Full wwPDB X-ray Structure Validation Report ⓘ

Nov 23, 2023 – 01:11 AM JST

PDB ID	:	7YOW
Title	:	Crystal structure of SARS-CoV-2 omicron variant spike receptor-binding domain (RBD) in complex with NCV2SG48 Fab
Authors	:	Yamamoto, A.; Higashiura, A.
Deposited on	:	2022-08-02
Resolution	:	3.30 Å(reported)

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

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

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

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

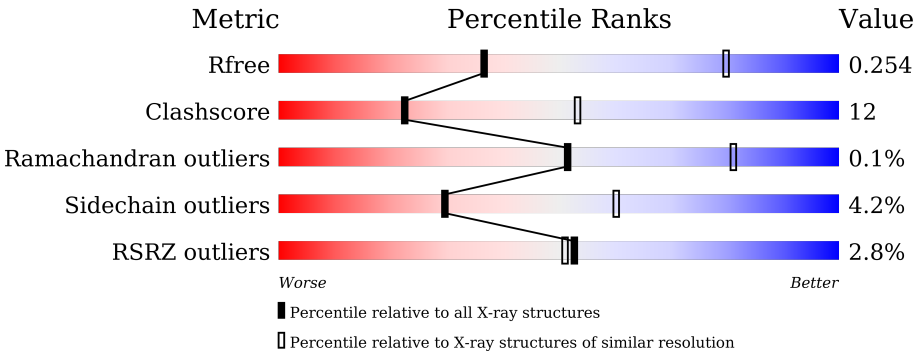
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	215	81% 18% •
1	L	215	% 73% 26% •
2	B	230	4% 63% 27% • 8%
2	H	230	2% 60% 29% • 8%
3	C	224	5% 60% 26% • 12%
3	R	224	3% 60% 25% • 12%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9650 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 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1636	1022	280	329	5			
1	A	215	Total	C	N	O	S	0	0	0
			1636	1022	280	329	5			

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	211	Total	C	N	O	S	0	0	0
			1581	1002	267	306	6			
2	B	212	Total	C	N	O	S	0	0	0
			1590	1008	269	307	6			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	196	Total	C	N	O	S	0	0	0
			1571	1012	265	286	8			
3	C	196	Total	C	N	O	S	0	0	0
			1576	1017	267	284	8			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	339	ASP	GLY	variant	UNP P0DTC2
R	371	LEU	SER	variant	UNP P0DTC2
R	373	PRO	SER	variant	UNP P0DTC2
R	375	PHE	SER	variant	UNP P0DTC2
R	417	ASN	LYS	variant	UNP P0DTC2
R	440	LYS	ASN	variant	UNP P0DTC2
R	446	SER	GLY	variant	UNP P0DTC2
R	477	ASN	SER	variant	UNP P0DTC2

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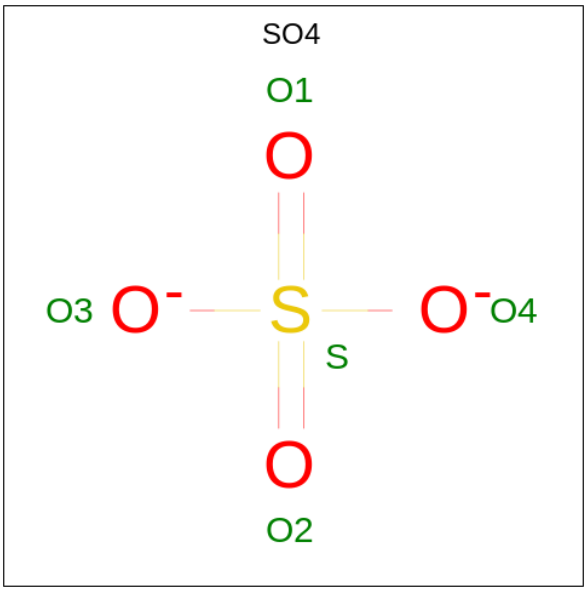
Chain	Residue	Modelled	Actual	Comment	Reference
R	478	LYS	THR	variant	UNP P0DTC2
R	484	ALA	GLU	variant	UNP P0DTC2
R	493	ARG	GLN	variant	UNP P0DTC2
R	496	SER	GLY	variant	UNP P0DTC2
R	498	ARG	GLN	variant	UNP P0DTC2
R	501	TYR	ASN	variant	UNP P0DTC2
R	505	HIS	TYR	variant	UNP P0DTC2
R	537	THR	-	expression tag	UNP P0DTC2
R	538	GLY	-	expression tag	UNP P0DTC2
R	539	HIS	-	expression tag	UNP P0DTC2
R	540	HIS	-	expression tag	UNP P0DTC2
R	541	HIS	-	expression tag	UNP P0DTC2
R	542	HIS	-	expression tag	UNP P0DTC2
R	543	HIS	-	expression tag	UNP P0DTC2
R	544	HIS	-	expression tag	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	537	THR	-	expression tag	UNP P0DTC2
C	538	GLY	-	expression tag	UNP P0DTC2
C	539	HIS	-	expression tag	UNP P0DTC2
C	540	HIS	-	expression tag	UNP P0DTC2
C	541	HIS	-	expression tag	UNP P0DTC2
C	542	HIS	-	expression tag	UNP P0DTC2
C	543	HIS	-	expression tag	UNP P0DTC2
C	544	HIS	-	expression tag	UNP P0DTC2

