98	0.63
1:A:114:TYR:HA	1:A:117:PHE:CE2	2.33	0.63
1:J:35:GLN:HB3	2:L:119:ILE:HD13	1.81	0.63
2:F:18:HIS:CD2	2:F:92:TYR:HE2	2.17	0.62
1:D:331:LEU:C	1:D:331:LEU:HD23	2.24	0.62
2:E:93:LEU:HD22	2:E:99:TYR:CE2	2.35	0.62
2:L:69:GLU:H	2:L:69:GLU:CD	2.06	0.62
2:I:52:SER:CB	2:I:87:THR:CG2	2.75	0.62
2:L:42:VAL:CG2	2:L:119:ILE:HG23	2.30	0.62
2:L:46:PRO:O	2:L:47:THR:HB	1.98	0.61
1:B:85:LEU:C	1:B:85:LEU:CD2	2.73	0.61
1:C:282:THR:HG23	2:F:88:ILE:HD11	1.82	0.60
1:J:35:GLN:HB3	2:L:119:ILE:CD1	2.32	0.60
1:B:73:ARG:NE	2:E:115:SER:O	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:84:TRP:CZ3	1:H:92:LYS:HB2	2.37	0.59
2:E:42:VAL:HG22	2:E:119:ILE:HG21	1.84	0.59
1:J:34:GLU:HB2	1:J:37:GLN:HG3	1.84	0.59
1:G:34:GLU:OE1	2:I:120:SER:HB2	2.01	0.59
1:A:32:GLY:HA3	1:A:37:GLN:CD	2.28	0.58
2:L:101:ILE:HB	2:L:121:ILE:CG2	2.34	0.58
1:J:99:ASN:OD1	1:J:103:GLN:NE2	2.37	0.57
1:G:39:ASN:HB3	1:H:73:ARG:HH22	1.68	0.57
2:I:75:PRO:HG3	2:L:104:TYR:CD2	2.40	0.57
2:F:70:ILE:HD12	2:F:70:ILE:H	1.67	0.57
2:F:68:TYR:O	2:F:91:ASN:HA	2.04	0.57
1:D:264:ALA:O	1:D:296:THR:N	2.27	0.56
1:B:88:THR:HG23	2:E:112:TRP:CD1	2.41	0.56
1:G:39:ASN:HB3	1:H:73:ARG:NH2	2.20	0.56
1:A:88:THR:HA	1:B:88:THR:HG22	1.88	0.56
2:E:42:VAL:HG23	2:E:119:ILE:CG2	2.16	0.56
1:G:88:THR:OG1	1:H:88:THR:HG22	2.07	0.55
1:K:43:GLN:HE22	1:K:118:PRO:HD2	1.71	0.55
2:L:52:SER:CB	2:L:87:THR:HG22	2.18	0.55
1:K:32:GLY:HA3	1:K:37:GLN:OE1	2.07	0.55
1:A:117:PHE:HB2	1:A:118:PRO:HD2	1.87	0.55
1:G:23:ASN:HB2	1:G:46:ILE:O	2.07	0.55
2:F:18:HIS:NE2	2:F:92:TYR:HE2	2.05	0.55
1:J:68:PHE:O	1:J:72:SER:HB3	2.06	0.55
2:E:49:HIS:NE2	2:E:123:TYR:CE2	2.73	0.54
1:C:281:GLN:HB2	2:F:86:GLY:O	2.06	0.54
1:J:79:THR:HB	1:J:80:PRO:CD	2.35	0.54
1:C:307:PHE:O	1:C:337:ILE:HD13	2.07	0.54
2:L:97:VAL:HG23	2:L:99:TYR:CE1	2.42	0.54
1:K:73:ARG:NE	2:L:115:SER:O	2.33	0.54
2:I:52:SER:CA	2:I:87:THR:HG22	2.37	0.54
2:I:65:ILE:O	2:I:78:GLU:HA	2.07	0.53
1:A:79:THR:HB	1:A:80:PRO:HD2	1.90	0.53
2:F:27:TYR:CE2	2:F:28:LYS:HG3	2.43	0.53
2:L:52:SER:HB3	2:L:87:THR:CG2	2.20	0.53
2:I:52:SER:HA	2:I:87:THR:HG22	1.89	0.53
1:G:114:TYR:HA	1:G:117:PHE:CE2	2.45	0.52
2:L:101:ILE:HB	2:L:121:ILE:HG22	1.90	0.52
1:A:42:ASP:C	1:A:42:ASP:OD1	2.52	0.52
2:F:70:ILE:HD11	2:F:92:TYR:HE1	1.74	0.52
1:C:277:ARG:HG3	1:C:292:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:SER:HB3	1:H:88:THR:O	2.10	0.52
