



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 12:44 AM EDT

PDB ID : 7S4S
Title : Crystal Structure of SARS-CoV-2 S receptor-binding domain (RBD) in complex CoV11 Fab
Authors : Tolbert, W.D.; Pazgier, M.
Deposited on : 2021-09-09
Resolution : 2.05 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 : 2.35.1
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) : 2.35.1

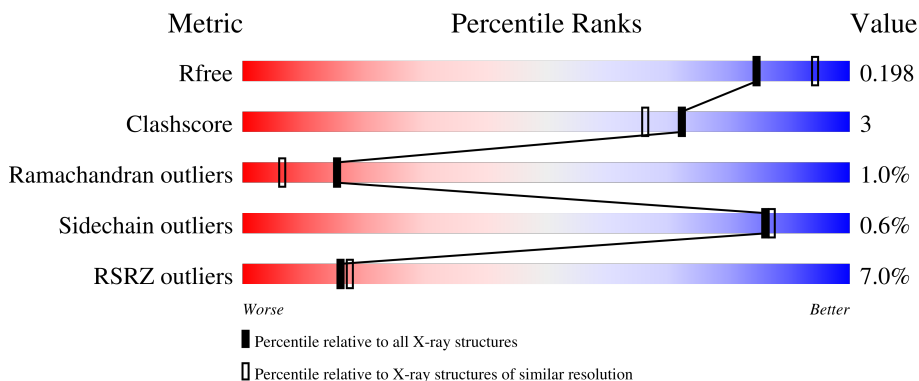
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	231	
2	H	221	
3	L	216	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	H	302	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5479 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	193	1535	983	256	288	8	0	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	542	SER	-	expression tag	UNP P0DTC2
A	543	GLY	-	expression tag	UNP P0DTC2
A	544	HIS	-	expression tag	UNP P0DTC2
A	545	HIS	-	expression tag	UNP P0DTC2
A	546	HIS	-	expression tag	UNP P0DTC2
A	547	HIS	-	expression tag	UNP P0DTC2
A	548	HIS	-	expression tag	UNP P0DTC2
A	549	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called CoV11 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1635	1032	275	322	6	0	1	0

- Molecule 3 is a protein called CoV11 light chain.

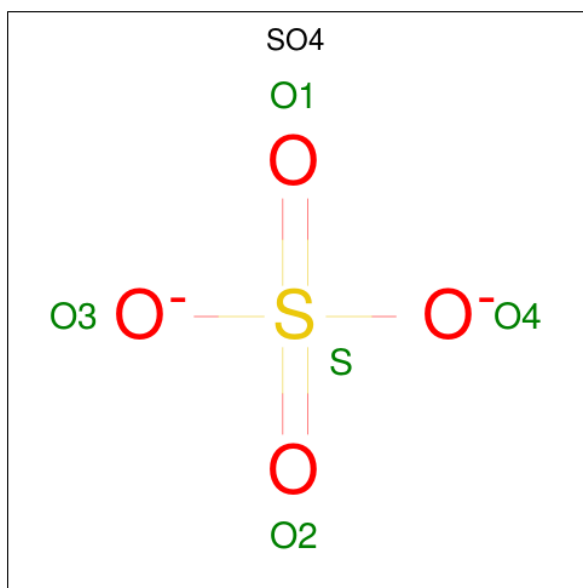
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	215	1687	1050	290	342	5	0	5	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



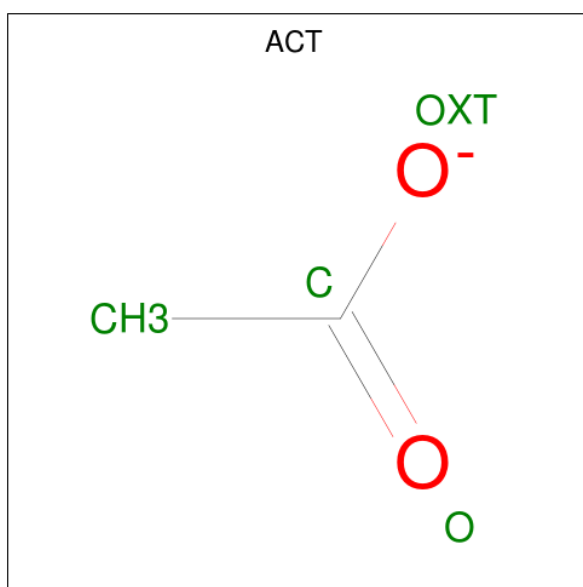
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
5	H	1	5	4	1	0	0
5	L	1	5	4	1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	1	Total O S 5 4 1	0	0
5	L	1	Total O S 5 4 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	H	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0
6	L	1	Total C O 4 2 2	0	0

