



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:51 PM UTC

PDB ID : 6ZSL / pdb_00006zsl
Title : Crystal structure of the SARS-CoV-2 helicase at 1.94 Angstrom resolution
Authors : Newman, J.A.; Yosaatmadja, Y.; Douangamath, A.; Arrowsmith, C.H.; von Delft, F.; Edwards, A.; Bountra, C.; Gileadi, O.
Deposited on : 2020-07-15
Resolution : 1.94 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

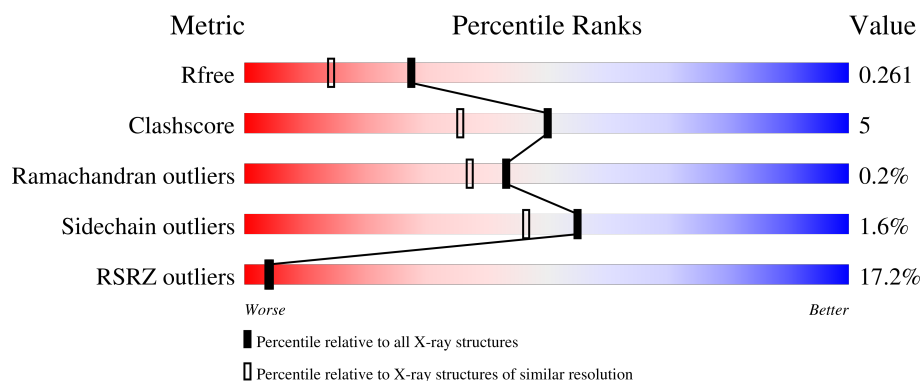
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	603	16% 84% 11% 5%
1	B	603	17% 83% 13% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9407 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 SARS-CoV-2 helicase NSP13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	585	Total	C	N	O	S	0	1	0
			4508	2875	750	848	35			
1	A	572	Total	C	N	O	S	0	0	0
			4417	2816	737	832	32			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP P0DTD1
B	0	MET	-	expression tag	UNP P0DTD1
A	-1	SER	-	expression tag	UNP P0DTD1
A	0	MET	-	expression tag	UNP P0DTD1

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		

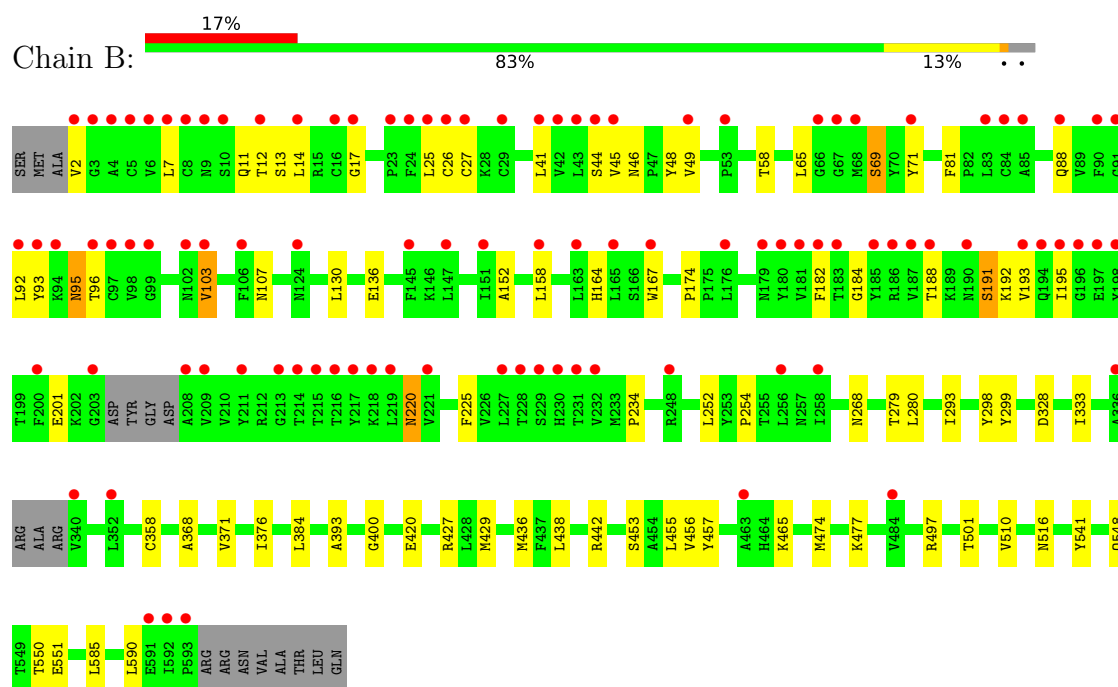
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	250	Total	O	0	0
			250	250		
4	A	206	Total	O	0	0
			206	206		