2:I:94:LYS:HB3	2:I:95:PRO:CD	2.40	0.52
1:B:112:ASP:CG	1:B:115:LYS:HE3	2.35	0.51
2:L:59:LYS:HB3	2:L:108:LYS:HD2	1.92	0.51
1:C:360:TYR:HA	1:C:363:PHE:CE1	2.45	0.51
2:F:18:HIS:NE2	2:F:92:TYR:CE2	2.79	0.51
1:H:43:GLN:HG3	1:H:117:PHE:CE2	2.45	0.51
2:L:69:GLU:N	2:L:69:GLU:OE1	2.42	0.51
2:E:101:ILE:HD12	2:E:101:ILE:H	1.76	0.51
2:F:33:ARG:HH11	2:E:75:PRO:HG2	1.75	0.51
1:J:63:PRO:HA	1:K:14:GLN:O	2.11	0.51
2:E:101:ILE:CD1	2:E:123:TYR:CD1	2.93	0.50
1:A:39:ASN:OD1	1:A:39:ASN:C	2.55	0.50
1:K:44:GLU:HG3	1:K:47:ARG:HH21	1.72	0.50
1:J:84:TRP:CZ3	1:K:92:LYS:HB2	2.46	0.50
2:F:70:ILE:CD1	2:F:92:TYR:CE1	2.95	0.50
1:H:43:GLN:HG3	1:H:117:PHE:CZ	2.47	0.49
2:F:18:HIS:CD2	2:F:92:TYR:CE2	2.99	0.49
2:I:55:ASN:OD1	2:I:55:ASN:C	2.56	0.49
1:C:334:THR:OG1	1:D:334:THR:HG22	2.12	0.49
1:G:63:PRO:HA	1:H:14:GLN:O	2.12	0.49
2:E:101:ILE:HD12	2:E:101:ILE:N	2.27	0.49
1:K:43:GLN:NE2	1:K:118:PRO:HD2	2.28	0.48
1:H:13:ARG:NH2	1:H:28:PHE:O	2.36	0.48
1:H:78:VAL:HG22	1:H:83:THR:HG23	1.95	0.48
1:H:97:ASP:OD1	1:H:98:PRO:HD2	2.13	0.48
1:H:106:LEU:O	1:H:110:HIS:HD2	1.96	0.48
2:F:70:ILE:N	2:F:70:ILE:CD1	2.74	0.48
2:I:104:TYR:CD2	2:L:75:PRO:HG3	2.48	0.48
2:F:70:ILE:CD1	2:F:92:TYR:HE1	2.27	0.48
1:C:353:LEU:HB3	1:D:322:MET:HE1	1.96	0.47
1:G:13:ARG:HG3	1:G:13:ARG:NH1	2.29	0.47
2:E:104:TYR:CD1	2:E:118:PRO:HB3	2.50	0.47
2:F:19:LEU:HD23	2:F:58:THR:HG22	1.97	0.47
2:F:33:ARG:HH12	2:E:75:PRO:HD2	1.77	0.47
1:G:79:THR:HB	1:G:80:PRO:HD2	1.97	0.47
1:J:55:TRP:N	1:J:56:PRO:CD	2.77	0.47
2:I:51:ILE:CD1	2:I:101:ILE:HD13	2.43	0.47
1:G:87:TYR:CZ	1:H:89:GLY:HA3	2.50	0.47
2:F:44:PRO:HG3	2:E:104:TYR:CD2	2.50	0.46
2:F:93:ARG:O	2:F:93:ARG:HG3	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLY:HA3	1:B:37:GLN:OE1	2.15	0.46
1:G:31:ARG:HA	1:G:38:GLY:O	2.15	0.46
1:J:59:ALA:C	1:J:61:PHE:H	2.23	0.46
2:L:51:ILE:N	2:L:88:ALA:O	2.28	0.46
1:C:285:ASN:C	1:C:285:ASN:OD1	2.58	0.46
2:E:53:TRP:O	2:E:86:SER:HB2	2.15	0.46
1:G:20:LYS:HE2	1:G:48:GLN:HG2	1.97	0.46
2:I:52:SER:HB3	2:I:87:THR:HG21	1.95	0.46
1:D:341:ASP:HA	1:D:346:PHE:CD2	2.51	0.46
1:J:101:LYS:O	1:J:105:ILE:HD12	2.15	0.46
2:E:65:ILE:HA	2:E:102:THR:O	2.16	0.46
1:B:88:THR:CG2	2:E:112:TRP:CD1	2.99	0.46
1:K:43:GLN:HG2	1:K:117:PHE:CZ	2.51	0.45
1:G:42:ASP:OD2	1:G:109:LYS:HE2	2.17	0.45
2:I:41:VAL:HG21	2:I:119:ILE:HD12	1.97	0.45
