



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:25 PM UTC

PDB ID : 9I4V / pdb_00009i4v
Title : Crystal structure of the SARS-CoV-2 helicase NSP13
Authors : Kloskowski, P.; Neumann, P.; Ficner, R.
Deposited on : 2025-01-27
Resolution : 2.33 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

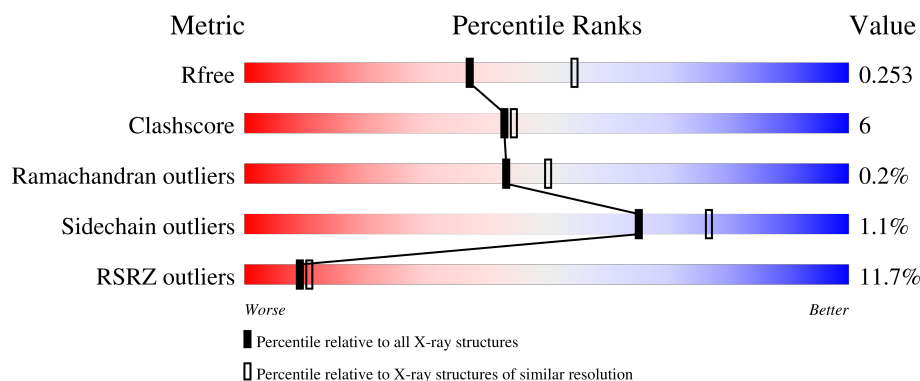
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	<div> <div>18%</div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	B	603	<div> <div>4%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>

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
2	ZN	A	703	-	-	X	-
2	ZN	B	702	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9066 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	A	570	Total	C	N	O	S	0	0	0
			4398	2801	735	830	32			
1	B	585	Total	C	N	O	S	0	2	0
			4513	2878	751	849	35			

There are 4 discrepancies between the modelled and reference sequences:

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

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

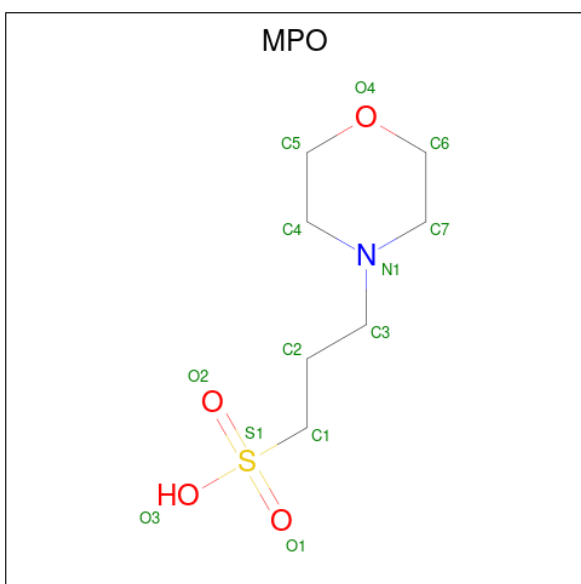
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

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



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

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

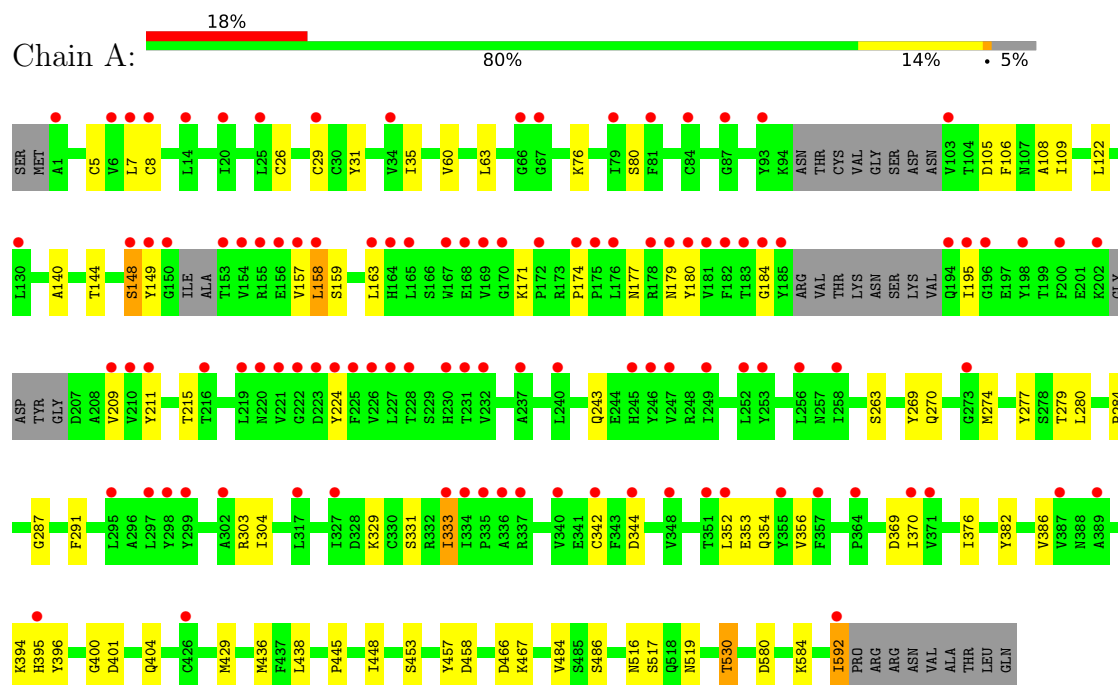
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	64	Total	O	0	0
			64	64		