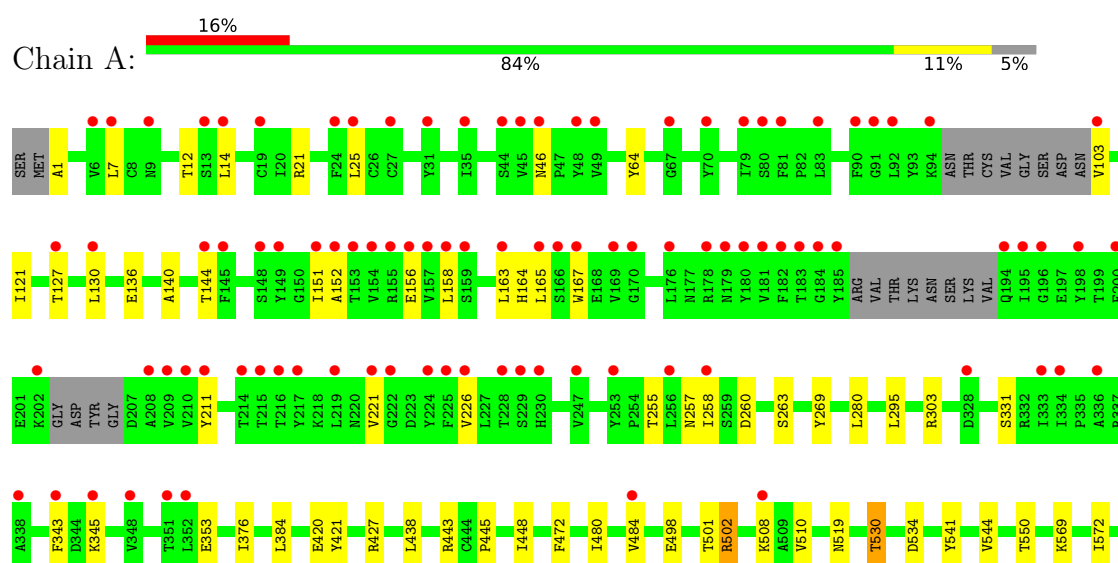
3 Residue-property plots

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: SARS-CoV-2 helicase NSP13



• Molecule 1: SARS-CoV-2 helicase NSP13





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.15Å 70.12Å 84.56Å 102.47° 95.65° 112.79°	Depositor
Resolution (Å)	57.56 – 1.94 57.56 – 1.94	Depositor EDS
% Data completeness (in resolution range)	97.3 (57.56-1.94) 89.5 (57.56-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.209 , 0.253 (Not available) , 0.261	Depositor DCC
R_{free} test set	4194 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: PO4, ZN

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	0.22	0/4517	0.42	0/6156
1	B	0.25	0/4610	0.46	0/6283
All	All	0.24	0/9127	0.44	0/12439

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

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	4417	0	4321	39	2
1	B	4508	0	4423	53	1
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	0	0
4	A	206	0	0	5	0
4	B	250	0	0	6	0
All	All	9407	0	8744	93	2

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 5.