1:K:43:GLN:HG2	1:K:117:PHE:CE1	2.52	0.45
2:E:50:LEU:HD23	2:E:89:THR:HG22	1.98	0.45
1:K:88:THR:HG23	2:L:112:TRP:CD1	2.51	0.45
1:A:41:GLY:O	1:A:113:ALA:HB3	2.17	0.45
1:A:69:PHE:O	1:B:40:PHE:HB3	2.17	0.45
1:B:45:LEU:HD12	1:B:45:LEU:O	2.16	0.45
1:C:326:PRO:O	1:C:327:SER:C	2.60	0.45
2:L:49:HIS:O	2:L:89:THR:HA	2.16	0.45
1:J:25:THR:HA	1:J:29:GLY:O	2.17	0.45
2:L:66:THR:HA	2:L:77:GLN:O	2.16	0.44
1:K:87:TYR:O	1:K:87:TYR:CD1	2.71	0.44
1:C:357:ILE:CD1	1:D:322:MET:HE2	2.47	0.44
1:J:114:TYR:HA	1:J:117:PHE:CZ	2.53	0.44
2:L:101:ILE:CD1	2:L:121:ILE:HG23	2.45	0.44
1:C:258:PRO:O	1:C:259:ARG:C	2.61	0.44
1:A:63:PRO:HA	1:B:14:GLN:O	2.18	0.44
1:A:84:TRP:CZ2	2:E:41:VAL:HG12	2.53	0.44
1:D:331:LEU:C	1:D:331:LEU:CD2	2.90	0.43
2:F:35:THR:HA	2:F:46:GLN:O	2.18	0.43
1:A:12:PRO:O	1:A:13:ARG:C	2.60	0.43
2:I:104:TYR:CD1	2:I:118:PRO:HB3	2.53	0.43
1:J:69:PHE:O	1:K:40:PHE:HB3	2.18	0.43
1:A:61:PHE:O	1:A:91:ILE:HD13	2.17	0.43
1:A:88:THR:HG23	1:B:88:THR:HG21	2.00	0.43
1:B:95:ASP:HA	1:B:100:PHE:CD1	2.53	0.43
1:J:76:MET:HE1	1:K:104:VAL:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:51:ILE:O	2:L:87:THR:HA	2.19	0.43
1:A:32:GLY:HA3	1:A:37:GLN:HE22	1.76	0.43
2:F:33:ARG:CD	2:F:47:GLU:OE2	2.66	0.43
1:J:33:PRO:O	2:L:117:GLY:HA3	2.19	0.43
2:F:11:VAL:HG23	2:F:88:ILE:HG23	1.92	0.43
2:E:101:ILE:HD11	2:E:123:TYR:HD1	1.77	0.43
2:L:90:ILE:HG22	2:L:93:LEU:HD23	2.00	0.43
1:G:89:GLY:HA3	1:H:87:TYR:CZ	2.54	0.42
1:D:301:TRP:N	1:D:302:PRO:CD	2.82	0.42
2:F:33:ARG:NH1	2:E:75:PRO:CD	2.80	0.42
1:A:45:LEU:O	1:A:46:ILE:C	2.62	0.42
2:I:66:THR:HG21	2:L:75:PRO:HB3	2.02	0.42
2:E:92:GLY:O	2:E:93:LEU:CB	2.67	0.42
1:K:88:THR:CG2	2:L:112:TRP:CD1	3.03	0.42
1:C:353:LEU:O	1:C:357:ILE:HG13	2.20	0.42
1:B:99:ASN:O	1:B:100:PHE:C	2.61	0.42
2:E:94:LYS:HA	2:E:95:PRO:HD3	1.85	0.41
1:J:50:THR:HG22	1:J:55:TRP:CE2	2.55	0.41
2:L:46:PRO:HA	2:L:49:HIS:HA	2.01	0.41
1:D:358:ASP:CG	1:D:361:LYS:HE3	2.44	0.41
1:A:24:VAL:HB	1:A:46:ILE:HA	2.02	0.41
1:B:85:LEU:HD23	1:B:86:THR:N	2.35	0.41
1:J:34:GLU:OE1	2:L:120:SER:N	2.53	0.41
1:K:20:LYS:HE3	1:K:48:GLN:HG2	2.02	0.41
1:A:34:GLU:OE2	2:E:120:SER:OG	2.35	0.41
2:L:64:ARG:HG2	2:L:80:THR:HG22	2.02	0.41
1:C:277:ARG:CG	1:C:292:ILE:HD11	2.51	0.41
1:C:330:TRP:CZ2	2:F:10:VAL:HG12	2.56	0.41
2:I:66:THR:HA	2:I:77:GLN:O	2.21	0.41
1:J:59:ALA:C	1:J:61:PHE:N	2.78	0.41
1:K:71:MET:HE3	1:K:71:MET:HB2	1.87	0.41