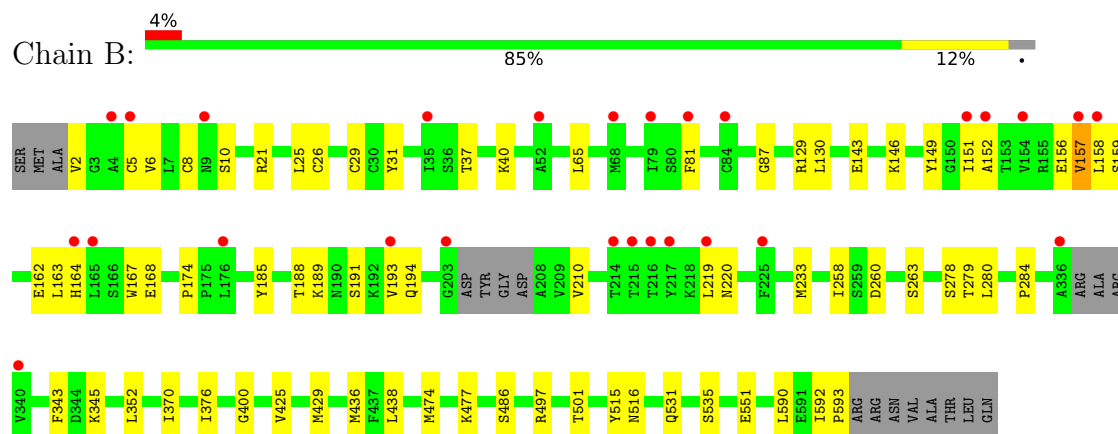
3 Residue-property plots

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	59.30Å 70.69Å 86.22Å 103.70° 95.24° 112.12°	Depositor
Resolution (Å)	45.60 – 2.33 45.60 – 2.33	Depositor EDS
% Data completeness (in resolution range)	92.8 (45.60-2.33) 92.8 (45.60-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.213 , 0.254 0.213 , 0.253	Depositor DCC
R_{free} test set	2510 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 65.9	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	0.95	EDS
Total number of atoms	9066	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: PO4, MPO, 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	0/4496	0.56	1/6126 (0.0%)
1	B	0.20	0/4618	0.54	0/6294
All	All	0.21	0/9114	0.55	1/12420 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	TYR	N-CA-C	-5.13	101.75	109.85

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	4398	0	4298	61	0
1	B	4513	0	4430	50	0
2	A	3	0	0	2	0
2	B	3	0	0	2	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
4	A	13	0	15	0	0
4	B	13	0	14	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	39	0	0	1	0
5	B	64	0	0	1	0
All	All	9066	0	8757	109	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 6.