All (93) 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:12:THR:HG22	1:A:14:LEU:H	1.40	0.85
1:B:27:CYS:SG	4:B:915:HOH:O	2.32	0.83
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.68	0.76
1:B:201:GLU:OE2	4:B:801:HOH:O	2.08	0.72
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.74	0.67
1:A:12:THR:HG21	1:A:25:LEU:O	1.95	0.66
1:B:2:VAL:N	4:B:806:HOH:O	2.30	0.63
1:A:534:ASP:OD2	4:A:801:HOH:O	2.17	0.60
1:B:510:VAL:HG21	1:B:541:TYR:CD1	2.38	0.59
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.25	0.58
1:A:7:LEU:HD13	1:A:103:VAL:HG22	1.85	0.58
1:B:279:THR:HB	1:B:429:MET:HE2	1.87	0.57
1:A:498:GLU:HB3	1:A:502:ARG:HH22	1.70	0.57
1:B:12:THR:HG22	1:B:14:LEU:H	1.69	0.56
1:B:44:SER:OG	1:B:45:VAL:N	2.34	0.56
1:A:480:ILE:HG12	1:A:550:THR:HG22	1.88	0.56
1:B:12:THR:HG21	1:B:25:LEU:O	2.05	0.55
1:B:48:TYR:O	4:B:802:HOH:O	2.18	0.53
1:A:303:ARG:NH1	1:A:353:GLU:O	2.41	0.53
1:B:13:SER:O	1:B:44:SER:HA	2.08	0.52
1:A:21:ARG:NE	1:A:136:GLU:OE2	2.39	0.52
1:B:516:ASN:ND2	4:B:814:HOH:O	2.42	0.52
1:A:584:LYS:NZ	4:A:813:HOH:O	2.42	0.52
1:B:95:ASN:OD1	1:B:95:ASN:N	2.31	0.51
1:A:1:ALA:N	4:A:810:HOH:O	2.40	0.51
1:A:510:VAL:HG21	1:A:541:TYR:CD1	2.46	0.51
1:A:163:LEU:HD23	1:A:211:TYR:CD2	2.46	0.51
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.94	0.50
1:B:7:LEU:HD21	1:B:130:LEU:HD21	1.93	0.49
1:B:376:ILE:HD11	1:B:384:LEU:HD21	1.93	0.49
1:B:497:ARG:O	1:B:501:THR:HG23	2.12	0.48
1:B:11:GLN:HG2	1:B:93:TYR:CD2	2.48	0.48
1:B:49:VAL:HG23	1:B:58:THR:HG22	1.95	0.48
1:A:152:ALA:HB1	1:A:165:LEU:HD22	1.96	0.48
1:B:17:GLY:HA3	1:B:41:LEU:HD23	1.96	0.47
1:B:69:SER:HB2	1:B:71:TYR:CE2	2.49	0.47
1:A:260:ASP:HA	1:A:263:SER:OG	2.15	0.47
1:B:455:LEU:HG	1:B:456:VAL:HG13	1.96	0.47
1:B:158:LEU:HD13	1:B:164:HIS:HB2	1.97	0.46
1:B:268:ASN:ND2	1:B:436:MET:HG2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:LYS:NZ	4:B:822:HOH:O	2.47	0.46
1:A:121:ILE:HG23	1:A:421:TYR:CE1	2.50	0.46
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.46	0.46
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.51	0.46
1:A:508:LYS:HB2	1:A:508:LYS:HE3	1.76	0.45
1:B:279:THR:HB	1:B:429:MET:CE	2.46	0.45
1:B:12:THR:HG21	1:B:26:CYS:HA	1.97	0.45
1:B:252:LEU:HB3	1:B:299:TYR:CD1	2.51	0.45
1:B:254:PRO:HB3	1:B:298:TYR:CE2	2.52	0.45
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.52	0.45
3:A:705:PO4:O4	4:A:802:HOH:O	2.21	0.45
1:A:156:GLU:HA	1:A:221:VAL:HG22	1.98	0.45
1:A:343:PHE:CE2	1:A:345:LYS:HB2	2.52	0.45
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.52	0.45
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.98	0.44
1:A:127:THR:HG22	1:A:130:LEU:HB2	1.98	0.44
1:A:158:LEU:HD11	1:A:164:HIS:CE1	2.52	0.44
1:A:420:GLU:OE1	1:A:427:ARG:NH1	2.50	0.44
1:A:255:THR:HG22	1:A:257:ASN:H	1.83	0.43
1:A:443:ARG:HG3	1:A:569:LYS:HG2	2.00	0.43
1:A:151:ILE:HG12	1:A:226:VAL:HG22	2.00	0.43
1:A:544:VAL:O	1:A:572:ILE:HA	2.19	0.43
1:A:472:PHE:HB3	1:A:590:LEU:HG	2.00	0.43
1:B:7:LEU:HD12	1:B:103:VAL:HG22	2.00	0.43
1:B:220:ASN:OD1	1:B:220:ASN:N	2.51	0.42
1:B:333:ILE:HB	1:B:358:CYS:SG	2.58	0.42
1:B:453:SER:HA	1:B:457:TYR:HB2	2.01	0.42
1:A:127:THR:HG23	1:A:130:LEU:H	1.84	0.42
1:B:280:LEU:HD11	1:B:438:LEU:HG	2.01	0.42
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	2.00	0.42
1:B:136:GLU:CD	1:B:234:PRO:HA	2.45	0.42
1:A:140:ALA:O	1:A:144:THR:HG23	2.19	0.42
1:B:13:SER:HB2	1:B:92:LEU:HB2	2.00	0.42
1:B:371:VAL:HG23	1:B:393:ALA:HB2	2.02	0.42
1:A:269:TYR:CD1	1:A:295:LEU:HD13	2.55	0.42
1:A:376:ILE:HD11	1:A:384:LEU:HD21	2.01	0.42
1:B:167:TRP:CZ3	1:B:174:PRO:HD2	2.54	0.42
1:B:368:ALA:O	1:B:393:ALA:HA	2.19	0.42
1:A:592:ILE:HD12	1:A:592:ILE:HA	1.86	0.42
1:B:27:CYS:HB3	1:B:88:GLN:HB3	2.02	0.42
1:B:420:GLU:OE1	1:B:427:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:CG2	1:B:26:CYS:HA	2.51	0.41
1:B:184:GLY:C	1:B:195:ILE:HG22	2.45	0.41
1:A:480:ILE:HD11	4:A:852:HOH:O	2.21	0.41
1:B:182:PHE:HB3	1:B:225:PHE:HB3	2.02	0.41
1:B:548:GLN:HG2	1:B:550:THR:O	2.21	0.41
1:A:519:ASN:HB3	1:A:530:THR:HG23	2.01	0.41
1:B:280:LEU:HB2	1:B:436:MET:HE3	2.03	0.41
1:A:498:GLU:HB3	1:A:502:ARG:NH2	2.34	0.40
1:B:103:VAL:HG12	1:B:107:ASN:ND2	2.36	0.40
1:B:7:LEU:CD2	1:B:130:LEU:HD21	2.50	0.40
1:B:12:THR:HG22	1:B:13:SER:N	2.37	0.40
1:B:585:LEU:HD23	1:B:585:LEU:HA	1.95	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:ARG:NH1	1:A:501:THR:O[1_666]	2.14	0.06
1:A:64:TYR:OH	1:A:345:LYS:NZ[1_665]	2.17	0.03