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

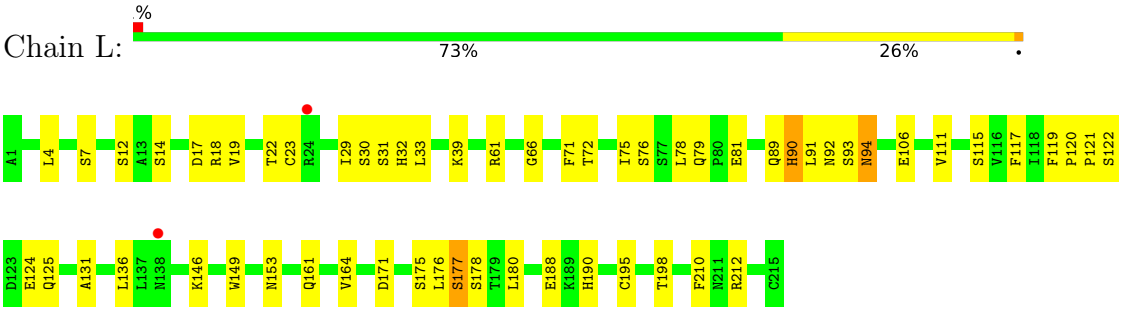


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	L	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	H	1	Total O S 5 4 1	0	0
4	R	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0

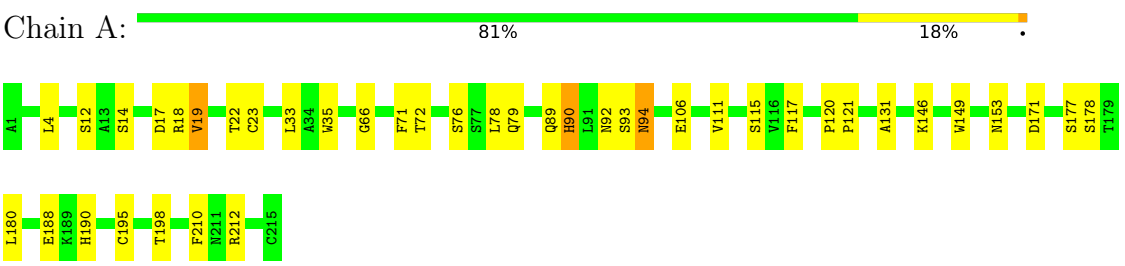
3 Residue-property plots (i)

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.