All (109) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD11	1:B:162:GLU:HB2	1.46	0.98
1:A:26:CYS:HG	2:A:703:ZN:ZN	0.82	0.87
1:B:6:VAL:O	1:B:129:ARG:HD3	1.79	0.81
1:B:279:THR:HB	1:B:429:MET:HE2	1.65	0.78
1:B:26:CYS:SG	2:B:702:ZN:ZN	1.73	0.76
1:A:26:CYS:SG	2:A:703:ZN:ZN	1.76	0.74
1:B:474[B]:MET:HG2	1:B:590:LEU:HB2	1.71	0.73
1:A:76:LYS:HE2	1:A:80:SER:HB2	1.75	0.67
1:B:516[A]:ASN:ND2	4:B:706:MPO:O2	2.28	0.66
1:A:280:LEU:HB2	1:A:436:MET:HE3	1.80	0.64
1:B:2:VAL:N	5:B:802:HOH:O	2.32	0.63
1:B:37:THR:O	1:B:40:LYS:NZ	2.32	0.63
1:A:158:LEU:HD12	1:A:159:SER:HB3	1.81	0.62
1:B:26:CYS:HG	2:B:702:ZN:ZN	1.11	0.62
1:A:31:TYR:O	1:A:35:ILE:HG13	2.00	0.61
1:A:333:ILE:HD13	1:A:356:VAL:HG13	1.83	0.60
1:B:280:LEU:HB2	1:B:436:MET:HE3	1.84	0.59
1:A:519:ASN:HB3	1:A:530:THR:HG21	1.84	0.59
1:B:5:CYS:SG	1:B:25:LEU:HA	2.43	0.59
1:B:352:LEU:H	1:B:352:LEU:HD23	1.70	0.57
1:A:8:CYS:SG	1:A:26:CYS:SG	3.03	0.56
1:A:519:ASN:HB3	1:A:530:THR:CG2	2.36	0.56
1:A:303:ARG:NH1	1:A:353:GLU:O	2.38	0.56
1:A:26:CYS:SG	1:A:29:CYS:HB2	2.46	0.56
1:B:163:LEU:HD11	1:B:219:LEU:HD11	1.87	0.55
1:A:329:LYS:HE3	1:A:354:GLN:H	1.71	0.55
1:B:531:GLN:HG2	1:B:535:SER:OG	2.06	0.55
1:B:158:LEU:HD12	1:B:159:SER:N	2.22	0.55
1:A:369:ASP:HA	1:A:394:LYS:HE3	1.89	0.54
1:A:26:CYS:SG	1:A:29:CYS:CB	2.95	0.54
1:A:280:LEU:HD11	1:A:438:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:HD11	1:A:122:LEU:HG	1.89	0.54
1:A:382:TYR:O	1:A:386:VAL:HG23	2.07	0.54
1:B:477:LYS:NZ	1:B:551:GLU:OE2	2.37	0.53
1:B:149:TYR:CD2	1:B:174:PRO:HB3	2.44	0.53
1:A:149:TYR:CD2	1:A:174:PRO:HB3	2.43	0.53
1:B:188:THR:HG1	1:B:191:SER:C	2.13	0.53
1:B:188:THR:N	1:B:191:SER:O	2.36	0.53
1:A:7:LEU:HD21	1:A:106:PHE:CD2	2.45	0.51
1:A:215:THR:HG22	1:B:193:VAL:HG21	1.92	0.50
1:B:143:GLU:HA	1:B:146:LYS:HE2	1.94	0.50
1:A:148:SER:O	1:A:171:LYS:HD3	2.12	0.50
1:B:280:LEU:HD11	1:B:438:LEU:HG	1.94	0.50
1:A:352:LEU:HG	1:B:233:MET:HE1	1.93	0.49
1:A:331:SER:HB2	1:A:353:GLU:HG3	1.93	0.49
1:A:184:GLY:C	1:A:195:ILE:HG12	2.38	0.49
1:B:343:PHE:CE2	1:B:345:LYS:HB2	2.47	0.49
1:A:466:ASP:OD1	1:A:467:LYS:N	2.43	0.48
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.48	0.48
1:B:156:GLU:OE1	1:B:164:HIS:ND1	2.45	0.48
1:A:108:ALA:HB3	1:A:122:LEU:HD21	1.96	0.48
1:B:157:VAL:HA	1:B:163:LEU:HD23	1.96	0.47
1:A:177:ASN:OD1	1:A:179:ASN:N	2.42	0.47
1:A:163:LEU:HG	1:A:211:TYR:CD1	2.49	0.47
1:A:333:ILE:CD1	1:A:356:VAL:HG13	2.45	0.46
1:B:188:THR:O	1:B:189:LYS:C	2.59	0.46
1:B:185:TYR:CE2	1:B:194:GLN:HG2	2.50	0.46
1:B:8:CYS:SG	1:B:26:CYS:SG	3.04	0.46