2:L:65:ILE:HD13	2:L:81:VAL:HG21	2.03	0.41
1:B:43:GLN:HG2	1:B:117:PHE:CE2	2.56	0.41
2:E:45:THR:HA	2:E:46:PRO:HD3	1.91	0.41
1:B:43:GLN:HG2	1:B:117:PHE:CZ	2.56	0.40
1:B:55:TRP:N	1:B:56:PRO:CD	2.85	0.40
2:E:101:ILE:CD1	2:E:121:ILE:HG23	2.47	0.40
2:I:97:VAL:HG23	2:I:99:TYR:CE1	2.56	0.40
1:D:363:PHE:HA	1:D:364:PRO:HD3	1.94	0.40
2:F:44:PRO:HD2	2:E:64:ARG:HH11	1.82	0.40
1:G:35:GLN:HB2	2:I:117:GLY:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:THR:OG1	1:H:88:THR:CG2	2.70	0.40
1:H:58:ILE:HG13	1:H:106:LEU:HD21	2.04	0.40
2:I:52:SER:HB2	2:I:87:THR:HG22	1.94	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	108/122 (88%)	102 (94%)	6 (6%)	0	100	100
1	B	109/122 (89%)	105 (96%)	4 (4%)	0	100	100
1	C	106/122 (87%)	102 (96%)	4 (4%)	0	100	100
1	D	112/122 (92%)	109 (97%)	3 (3%)	0	100	100
1	G	107/122 (88%)	104 (97%)	3 (3%)	0	100	100
1	H	111/122 (91%)	105 (95%)	6 (5%)	0	100	100
1	J	108/122 (88%)	98 (91%)	10 (9%)	0	100	100
1	K	108/122 (88%)	104 (96%)	4 (4%)	0	100	100
2	E	80/94 (85%)	71 (89%)	8 (10%)	1 (1%)	9	13
2	F	80/94 (85%)	75 (94%)	5 (6%)	0	100	100
2	I	80/94 (85%)	72 (90%)	8 (10%)	0	100	100
2	L	80/94 (85%)	74 (92%)	4 (5%)	2 (2%)	4	4
All	All	1189/1352 (88%)	1121 (94%)	65 (6%)	3 (0%)	36	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	92	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	93	LEU
2	L	70	THR

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	92/99 (93%)	91 (99%)	1 (1%)	65	81
1	B	92/99 (93%)	89 (97%)	3 (3%)	33	53
1	C	90/99 (91%)	89 (99%)	1 (1%)	65	81
1	D	93/99 (94%)	91 (98%)	2 (2%)	45	66
1	G	91/99 (92%)	89 (98%)	2 (2%)	45	66
1	H	93/99 (94%)	89 (96%)	4 (4%)	26	42
1	J	91/99 (92%)	85 (93%)	6 (7%)	15	25
1	K	92/99 (93%)	92 (100%)	0	100	100
2	E	73/82 (89%)	67 (92%)	6 (8%)	10	17
2	F	73/82 (89%)	67 (92%)	6 (8%)	10	17
2	I	73/82 (89%)	69 (94%)	4 (6%)	19	32
2	L	73/82 (89%)	67 (92%)	6 (8%)	10	17
All	All	1026/1120 (92%)	985 (96%)	41 (4%)	28	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	327	SER
1	D	322	MET
1	D	334	THR
2	F	16	THR
2	F	33	ARG
2	F	43	SER
2	F	60	SER
2	F	66	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	70	ILE
1	A	36	THR
1	B	20	LYS
1	B	76	MET
1	B	85	LEU
2	E	70	THR
2	E	74	SER
2	E	101	ILE
2	E	106	VAL
2	E	119	ILE
2	E	122	ASN
1	G	81	SER
1	G	106	LEU
1	H	31	ARG
1	H	72	SER
1	H	79	THR
1	H	88	THR
2	I	47	THR