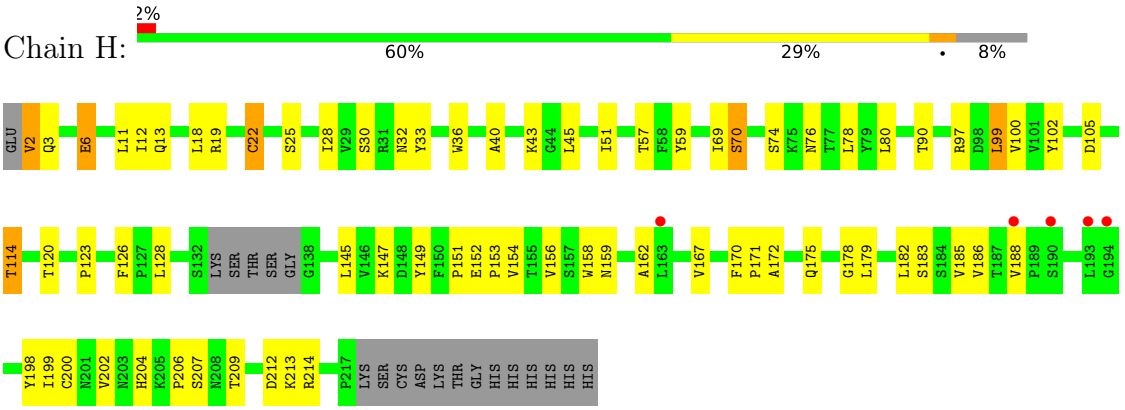
• Molecule 1: Fab Light chain



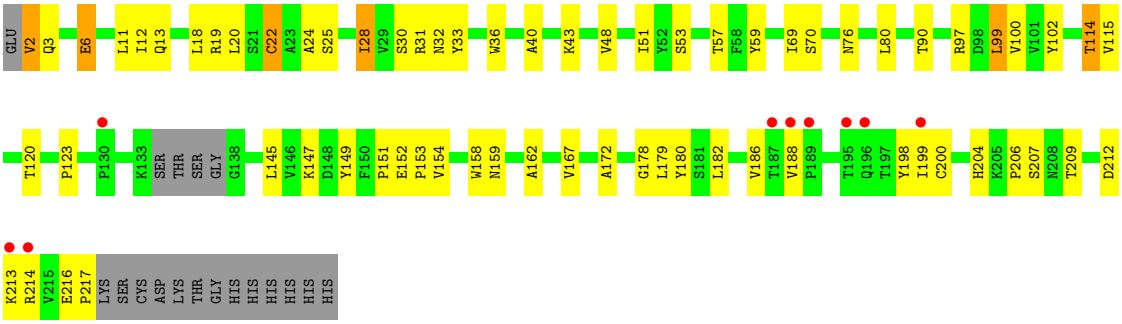
• Molecule 1: Fab Light chain



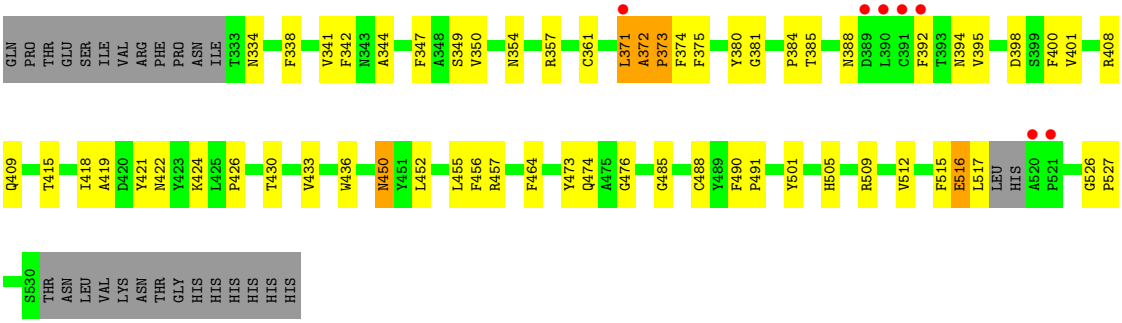
• Molecule 2: Fab Heavy chain



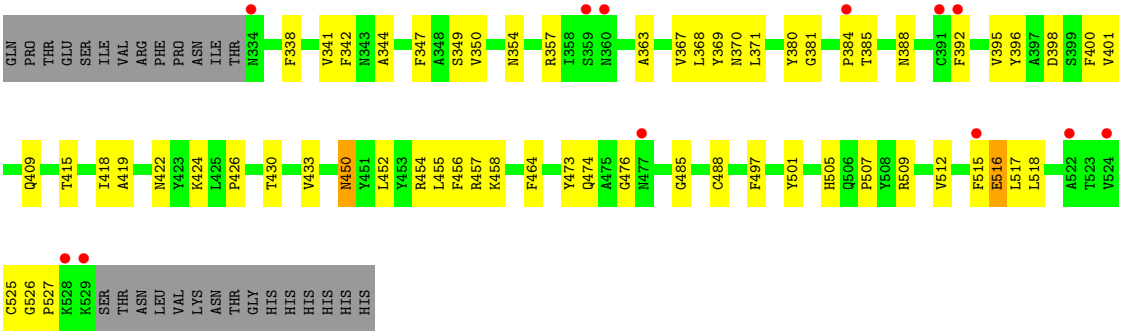
• Molecule 2: Fab Heavy chain



• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.55Å 115.68Å 99.49Å 90.00° 105.89° 90.00°	Depositor
Resolution (Å)	47.84 – 3.30 47.84 – 3.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (47.84-3.30) 97.7 (47.84-3.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.208 , 0.254 0.208 , 0.254	Depositor DCC
R_{free} test set	1482 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	105.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 66.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9650	wwPDB-VP
Average B, all atoms (Å^2)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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: 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	0.43	0/1671	0.59	0/2270
1	L	0.44	0/1671	0.60	0/2270
2	B	0.43	0/1626	0.61	0/2215
2	H	0.43	0/1617	0.62	0/2204
3	C	0.46	0/1623	0.62	0/2207
3	R	0.49	0/1616	0.62	0/2196
All	All	0.45	0/9824	0.61	0/13362

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	L	0	1
2	B	0	1
2	H	0	1
3	R	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	94	ASN	Peptide
2	B	99	LEU	Peptide