1:A:287:GLY:HA2	5:A:818:HOH:O	2.15	0.46
1:B:497:ARG:O	1:B:501:THR:HG23	2.16	0.46
1:B:31:TYR:CE1	1:B:87:GLY:HA2	2.50	0.46
1:B:343:PHE:CZ	1:B:345:LYS:HB2	2.50	0.46
1:A:592:ILE:HD12	1:A:592:ILE:HA	1.74	0.45
1:A:163:LEU:N	1:A:209:VAL:O	2.43	0.45
1:A:270:GLN:O	1:A:274:MET:HG3	2.17	0.45
1:A:329:LYS:HD2	1:A:329:LYS:HA	1.76	0.45
1:A:277:TYR:HA	1:A:396:TYR:O	2.17	0.45
1:B:486:SER:OG	1:B:515:TYR:HB3	2.16	0.45
1:A:376:ILE:HG22	1:A:400:GLY:HA3	1.98	0.45
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.51	0.45
1:A:174:PRO:HB2	1:A:180:TYR:HD2	1.81	0.45
1:B:151:ILE:HG13	1:B:168:GLU:OE1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ILE:HG22	1:B:400:GLY:HA3	1.99	0.44
1:A:269:TYR:OH	1:A:291:PHE:O	2.22	0.44
1:A:445:PRO:HD2	1:A:448:ILE:HD12	1.99	0.44
1:A:401:ASP:HB3	1:A:404:GLN:HG3	1.99	0.44
1:B:260:ASP:HA	1:B:263:SER:OG	2.18	0.44
1:A:5:CYS:SG	1:A:26:CYS:SG	3.15	0.44
1:A:179:ASN:C	1:A:180:TYR:HD1	2.26	0.44
1:A:157:VAL:HA	1:A:163:LEU:HD23	2.00	0.43
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.75	0.43
1:A:453:SER:HA	1:A:457:TYR:HB2	2.00	0.43
1:B:352:LEU:H	1:B:352:LEU:CD2	2.31	0.43
1:B:592:ILE:HA	1:B:593:PRO:HD3	1.86	0.43
1:A:140:ALA:O	1:A:144:THR:HG23	2.19	0.43
1:A:333:ILE:HD12	1:A:333:ILE:N	2.34	0.43
1:A:580:ASP:OD1	1:A:584:LYS:HE2	2.19	0.43
1:B:188:THR:OG1	1:B:191:SER:O	2.20	0.42
1:B:425:VAL:HG12	1:B:429:MET:HE3	2.02	0.42
1:A:516:ASN:O	1:A:519:ASN:HB2	2.19	0.42
1:B:8:CYS:SG	1:B:10:SER:HB2	2.60	0.42
1:A:279:THR:HB	1:A:429:MET:HE2	2.02	0.42
1:A:284:PRO:HA	3:A:705:PO4:O1	2.20	0.41
1:A:486:SER:HB3	1:A:517:SER:HG	1.84	0.41
1:A:344:ASP:CG	1:A:344:ASP:O	2.63	0.41
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.92	0.41
1:B:21:ARG:HA	1:B:21:ARG:HD2	1.69	0.41
1:B:158:LEU:HD23	1:B:164:HIS:NE2	2.34	0.41
1:B:284:PRO:HA	3:B:705:PO4:O1	2.21	0.41
1:A:60:VAL:HA	1:A:63:LEU:HD12	2.02	0.41
1:A:344:ASP:O	1:A:344:ASP:OD1	2.38	0.41
1:A:184:GLY:O	1:A:195:ILE:HG12	2.20	0.41
1:B:26:CYS:SG	1:B:29:CYS:SG	3.18	0.41
1:A:304:ILE:HD12	1:A:370:ILE:HB	2.03	0.41
1:B:220:ASN:OD1	1:B:220:ASN:N	2.46	0.40
1:A:370:ILE:HG23	1:A:395:HIS:HB2	2.03	0.40
1:A:105:ASP:O	1:A:109:ILE:HD12	2.21	0.40
1:B:162:GLU:HG3	1:B:210:VAL:HG22	2.03	0.40
1:A:243:GLN:HB2	1:A:277:TYR:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	560/603 (93%)	534 (95%)	24 (4%)	2 (0%)	30	32
1	B	581/603 (96%)	560 (96%)	21 (4%)	0	100	100
All	All	1141/1206 (95%)	1094 (96%)	45 (4%)	2 (0%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	SER
1	A	484	VAL