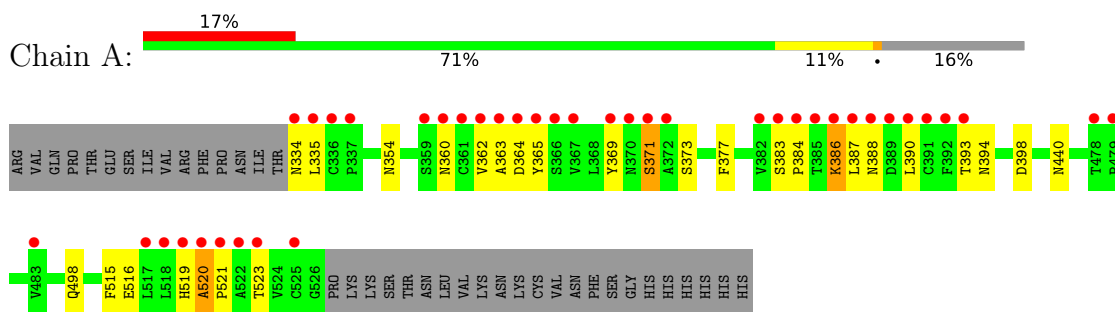
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	123	Total O 123 123	0	0
7	H	194	Total O 194 194	0	0
7	L	250	Total O 250 250	0	0

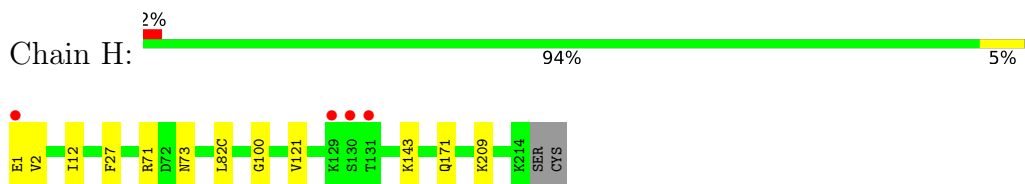
3 Residue-property plots [i](#)

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.

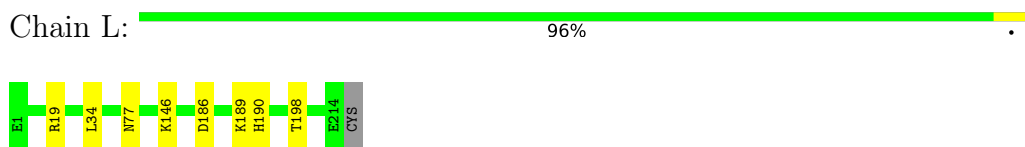
- Molecule 1: Spike protein S1



- Molecule 2: CoV11 heavy chain



- Molecule 3: CoV11 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.06Å 111.26Å 142.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.90 – 2.05 35.90 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.2 (35.90-2.05) 95.2 (35.90-2.05)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.05Å)	Xtrriage
Refinement program	PHENIX (1.17.1_3660: ???), REFMAC 5.8.0258	Depositor
R, R_{free}	0.166 , 0.198 0.166 , 0.198	Depositor DCC
R_{free} test set	2710 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.9	Xtrriage
Anisotropy	0.034	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5479	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, ACT, 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	0.44	0/1578	0.60	0/2147
2	H	0.45	0/1671	0.62	0/2275
3	L	0.47	0/1723	0.62	0/2338
All	All	0.46	0/4972	0.61	0/6760

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1535	0	1449	22	0
2	H	1635	0	1618	6	0
3	L	1687	0	1631	5	0
4	A	14	0	13	0	0
5	A	5	0	0	0	0
5	H	5	0	0	0	0
5	L	15	0	0	0	0
6	A	4	0	3	0	0
6	H	4	0	3	2	0
6	L	8	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	123	0	0	3	0
7	H	194	0	0	0	0
7	L	250	0	0	2	0
All	All	5479	0	4723	33	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 3.