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Mol	Chain	Res	Type	Group
2	H	99	LEU	Peptide
1	L	94	ASN	Peptide
3	R	372	ALA	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	1636	0	1602	21	0
1	L	1636	0	1602	38	0
2	B	1590	0	1570	45	0
2	H	1581	0	1557	52	0
3	C	1576	0	1513	39	0
3	R	1571	0	1506	38	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	H	15	0	0	0	0
4	L	15	0	0	1	0
4	R	5	0	0	0	0
All	All	9650	0	9350	221	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 (221) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:THR:HG23	2:B:114:THR:HA	1.60	0.84
2:H:90:THR:HG23	2:H:114:THR:HA	1.60	0.83
2:H:199:ILE:HD11	2:H:212:ASP:HB3	1.61	0.82
2:H:59:TYR:HE1	2:H:69:ILE:HG22	1.46	0.81
3:R:372:ALA:O	3:R:374:PHE:N	2.14	0.81
2:H:11:LEU:HB2	2:H:151:PRO:HG3	1.63	0.80
1:L:66:GLY:HA3	1:L:71:PHE:HA	1.65	0.79
2:B:59:TYR:HE1	2:B:69:ILE:HG22	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ILE:HD11	2:B:212:ASP:HB3	1.64	0.78
1:L:18:ARG:HG3	1:L:76:SER:HA	1.65	0.77
2:B:204:HIS:HD1	2:B:207:SER:HG	1.31	0.77
1:A:66:GLY:HA3	1:A:71:PHE:HA	1.66	0.77
2:B:11:LEU:HB2	2:B:151:PRO:HG3	1.68	0.76
1:A:18:ARG:HG3	1:A:76:SER:HA	1.68	0.74
1:L:22:THR:HG22	1:L:72:THR:HG22	1.72	0.71
2:B:51:ILE:HD12	2:B:57:THR:HG22	1.73	0.70
1:L:92:ASN:ND2	1:L:94:ASN:O	2.25	0.70
3:C:516:GLU:HG3	3:C:518:LEU:HG	1.75	0.69
2:H:28:ILE:O	2:H:32:ASN:ND2	2.26	0.69
1:A:92:ASN:ND2	1:A:94:ASN:O	2.26	0.68
2:H:51:ILE:HD12	2:H:57:THR:HG22	1.74	0.68
3:R:392:PHE:HA	3:R:517:LEU:HD13	1.76	0.67
3:R:371:LEU:HD11	3:R:374:PHE:HB3	1.77	0.67
3:R:374:PHE:HA	3:R:436:TRP:HB3	1.78	0.65
3:R:418:ILE:HA	3:R:422:ASN:HD22	1.61	0.65
1:L:190:HIS:O	1:L:212:ARG:NH1	2.29	0.65
3:C:392:PHE:HA	3:C:517:LEU:HD13	1.78	0.65
3:C:384:PRO:O	3:C:385:THR:OG1	2.14	0.65
2:B:28:ILE:O	2:B:32:ASN:ND2	2.30	0.65
3:C:388:ASN:HB3	3:C:527:PRO:HD2	1.78	0.64
1:A:190:HIS:O	1:A:212:ARG:NH1	2.30	0.64
3:R:388:ASN:HB3	3:R:527:PRO:HD2	1.78	0.63
1:A:22:THR:HG22	1:A:72:THR:HG22	1.81	0.62
3:R:384:PRO:O	3:R:385:THR:OG1	2.18	0.62
2:H:154:VAL:HG12	2:H:204:HIS:CD2	2.35	0.62
2:B:154:VAL:HG12	2:B:204:HIS:CD2	2.35	0.62
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.34	0.61
1:L:136:LEU:HD11	2:H:185:VAL:HG21	1.81	0.61
2:H:158:TRP:CZ3	2:H:200:CYS:HB3	2.36	0.61
3:C:349:SER:HB3	3:C:452:LEU:H	1.66	0.61
3:C:347:PHE:CE2	3:C:509:ARG:HB3	2.36	0.60
3:C:419:ALA:O	3:C:424:LYS:HD2	2.01	0.60
3:C:357:ARG:HH11	3:C:357:ARG:HB3	1.67	0.60
3:R:349:SER:HB3	3:R:452:LEU:H	1.67	0.60
3:C:409:GLN:HB3	3:C:419:ALA:HB2	1.83	0.59
3:R:357:ARG:HH11	3:R:357:ARG:HB3	1.68	0.59
3:R:347:PHE:CE2	3:R:509:ARG:HB3	2.38	0.59
3:C:418:ILE:HA	3:C:422:ASN:HD22	1.68	0.59
2:B:59:TYR:CE1	2:B:69:ILE:HG22	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:6:GLU:HB3	2:H:22:CYS:HB2	1.84	0.58