2	I	76	VAL
2	I	120	SER
2	I	124	ARG
1	J	30	ARG
1	J	80	PRO
1	J	81	SER
1	J	85	LEU
1	J	88	THR
1	J	101	LYS
2	L	65	ILE
2	L	69	GLU
2	L	70	THR
2	L	100	THR
2	L	119	ILE
2	L	122	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	272	GLN
1	C	303	GLN
1	D	294	GLN
1	A	99	ASN
1	A	108	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	43	GLN
1	G	26	GLN
2	I	49	HIS
1	J	103	GLN
1	K	43	GLN
1	K	57	GLN
1	K	103	GLN

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](#)

4 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	SO4	H	201	-	4,4,4	0.27	0	6,6,6	0.23	0
3	SO4	D	401	-	4,4,4	0.38	0	6,6,6	0.15	0
3	SO4	B	201	-	4,4,4	0.22	0	6,6,6	0.21	0
3	SO4	K	201	-	4,4,4	0.40	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	SO4	1	0
3	K	201	SO4	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	110/122 (90%)	0.83	17 (15%) 5 4	19, 39, 65, 92	0
1	B	111/122 (90%)	0.54	4 (3%) 46 42	22, 34, 54, 104	0
1	C	108/122 (88%)	0.41	4 (3%) 45 41	18, 32, 51, 70	0
1	D	114/122 (93%)	0.46	6 (5%) 32 28	17, 30, 62, 125	0
1	G	109/122 (89%)	0.64	5 (4%) 37 33	22, 35, 58, 96	0
1	H	113/122 (92%)	0.64	9 (7%) 18 15	22, 33, 57, 104	0
1	J	110/122 (90%)	1.39	31 (28%) 1 1	29, 48, 75, 92	0
1	K	110/122 (90%)	0.79	5 (4%) 38 34	29, 41, 61, 85	0
2	E	84/94 (89%)	1.09	13 (15%) 5 4	24, 40, 63, 82	0
2	F	84/94 (89%)	1.04	12 (14%) 6 4	20, 38, 68, 85	0
2	I	84/94 (89%)	1.34	23 (27%) 1 1	27, 48, 76, 93	0
2	L	84/94 (89%)	1.70	30 (35%) 1 0	29, 50, 75, 87	0
All	All	1221/1352 (90%)	0.87	159 (13%) 7 5	17, 38, 70, 125	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	252	ALA	6.7
1	J	8	ALA	6.3
1	D	251	ALA	5.9
1	H	8	ALA	5.6
1	J	99	ASN	5.4
1	H	6	ALA	5.4
2	L	123	TYR	5.4
2	I	47	THR	5.3
1	B	10	LYS	4.9
1	A	118	PRO	4.9
1	D	254	ALA	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	9	SER	4.8
2	I	70	THR	4.6
2	E	95	PRO	4.4
1	G	10	LYS	4.3
2	F	65	GLY	4.3
2	F	64	PRO	4.3
2	I	97	VAL	4.2
1	J	79	THR	4.1
2	L	47	THR	4.0
2	L	71	GLY	3.9
1	J	43	GLN	3.9
2	L	124	ARG	3.8
1	C	363	PHE	3.8
1	J	80	PRO	3.8
1	K	10	LYS	3.8
1	K	109	LYS	3.7
2	L	90	ILE	3.7
2	F	40	GLY	3.7
2	F	93	ARG	3.5
2	E	109	ARG	3.5
1	A	9	SER	3.5
1	B	47	ARG	3.4
1	A	10	LYS	3.3
1	J	10	LYS	3.3
2	E	124	ARG	3.3
2	I	124	ARG	3.3
2	I	86	SER	3.3
2	I	95	PRO	3.3
2	L	45	THR	3.3
2	L	70	THR	3.3
1	C	256	LYS	3.3
1	K	9	SER	3.2
1	J	52	TYR	3.2
1	J	11	LYS	3.2
1	A	30	ARG	3.2