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	564/603 (94%)	547 (97%)	16 (3%)	1 (0%)	43	37
1	B	580/603 (96%)	553 (95%)	26 (4%)	1 (0%)	43	37
All	All	1144/1206 (95%)	1100 (96%)	42 (4%)	2 (0%)	43	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	484	VAL
1	B	191	SER

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	485/525 (92%)	481 (99%)	4 (1%)	73	71
1	B	498/525 (95%)	486 (98%)	12 (2%)	43	31
All	All	983/1050 (94%)	967 (98%)	16 (2%)	55	46

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	ASN
1	B	69	SER
1	B	95	ASN
1	B	96	THR
1	B	103	VAL
1	B	188	THR
1	B	191	SER
1	B	192	LYS
1	B	193	VAL
1	B	220	ASN
1	B	293	ILE
1	B	328	ASP
1	A	46	ASN
1	A	258	ILE
1	A	502	ARG
1	A	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	164	HIS

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	245	HIS
1	B	268	ASN
1	B	404	GLN
1	B	459	ASN
1	B	470	GLN
1	A	164	HIS
1	A	220	ASN
1	A	257	ASN
1	A	275	GLN
1	A	404	GLN
1	A	459	ASN
1	A	531	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](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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	PO4	B	705	-	4,4,4	1.12	0	6,6,6	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	A	705	-	4,4,4	0.97	0	6,6,6	0.47	0
3	PO4	A	704	-	4,4,4	1.10	0	6,6,6	0.70	0
3	PO4	B	704	-	4,4,4	1.07	0	6,6,6	0.62	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
3	A	705	PO4	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	572/603 (94%)	1.12	98 (17%) 4 4	32, 52, 97, 110	0
1	B	585/603 (97%)	0.92	101 (17%) 4 4	24, 45, 84, 104	1 (0%)
All	All	1157/1206 (95%)	1.02	199 (17%) 4 4	24, 49, 92, 110	1 (0%)