3:C:350:VAL:HG22	3:C:422:ASN:HB3	1.84	0.58
3:R:456:PHE:HB3	3:R:473:TYR:CD2	2.38	0.57
3:R:409:GLN:HB3	3:R:419:ALA:HB2	1.85	0.57
3:R:419:ALA:O	3:R:424:LYS:HD2	2.04	0.57
3:C:363:ALA:N	3:C:525:CYS:O	2.34	0.57
3:C:395:VAL:HG22	3:C:515:PHE:HD1	1.70	0.57
3:R:395:VAL:HG22	3:R:515:PHE:HD1	1.71	0.56
3:C:456:PHE:HB3	3:C:473:TYR:CD2	2.41	0.56
2:H:18:LEU:HD12	2:H:19:ARG:H	1.71	0.55
1:L:119:PHE:CD1	2:H:128:LEU:HB3	2.42	0.55
1:A:149:TRP:CG	1:A:180:LEU:HD12	2.42	0.54
3:R:350:VAL:HG22	3:R:422:ASN:HB3	1.87	0.54
2:B:123:PRO:HD2	2:B:209:THR:HG21	1.90	0.54
2:H:99:LEU:O	2:H:102:TYR:N	2.38	0.54
3:C:381:GLY:HA3	3:C:430:THR:HG22	1.90	0.54
1:A:120:PRO:HB3	1:A:210:PHE:CZ	2.43	0.53
1:L:120:PRO:HB3	1:L:210:PHE:CZ	2.44	0.53
3:R:381:GLY:HA3	3:R:430:THR:HG22	1.91	0.53
1:L:122:SER:OG	2:H:126:PHE:HB3	2.08	0.53
2:B:28:ILE:HA	2:B:76:ASN:OD1	2.08	0.53
2:H:123:PRO:HD2	2:H:209:THR:HG21	1.91	0.53
2:B:40:ALA:HB3	2:B:43:LYS:HB2	1.92	0.52
1:L:30:SER:HB2	3:R:501:TYR:OH	2.10	0.52
3:C:485:GLY:H	3:C:488:CYS:HB2	1.75	0.52
2:B:18:LEU:HD12	2:B:19:ARG:H	1.74	0.52
2:B:158:TRP:CZ3	2:B:200:CYS:HB3	2.45	0.52
1:A:146:LYS:HB3	1:A:198:THR:HB	1.92	0.51
1:A:149:TRP:CD2	1:A:180:LEU:HD12	2.45	0.51
1:L:119:PHE:CG	2:H:128:LEU:HD13	2.45	0.51
2:H:145:LEU:HD21	2:H:147:LYS:HB2	1.92	0.51
2:B:6:GLU:HB3	2:B:22:CYS:HB2	1.92	0.51
2:B:33:TYR:CD2	2:B:100:VAL:HG23	2.45	0.50
3:R:373:PRO:HB2	3:R:375:PHE:CZ	2.46	0.50
2:H:40:ALA:HB3	2:H:43:LYS:HB2	1.93	0.50
3:C:357:ARG:HB3	3:C:357:ARG:NH1	2.27	0.50
3:R:357:ARG:HB3	3:R:357:ARG:NH1	2.25	0.50
2:B:36:TRP:NE1	2:B:80:LEU:HB2	2.26	0.50
1:L:149:TRP:CD2	1:L:180:LEU:HD12	2.47	0.50
2:H:28:ILE:HA	2:H:76:ASN:OD1	2.11	0.50
2:B:3:GLN:HB3	2:B:25:SER:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:175:SER:O	2:H:170:PHE:HE1	1.95	0.49
1:A:121:PRO:HG3	1:A:131:ALA:HB1	1.94	0.49
3:C:363:ALA:O	3:C:526:GLY:HA2	2.13	0.49
3:R:426:PRO:HD3	3:R:464:PHE:CE2	2.47	0.49
3:C:338:PHE:O	3:C:342:PHE:HD2	1.95	0.49
2:H:36:TRP:NE1	2:H:80:LEU:HB2	2.27	0.49
3:R:338:PHE:O	3:R:342:PHE:HD2	1.96	0.49
2:H:33:TYR:CD2	2:H:100:VAL:HG23	2.48	0.48
3:C:426:PRO:HD3	3:C:464:PHE:CE2	2.48	0.48
2:H:3:GLN:HB3	2:H:25:SER:HB3	1.95	0.48
2:H:97:ARG:CZ	2:H:99:LEU:HD21	2.44	0.48
3:R:433:VAL:HG13	3:R:512:VAL:HG22	1.95	0.48
1:L:39:LYS:NZ	1:L:81:GLU:O	2.26	0.48
3:C:497:PHE:CD1	3:C:507:PRO:HD3	2.48	0.48
1:L:124:GLU:HG2	2:H:213:LYS:NZ	2.29	0.48
2:B:99:LEU:O	2:B:102:TYR:N	2.38	0.48
3:C:501:TYR:HB3	3:C:505:HIS:HB2	1.96	0.47
1:A:92:ASN:OD1	1:A:93:SER:N	2.48	0.47
3:R:501:TYR:HB3	3:R:505:HIS:HB2	1.96	0.47
2:B:154:VAL:HG12	2:B:204:HIS:HD2	1.77	0.47
1:L:12:SER:HA	1:L:106:GLU:O	2.15	0.47
2:H:167:VAL:HG22	2:H:186:VAL:HB	1.97	0.47
2:B:145:LEU:HD21	2:B:147:LYS:HB2	1.97	0.46