2	F	66	VAL	3.2
2	I	96	GLY	3.1
2	F	14	THR	3.1
1	J	53	LYS	3.1
2	L	95	PRO	3.1
2	L	68	GLY	3.1
2	L	69	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	122	ASN	3.1
1	D	256	LYS	3.0
1	J	98	PRO	3.0
2	F	68	TYR	3.0
1	J	47	ARG	3.0
2	L	91	SER	3.0
2	E	96	GLY	3.0
2	L	108	LYS	2.9
1	A	17	THR	2.9
1	B	8	ALA	2.9
1	C	257	LYS	2.9
1	A	43	GLN	2.9
1	A	117	PHE	2.9
2	E	97	VAL	2.8
1	H	11	LYS	2.8
2	F	63	LYS	2.8
2	L	98	ASP	2.8
1	J	54	HIS	2.8
2	L	92	GLY	2.8
2	L	96	GLY	2.7
1	D	255	SER	2.7
2	L	50	LEU	2.7
1	K	57	GLN	2.7
2	F	61	GLY	2.7
1	G	80	PRO	2.7
2	L	40	GLU	2.7
1	J	81	SER	2.7
2	L	100	THR	2.7
2	I	99	TYR	2.7
2	L	49	HIS	2.7
2	E	51	ILE	2.6
2	I	119	ILE	2.6
1	J	30	ARG	2.6
2	L	93	LEU	2.6
1	D	253	GLU	2.6
1	H	57	GLN	2.6
2	E	94	LYS	2.6
2	I	123	TYR	2.6
1	J	96	LYS	2.6
1	B	13	ARG	2.6
2	I	61	ARG	2.6
2	I	93	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	78	VAL	2.6
1	H	81	SER	2.6
2	I	71	GLY	2.5
1	J	117	PHE	2.5
2	E	91	SER	2.5
2	E	47	THR	2.5
1	J	13	ARG	2.5
1	K	30	ARG	2.5
1	H	96	LYS	2.5
1	J	21	ALA	2.5
1	G	20	LYS	2.5
1	J	82	GLY	2.4
1	G	11	LYS	2.4
1	J	12	PRO	2.4
2	L	121	ILE	2.4
2	E	123	TYR	2.4
1	H	10	LYS	2.4
1	J	44	GLU	2.4
1	J	57	GLN	2.4
2	L	43	VAL	2.4
2	I	94	LYS	2.4
2	F	92	TYR	2.4
2	I	90	ILE	2.3
1	J	26	GLN	2.3
1	J	20	LYS	2.3
2	L	99	TYR	2.3
1	A	20	LYS	2.3
1	A	53	LYS	2.3
1	A	44	GLU	2.3
2	I	69	GLU	2.3
1	A	13	ARG	2.3
2	I	89	THR	2.2
1	A	11	LYS	2.2
2	E	101	ILE	2.2
1	J	24	VAL	2.2
1	H	54	HIS	2.2
2	I	40	GLU	2.2
2	L	88	ALA	2.2
1	H	9	SER	2.2
1	A	56	PRO	2.2
2	L	94	LYS	2.2
1	A	116	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	62	LEU	2.2
2	E	99	TYR	2.2
1	A	47	ARG	2.2
1	A	54	HIS	2.1
1	A	79	THR	2.1
1	J	17	THR	2.1
2	F	16	THR	2.1
2	I	87	THR	2.1
2	I	51	ILE	2.1
2	E	121	ILE	2.1
1	J	46	ILE	2.1
1	J	22	TYR	2.1
2	L	74	SER	2.1
2	I	50	LEU	2.1
1	J	94	ASP	2.1
1	C	289	GLN	2.0
2	L	44	ALA	2.0
2	I	72	GLY	2.0
2	I	64	ARG	2.0
2	L	97	VAL	2.0
1	J	65	ALA	2.0
2	L	85	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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, 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	B-factors(Å ²)	Q<0.9
3	SO4	K	201	5/5	0.92	0.12	40,43,50,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	H	201	5/5	0.95	0.11	39,43,49,50	0
3	SO4	D	401	5/5	0.97	0.07	35,38,42,47	0
3	SO4	B	201	5/5	0.98	0.05	32,33,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.