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	ILE	7.0
1	A	157	VAL	6.0
1	A	221	VAL	5.7
1	A	169	VAL	5.3
1	A	152	ALA	5.3
1	A	81	PHE	5.2
1	B	214	THR	5.1
1	A	151	ILE	4.9
1	A	225	PHE	4.8
1	B	193	VAL	4.6
1	B	217	TYR	4.5
1	B	195	ILE	4.5
1	A	228	THR	4.2
1	A	219	LEU	4.2
1	A	200	PHE	4.2
1	B	45	VAL	4.2
1	B	187	VAL	4.2
1	B	4	ALA	4.1
1	B	229	SER	4.0
1	A	195	ILE	4.0
1	B	2	VAL	3.9
1	A	336	ALA	3.9
1	B	98	VAL	3.9
1	A	154	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	229	SER	3.8
1	A	185	TYR	3.8
1	B	91	GLY	3.8
1	B	336	ALA	3.7
1	B	221	VAL	3.7
1	A	158	LEU	3.7
1	A	352	LEU	3.7
1	A	182	PHE	3.7
1	B	215	THR	3.6
1	A	224	TYR	3.6
1	A	333	ILE	3.6
1	A	167	TRP	3.6
1	B	67	GLY	3.5
1	A	153	THR	3.5
1	B	92	LEU	3.5
1	B	180	TYR	3.5
1	B	83	LEU	3.5
1	B	196	GLY	3.4
1	A	94	LYS	3.4
1	B	93	TYR	3.3
1	A	247	VAL	3.3
1	B	208	ALA	3.3
1	B	14	LEU	3.3
1	B	53	PRO	3.3
1	A	149	TYR	3.3
1	B	230	HIS	3.3
1	A	170	GLY	3.3
1	B	227	LEU	3.2
1	A	338	ALA	3.2
1	A	210	VAL	3.2
1	A	215	THR	3.2
1	A	196	GLY	3.1
1	A	217	TYR	3.1
1	B	25	LEU	3.1
1	B	340	VAL	3.0
1	A	14	LEU	3.0
1	B	219	LEU	3.0
1	A	176	LEU	3.0
1	A	103	VAL	3.0
1	A	208	ALA	3.0
1	A	79	ILE	3.0
1	B	10	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	231	THR	2.9
1	B	84	CYS	2.9
1	B	7	LEU	2.9
1	A	163	LEU	2.9
1	A	165	LEU	2.9
1	B	9	ASN	2.9
1	A	194	GLN	2.9
1	B	163	LEU	2.9
1	A	156	GLU	2.9
1	B	27	CYS	2.9
1	A	178	ARG	2.9
1	A	256	LEU	2.9
1	A	209	VAL	2.8
1	A	211	TYR	2.8
1	B	97	CYS	2.8
1	B	258	ILE	2.8
1	B	3	GLY	2.8
1	A	67	GLY	2.8
1	A	222	GLY	2.8
1	A	230	HIS	2.8
1	B	209	VAL	2.8
1	A	184	GLY	2.8
1	B	185	TYR	2.8
1	A	92	LEU	2.8
1	A	6	VAL	2.8
1	A	155	ARG	2.7
1	B	8	CYS	2.7
1	B	256	LEU	2.7
1	A	226	VAL	2.7
1	B	26	CYS	2.7
1	A	7	LEU	2.7
1	A	9	ASN	2.7
1	B	85	ALA	2.7
1	B	211	TYR	2.7
1	A	91	GLY	2.7
1	A	145	PHE	2.7
1	B	96	THR	2.7
1	B	592	ILE	2.7
1	B	145	PHE	2.6
1	B	151	ILE	2.6
1	A	45	VAL	2.6
1	A	214	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	29	CYS	2.6
1	B	179	ASN	2.6
1	A	80	SER	2.6
1	B	200	PHE	2.6
1	A	90	PHE	2.6
1	B	12	THR	2.6