1:L:164:VAL:O	2:H:171:PRO:HG2	2.16	0.46
1:A:12:SER:HA	1:A:106:GLU:O	2.15	0.46
2:H:199:ILE:HB	2:H:214:ARG:HG2	1.97	0.46
2:B:199:ILE:HB	2:B:214:ARG:HG2	1.96	0.46
2:H:120:THR:HG22	2:H:207:SER:HB3	1.98	0.46
1:A:171:ASP:N	1:A:171:ASP:OD1	2.48	0.46
3:C:347:PHE:HB2	3:C:401:VAL:HG23	1.97	0.46
2:H:154:VAL:HG12	2:H:204:HIS:HD2	1.79	0.46
3:R:455:LEU:O	3:R:455:LEU:HD12	2.16	0.46
1:L:32:HIS:HB3	1:L:91:LEU:O	2.17	0.45
2:B:12:ILE:HD12	2:B:13:GLN:H	1.80	0.45
3:C:388:ASN:HA	3:C:526:GLY:HA3	1.98	0.45
2:B:152:GLU:HG2	2:B:180:TYR:CD2	2.51	0.45
1:L:89:GLN:HG2	1:L:90:HIS:N	2.31	0.45
1:L:146:LYS:HB3	1:L:198:THR:HB	1.98	0.45
2:H:145:LEU:CD2	2:H:147:LYS:HB2	2.46	0.45
1:A:4:LEU:HD22	1:A:23:CYS:SG	2.56	0.45
2:H:12:ILE:HD12	2:H:13:GLN:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ARG:CZ	3:C:458:LYS:HD3	2.46	0.45
2:B:159:ASN:HB2	2:B:162:ALA:HB3	1.98	0.45
3:R:485:GLY:H	3:R:488:CYS:HB2	1.82	0.45
1:L:149:TRP:CG	1:L:180:LEU:HD12	2.52	0.45
2:H:175:GLN:HE21	2:H:175:GLN:HB2	1.61	0.45
1:A:115:SER:HB3	1:A:117:PHE:CE2	2.51	0.45
3:R:450:ASN:N	3:R:450:ASN:OD1	2.50	0.45
3:R:388:ASN:HA	3:R:526:GLY:HA3	1.98	0.44
2:B:172:ALA:HA	2:B:182:LEU:HB3	1.98	0.44
3:C:474:GLN:HG2	3:C:476:GLY:O	2.17	0.44
3:C:367:VAL:O	3:C:368:LEU:HD23	2.17	0.44
1:L:161:GLN:HE22	2:H:175:GLN:HA	1.81	0.44
2:B:204:HIS:CD2	2:B:206:PRO:HD2	2.52	0.44
3:C:455:LEU:HD12	3:C:455:LEU:O	2.17	0.44
3:R:474:GLN:HG2	3:R:476:GLY:O	2.17	0.44
1:A:14:SER:O	1:A:17:ASP:HB2	2.18	0.44
2:B:152:GLU:OE1	2:B:153:PRO:HA	2.17	0.44
1:L:125:GLN:HB2	2:H:126:PHE:CD2	2.52	0.44
2:H:158:TRP:CH2	2:H:200:CYS:HB3	2.52	0.44
1:L:176:LEU:HD23	1:L:177:SER:N	2.33	0.44
2:H:11:LEU:HA	2:H:114:THR:O	2.18	0.44
2:H:149:TYR:OH	2:H:182:LEU:HD23	2.18	0.43
1:A:188:GLU:O	1:A:212:ARG:NH1	2.51	0.43
1:L:136:LEU:HD13	2:H:185:VAL:HG11	2.00	0.43
2:H:178:GLY:O	2:H:179:LEU:HD23	2.18	0.43
2:B:97:ARG:CZ	2:B:99:LEU:HD21	2.48	0.43
2:B:167:VAL:HG22	2:B:186:VAL:HB	2.00	0.43
3:R:347:PHE:HB2	3:R:401:VAL:HG23	1.99	0.43
2:B:36:TRP:O	2:B:48:VAL:HB	2.18	0.43
3:C:347:PHE:HE2	3:C:509:ARG:HB3	1.80	0.43
3:C:396:TYR:HE2	3:C:516:GLU:OE1	2.01	0.43
3:R:380:TYR:O	3:R:430:THR:HA	2.18	0.43
1:L:78:LEU:HD12	1:L:79:GLN:H	1.83	0.43
1:A:23:CYS:HB2	1:A:35:TRP:CH2	2.54	0.43
1:L:121:PRO:HG3	1:L:131:ALA:HB1	1.99	0.43
2:H:70:SER:O	2:H:78:LEU:HD12	2.19	0.43
1:L:171:ASP:OD1	1:L:171:ASP:N	2.52	0.43
1:L:14:SER:O	1:L:17:ASP:HB2	2.19	0.43
2:H:156:VAL:HG22	2:H:202:VAL:HG22	2.00	0.43
3:R:350:VAL:HA	3:R:400:PHE:HB2	2.00	0.43
1:L:4:LEU:HD22	1:L:23:CYS:SG	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD12	1:A:79:GLN:H	1.85	0.42
1:L:115:SER:HB3	1:L:117:PHE:CE2	2.54	0.42
2:H:172:ALA:HA	2:H:182:LEU:HB3	2.01	0.42
2:B:99:LEU:HB2	2:B:102:TYR:HB2	2.02	0.42