All (33) 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:A:520:ALA:HB1	1:A:521:PRO:HD2	1.64	0.79
1:A:387:LEU:HD21	1:A:515:PHE:CZ	2.21	0.76
1:A:386:LYS:O	1:A:390:LEU:CD2	2.37	0.73
3:L:190:HIS:ND1	7:L:402:HOH:O	2.28	0.66
3:L:19[A]:ARG:NH2	3:L:77:ASN:OD1	2.29	0.66
1:A:440:ASN:ND2	7:A:1102:HOH:O	2.27	0.63
1:A:393:THR:HG23	1:A:516:GLU:HG2	1.81	0.61
1:A:383:SER:O	1:A:386:LYS:HB3	2.02	0.60
1:A:360:ASN:N	1:A:523:THR:OG1	2.32	0.57
1:A:498:GLN:NE2	7:A:1107:HOH:O	2.36	0.57
1:A:371:SER:C	1:A:373:SER:H	2.10	0.55
1:A:363:ALA:O	1:A:364:ASP:HB3	2.06	0.53
1:A:364:ASP:HA	1:A:388:ASN:ND2	2.24	0.53
1:A:354:ASN:O	1:A:398:ASP:HA	2.11	0.51
1:A:390:LEU:N	1:A:390:LEU:HD22	2.26	0.51
2:H:71:ARG:HH11	6:H:302:ACT:C	2.24	0.51
1:A:369:TYR:HA	1:A:377:PHE:CE2	2.47	0.49
1:A:386:LYS:O	1:A:390:LEU:HD22	2.14	0.47
1:A:371:SER:HB3	1:A:373:SER:OG	2.14	0.46
3:L:77:ASN:ND2	7:L:406:HOH:O	2.36	0.46
1:A:386:LYS:O	1:A:390:LEU:HD23	2.12	0.45
2:H:2:VAL:HG22	2:H:27:PHE:CE2	2.51	0.45
2:H:121:VAL:O	2:H:209:LYS:NZ	2.36	0.45
1:A:334:ASN:O	1:A:362:VAL:HG12	2.18	0.43
1:A:365:TYR:CE1	1:A:387:LEU:HG	2.54	0.42
1:A:498:GLN:NE2	7:A:1104:HOH:O	2.32	0.42
1:A:386:LYS:HG3	1:A:390:LEU:HD21	2.01	0.42
2:H:73:ASN:HD21	6:H:302:ACT:C	2.32	0.42
1:A:394:ASN:O	1:A:516:GLU:HB3	2.20	0.41
2:H:143:LYS:NZ	2:H:171:GLN:OE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:186:ASP:HA	3:L:189:LYS:HD3	2.02	0.41
2:H:12:ILE:HG21	2:H:82(C):LEU:HD13	2.03	0.41
3:L:146:LYS:HB3	3:L:198:THR:HB	2.02	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	192/231 (83%)	171 (89%)	16 (8%)	5 (3%)	5 1
2	H	218/221 (99%)	213 (98%)	4 (2%)	1 (0%)	29 18
3	L	218/216 (101%)	214 (98%)	4 (2%)	0	100 100
All	All	628/668 (94%)	598 (95%)	24 (4%)	6 (1%)	15 6