1	B	43	LEU	2.5
1	A	345	LYS	2.5
1	A	46	ASN	2.5
1	A	181	VAL	2.5
1	B	5	CYS	2.5
1	B	232	VAL	2.5
1	B	66	GLY	2.5
1	B	186	ARG	2.5
1	B	44	SER	2.5
1	B	593	PRO	2.5
1	B	90	PHE	2.4
1	A	13	SER	2.4
1	A	202	LYS	2.4
1	B	167	TRP	2.4
1	B	6	VAL	2.4
1	B	198	TYR	2.4
1	B	352	LEU	2.4
1	A	328	ASP	2.4
1	A	348	VAL	2.4
1	B	176	LEU	2.4
1	A	216	THR	2.4
1	A	351	THR	2.4
1	B	194	GLN	2.4
1	B	102	ASN	2.4
1	B	41	LEU	2.3
1	B	147	LEU	2.3
1	B	158	LEU	2.3
1	B	188	THR	2.3
1	A	144	THR	2.3
1	A	179	ASN	2.3
1	B	181	VAL	2.3
1	A	44	SER	2.3
1	B	24	PHE	2.3
1	A	70	TYR	2.3
1	B	218	LYS	2.3
1	A	49	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	183	THR	2.3
1	A	48	TYR	2.3
1	B	23	PRO	2.3
1	B	203	GLY	2.3
1	B	591	GLU	2.3
1	B	103	VAL	2.3
1	B	228	THR	2.3
1	A	508	LYS	2.3
1	B	17	GLY	2.2
1	A	180	TYR	2.2
1	A	484	VAL	2.2
1	B	190	ASN	2.2
1	B	68	MET	2.2
1	A	591	GLU	2.2
1	A	27	CYS	2.2
1	A	130	LEU	2.2
1	A	159	SER	2.2
1	B	182	PHE	2.2
1	A	35	ILE	2.2
1	B	49	VAL	2.2
1	B	99	GLY	2.2
1	A	83	LEU	2.2
1	B	463	ALA	2.2
1	B	248	ARG	2.2
1	B	197	GLU	2.1
1	A	24	PHE	2.1
1	A	198	TYR	2.1
1	A	258	ILE	2.1
1	A	148	SER	2.1
1	A	166	SER	2.1
1	A	19	CYS	2.1
1	B	88	GLN	2.1
1	A	253	TYR	2.1
1	B	216	THR	2.1
1	B	94	LYS	2.1
1	B	16	CYS	2.1
1	A	343	PHE	2.1
1	B	71	TYR	2.1
1	A	31	TYR	2.1
1	B	183	THR	2.1
1	B	213	GLY	2.1
1	B	42	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	165	LEU	2.1
1	A	25	LEU	2.1
1	B	106	PHE	2.0
1	A	334	ILE	2.0
1	A	127	THR	2.0
1	B	484	VAL	2.0
1	B	124	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 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
2	ZN	B	702	1/1	0.94	0.07	66,66,66,66	0
3	PO4	B	705	5/5	0.94	0.10	43,45,54,63	0
3	PO4	A	705	5/5	0.96	0.07	38,40,48,53	0
3	PO4	A	704	5/5	0.97	0.06	40,42,46,47	0
3	PO4	B	704	5/5	0.97	0.07	36,39,44,51	0
2	ZN	B	701	1/1	0.98	0.05	47,47,47,47	0
2	ZN	A	703	1/1	0.98	0.05	70,70,70,70	0
2	ZN	A	702	1/1	0.99	0.04	45,45,45,45	0
2	ZN	B	703	1/1	0.99	0.03	68,68,68,68	0
2	ZN	A	701	1/1	0.99	0.03	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.