2:B:188:VAL:HG21	2:B:198:TYR:CE2	2.55	0.42
3:C:380:TYR:O	3:C:430:THR:HA	2.18	0.42
3:C:454:ARG:HD2	3:C:457:ARG:HD2	2.02	0.42
1:L:19:VAL:HG21	1:L:78:LEU:HD22	2.00	0.42
3:R:334:ASN:O	3:R:361:CYS:HA	2.19	0.42
2:B:120:THR:HG22	2:B:207:SER:HB3	2.01	0.42
3:C:450:ASN:N	3:C:450:ASN:OD1	2.52	0.42
2:H:123:PRO:HB3	2:H:149:TYR:HB3	2.01	0.42
2:B:188:VAL:HG11	2:B:198:TYR:CZ	2.54	0.42
2:H:188:VAL:HG21	2:H:198:TYR:CE2	2.55	0.42
1:L:92:ASN:OD1	1:L:93:SER:N	2.52	0.41
3:R:490:PHE:HA	3:R:491:PRO:HD3	1.94	0.41
2:H:159:ASN:HB2	2:H:162:ALA:HB3	2.01	0.41
2:H:2:VAL:N	2:H:25:SER:O	2.53	0.41
3:R:342:PHE:C	3:R:344:ALA:H	2.22	0.41
2:B:12:ILE:O	2:B:115:VAL:HA	2.19	0.41
2:B:199:ILE:HG13	2:B:213:LYS:O	2.20	0.41
3:C:433:VAL:HG13	3:C:512:VAL:HG22	2.02	0.41
1:L:29:ILE:H	1:L:29:ILE:HG13	1.75	0.41
2:B:149:TYR:OH	2:B:182:LEU:HD23	2.20	0.41
2:B:11:LEU:HA	2:B:114:THR:O	2.21	0.41
1:A:19:VAL:HG21	1:A:78:LEU:HD22	2.02	0.41
3:C:354:ASN:O	3:C:398:ASP:HA	2.21	0.41
2:H:45:LEU:HA	2:H:45:LEU:HD23	1.77	0.41
3:C:388:ASN:CB	3:C:527:PRO:HD2	2.49	0.41
1:L:31:SER:OG	4:L:301:SO4:O3	2.39	0.41
2:H:105:ASP:OD1	2:H:105:ASP:N	2.54	0.41
2:H:152:GLU:OE1	2:H:153:PRO:HA	2.21	0.41
2:H:204:HIS:CD2	2:H:206:PRO:HD2	2.56	0.41
3:R:354:ASN:O	3:R:398:ASP:HA	2.21	0.41
1:A:89:GLN:HG2	1:A:90:HIS:N	2.35	0.41
3:C:342:PHE:C	3:C:344:ALA:H	2.24	0.41
3:R:421:TYR:CD1	3:R:457:ARG:HB3	2.57	0.41
2:B:145:LEU:CD2	2:B:147:LYS:HB2	2.51	0.41
3:C:350:VAL:HA	3:C:400:PHE:HB2	2.03	0.41
3:C:368:LEU:HD22	3:C:371:LEU:HD23	2.03	0.40
1:L:61:ARG:O	1:L:75:ILE:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:394:ASN:HB2	3:R:516:GLU:OE2	2.22	0.40
3:R:395:VAL:HG22	3:R:515:PHE:CD1	2.53	0.40
2:B:2:VAL:N	2:B:25:SER:O	2.55	0.40
2:B:178:GLY:O	2:B:179:LEU:HD23	2.21	0.40
1:L:91:LEU:HD23	1:L:91:LEU:HA	1.86	0.40
1:L:188:GLU:O	1:L:212:ARG:NH1	2.54	0.40
2:B:24:ALA:HB3	2:B:76:ASN:ND2	2.36	0.40
2:B:216:GLU:HA	2:B:217:PRO:HD3	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	213/215 (99%)	193 (91%)	20 (9%)	0	100	100
1	L	213/215 (99%)	191 (90%)	22 (10%)	0	100	100
2	B	208/230 (90%)	192 (92%)	16 (8%)	0	100	100
2	H	207/230 (90%)	191 (92%)	16 (8%)	0	100	100
3	C	194/224 (87%)	181 (93%)	13 (7%)	0	100	100
3	R	192/224 (86%)	173 (90%)	18 (9%)	1 (0%)	29	61
All	All	1227/1338 (92%)	1121 (91%)	105 (9%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	R	373	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	187/187 (100%)	179 (96%)	8 (4%)	29	59
1	L	187/187 (100%)	179 (96%)	8 (4%)	29	59
2	B	177/193 (92%)	168 (95%)	9 (5%)	24	54
2	H	176/193 (91%)	168 (96%)	8 (4%)	27	58
3	C	171/198 (86%)	165 (96%)	6 (4%)	36	64
3	R	171/198 (86%)	165 (96%)	6 (4%)	36	64
All	All	1069/1156 (92%)	1024 (96%)	45 (4%)	30	60