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	ALA
1	A	371	SER
1	A	386	LYS
1	A	519	HIS
2	H	100	GLY
1	A	384	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	167/203 (82%)	166 (99%)	1 (1%)	86	87
2	H	183/184 (100%)	182 (100%)	1 (0%)	88	89
3	L	189/185 (102%)	188 (100%)	1 (0%)	88	89
All	All	539/572 (94%)	536 (99%)	3 (1%)	86	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	LEU
2	H	1	GLU
3	L	34	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	A	519	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
6	ACT	L	305	-	3,3,3	1.22	0	3,3,3	1.36	0
4	NAG	A	1001	1	14,14,15	0.33	0	17,19,21	0.68	1 (5%)
5	SO4	L	301	-	4,4,4	0.21	0	6,6,6	0.36	0
5	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.17	0
6	ACT	H	302	-	3,3,3	1.22	0	3,3,3	1.57	1 (33%)
5	SO4	H	301	-	4,4,4	0.19	0	6,6,6	0.11	0
6	ACT	L	304	-	3,3,3	1.36	0	3,3,3	1.44	0
5	SO4	L	303	-	4,4,4	0.15	0	6,6,6	0.24	0
6	ACT	A	1003	-	3,3,3	1.62	1 (33%)	3,3,3	1.58	0
5	SO4	A	1002	-	4,4,4	0.13	0	6,6,6	0.10	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1001	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1003	ACT	CH3-C	2.33	1.58	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAG	C1-O5-C5	2.32	115.34	112.19
6	H	302	ACT	O-C-CH3	-2.03	114.43	122.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
4	A	1001	NAG	O7-C7-N2-C2
4	A	1001	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	302	ACT	2	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	193/231 (83%)	0.80	40 (20%) 1 0	19, 35, 90, 117	0
2	H	219/221 (99%)	-0.16	4 (1%) 68 71	20, 27, 45, 99	0
3	L	215/216 (99%)	-0.24	0 100 100	17, 25, 41, 65	0
All	All	627/668 (93%)	0.11	44 (7%) 16 18	17, 27, 76, 117	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	387	LEU	8.4
1	A	369	TYR	7.6
1	A	518	LEU	7.3
1	A	519	HIS	7.1
1	A	517	LEU	5.9
1	A	365	TYR	5.9
1	A	372	ALA	5.7
1	A	521	PRO	5.7
1	A	525	CYS	5.1
1	A	389	ASP	5.0
1	A	520	ALA	4.8
1	A	371	SER	4.6
1	A	385	THR	4.4
1	A	370	ASN	4.3
1	A	366	SER	4.0
1	A	386	LYS	3.9
1	A	334	ASN	3.8
1	A	367	VAL	3.7
1	A	361	CYS	3.6
1	A	335	LEU	3.5
1	A	362	VAL	3.5
1	A	384	PRO	3.4
2	H	1	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	130	SER	3.4
1	A	360	ASN	3.2
1	A	364	ASP	3.2
1	A	522	ALA	3.2
1	A	382	VAL	3.2
1	A	390	LEU	3.1
1	A	523	THR	3.1
2	H	129	LYS	3.1
1	A	363	ALA	3.0
1	A	383	SER	3.0
1	A	393	THR	3.0
1	A	388	ASN	2.9
1	A	483	VAL	2.9
1	A	336	CYS	2.8
1	A	478	THR	2.6
2	H	131	THR	2.6
1	A	391	CYS	2.5
1	A	337	PRO	2.5
1	A	392	PHE	2.4
1	A	479	PRO	2.3
1	A	359	SER	2.3

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, 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(\AA^2)	Q<0.9
6	ACT	A	1003	4/4	0.63	0.22	55,55,57,59	0
6	ACT	H	302	4/4	0.78	0.24	64,66,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	1002	5/5	0.81	0.18	104,108,110,110	0
4	NAG	A	1001	14/15	0.82	0.37	75,81,90,97	0
6	ACT	L	305	4/4	0.82	0.17	79,79,79,82	0
5	SO4	H	301	5/5	0.89	0.37	100,100,102,102	0
5	SO4	L	303	5/5	0.95	0.17	71,75,79,80	0
5	SO4	L	302	5/5	0.95	0.09	66,66,71,72	0
6	ACT	L	304	4/4	0.96	0.14	32,34,37,46	0
5	SO4	L	301	5/5	0.99	0.08	28,30,34,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.