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	33	LEU
1	L	90	HIS
1	L	111	VAL
1	L	153	ASN
1	L	177	SER
1	L	178	SER
1	L	195	CYS
2	H	2	VAL
2	H	6	GLU
2	H	22	CYS
2	H	30	SER
2	H	70	SER
2	H	74	SER
2	H	114	THR
2	H	183	SER
3	R	341	VAL
3	R	371	LEU
3	R	408	ARG
3	R	415	THR
3	R	450	ASN
3	R	516	GLU

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Mol	Chain	Res	Type
1	A	19	VAL
1	A	33	LEU
1	A	90	HIS
1	A	111	VAL
1	A	153	ASN
1	A	177	SER
1	A	178	SER
1	A	195	CYS
2	B	2	VAL
2	B	6	GLU
2	B	20	LEU
2	B	22	CYS
2	B	28	ILE
2	B	30	SER
2	B	53	SER
2	B	70	SER
2	B	114	THR
3	C	341	VAL
3	C	369	TYR
3	C	370	ASN
3	C	415	THR
3	C	450	ASN
3	C	516	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (i)

12 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	$\#\|Z\| > 2$
4	SO4	C	602	-	4,4,4	0.16	0	6,6,6	0.07	0
4	SO4	H	303	-	4,4,4	0.17	0	6,6,6	0.20	0
4	SO4	R	601	-	4,4,4	0.16	0	6,6,6	0.24	0
4	SO4	H	301	-	4,4,4	0.21	0	6,6,6	0.26	0
4	SO4	L	302	-	4,4,4	0.16	0	6,6,6	0.17	0
4	SO4	A	302	-	4,4,4	0.23	0	6,6,6	0.28	0
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.23	0
4	SO4	H	302	-	4,4,4	0.20	0	6,6,6	0.14	0
4	SO4	B	301	-	4,4,4	0.19	0	6,6,6	0.24	0
4	SO4	C	601	-	4,4,4	0.17	0	6,6,6	0.33	0
4	SO4	L	303	-	4,4,4	0.12	0	6,6,6	0.22	0
4	SO4	L	301	-	4,4,4	0.15	0	6,6,6	0.16	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	301	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, 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	215/215 (100%)	0.00	0 100 100	76, 101, 129, 159	0
1	L	215/215 (100%)	0.00	2 (0%) 84 84	74, 101, 126, 157	0
2	B	212/230 (92%)	0.13	9 (4%) 36 34	69, 99, 139, 156	0
2	H	211/230 (91%)	0.12	5 (2%) 59 56	68, 99, 139, 159	0
3	C	196/224 (87%)	0.24	12 (6%) 21 20	74, 106, 148, 163	0
3	R	196/224 (87%)	0.13	7 (3%) 42 40	74, 104, 154, 165	0
All	All	1245/1338 (93%)	0.10	35 (2%) 53 51	68, 101, 141, 165	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	195	THR	4.7
3	C	391	CYS	3.9
3	R	389	ASP	3.6
2	B	188	VAL	3.3
3	R	391	CYS	3.2
3	C	392	PHE	3.2
2	H	194	GLY	3.1
3	R	390	LEU	3.0
3	C	334	ASN	3.0
2	H	193	LEU	2.9
2	B	187	THR	2.8
3	C	524	VAL	2.8
2	B	130	PRO	2.7
3	C	384	PRO	2.6
3	C	515	PHE	2.6
1	L	24	ARG	2.4
2	H	163	LEU	2.4
2	B	199	ILE	2.3
3	C	528	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	190	SER	2.3
3	C	359	SER	2.3
1	L	138	ASN	2.3
2	B	214	ARG	2.3
3	R	520	ALA	2.3
2	B	213	LYS	2.3
2	B	189	PRO	2.3
3	C	477	ASN	2.2
2	B	196	GLN	2.2
3	R	371	LEU	2.2
3	C	529	LYS	2.2
3	R	392	PHE	2.2
3	R	521	PRO	2.1
3	C	522	ALA	2.0
2	H	188	VAL	2.0
3	C	360	ASN	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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	SO4	A	302	5/5	0.43	0.38	157,164,199,200	0
4	SO4	H	303	5/5	0.62	0.31	145,150,186,186	0
4	SO4	H	302	5/5	0.75	0.27	147,148,178,182	0
4	SO4	C	602	5/5	0.76	0.39	155,167,177,191	0
4	SO4	H	301	5/5	0.79	0.31	112,123,162,165	0
4	SO4	B	301	5/5	0.84	0.23	116,129,135,165	0
4	SO4	L	301	5/5	0.85	0.29	137,141,168,172	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	L	303	5/5	0.85	0.37	143,151,181,187	0
4	SO4	C	601	5/5	0.86	0.28	127,145,159,165	0
4	SO4	L	302	5/5	0.88	0.17	136,142,158,167	0
4	SO4	A	301	5/5	0.92	0.16	116,139,156,163	0
4	SO4	R	601	5/5	0.96	0.12	122,128,146,147	0

6.5 Other polymers (i)

There are no such residues in this entry.