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	483/525 (92%)	476 (99%)	7 (1%)	59	71
1	B	499/525 (95%)	495 (99%)	4 (1%)	73	82
All	All	982/1050 (94%)	971 (99%)	11 (1%)	65	77

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	A	263	SER
1	A	333	ILE
1	A	342	CYS

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Mol	Chain	Res	Type
1	A	458	ASP
1	A	530	THR
1	A	592	ILE
1	B	157	VAL
1	B	258	ILE
1	B	278	SER
1	B	370	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	HIS
1	A	503	ASN
1	B	62	GLN
1	B	245	HIS
1	B	275	GLN
1	B	459	ASN
1	B	562	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
4	MPO	A	706	-	13,13,13	0.19	0	17,17,17	0.39	0
3	PO4	A	705	-	4,4,4	0.96	0	6,6,6	0.51	0
4	MPO	B	706	-	13,13,13	0.24	0	17,17,17	0.42	0
3	PO4	A	704	-	4,4,4	0.97	0	6,6,6	0.45	0
3	PO4	B	704	-	4,4,4	0.95	0	6,6,6	0.49	0
3	PO4	B	705	-	4,4,4	0.98	0	6,6,6	0.47	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	MPO	A	706	-	-	0/7/15/15	0/1/1/1
4	MPO	B	706	-	-	0/7/15/15	0/1/1/1

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	PO4	1	0
4	B	706	MPO	1	0
3	B	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	570/603 (94%)	1.05	108 (18%) 3 3	30, 80, 154, 181	0
1	B	585/603 (97%)	0.42	27 (4%) 37 43	25, 54, 96, 137	2 (0%)
All	All	1155/1206 (95%)	0.73	135 (11%) 9 11	25, 64, 138, 181	2 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	4.8
1	A	167	TRP	4.8
1	A	150	GLY	4.6
1	A	210	VAL	4.4
1	B	157	VAL	4.1
1	A	225	PHE	4.0
1	A	185	TYR	3.9
1	A	224	TYR	3.9
1	A	169	VAL	3.9
1	A	67	GLY	3.9
1	A	149	TYR	3.8
1	A	7	LEU	3.8
1	A	222	GLY	3.8
1	A	155	ARG	3.8
1	A	153	THR	3.8
1	B	164	HIS	3.7
1	A	156	GLU	3.6
1	A	226	VAL	3.6
1	A	252	LEU	3.6
1	A	103	VAL	3.6
1	B	336	ALA	3.6
1	A	184	GLY	3.6
1	A	592	ILE	3.5
1	A	200	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	165	LEU	3.5
1	A	352	LEU	3.5
1	A	163	LEU	3.4
1	A	333	ILE	3.3
1	B	217	TYR	3.3
1	A	227	LEU	3.3
1	A	389	ALA	3.2
1	A	8	CYS	3.2
1	A	182	PHE	3.2
1	A	183	THR	3.2
1	A	228	THR	3.1
1	A	340	VAL	3.0
1	A	344	ASP	3.0
1	A	157	VAL	3.0
1	A	1	ALA	2.9
1	A	223	ASP	2.9
1	A	164	HIS	2.9
1	A	176	LEU	2.9
1	A	249	ILE	2.9
1	A	348	VAL	2.8
1	A	302	ALA	2.8
1	A	336	ALA	2.8
1	A	387	VAL	2.8
1	A	258	ILE	2.8
1	B	158	LEU	2.8
1	B	225	PHE	2.7
1	A	148	SER	2.7
1	A	174	PRO	2.7
1	A	168	GLU	2.7
1	A	230	HIS	2.6
1	A	211	TYR	2.6
1	A	246	TYR	2.6
1	A	202	LYS	2.6
1	B	165	LEU	2.6
1	B	219	LEU	2.6
1	A	209	VAL	2.6
1	B	154	VAL	2.5
1	A	334	ILE	2.5
1	A	220	ASN	2.5
1	A	87	GLY	2.5
1	B	84	CYS	2.5
1	A	34	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	198	TYR	2.5
1	A	240	LEU	2.5
1	A	6	VAL	2.4
1	A	221	VAL	2.4
1	A	371	VAL	2.4
1	B	79	ILE	2.4
1	A	93	TYR	2.4
1	A	178	ARG	2.4
1	B	4	ALA	2.4
1	A	247	VAL	2.4
1	B	193	VAL	2.4
1	A	219	LEU	2.4
1	A	355	TYR	2.4
1	A	66	GLY	2.4
1	A	170	GLY	2.4
1	A	342	CYS	2.4
1	B	81	PHE	2.4
1	B	68	MET	2.4
1	A	175	PRO	2.4
1	A	327	ILE	2.4
1	A	25	LEU	2.4
1	A	426	CYS	2.3
1	A	335	PRO	2.3
1	A	196	GLY	2.3
1	A	245	HIS	2.3
1	A	370	ILE	2.3
1	B	176	LEU	2.3
1	A	273	GLY	2.3
1	B	152	ALA	2.3
1	A	180	TYR	2.3
1	A	299	TYR	2.3
1	B	215	THR	2.3
1	A	79	ILE	2.3
1	A	357	PHE	2.2
1	A	179	ASN	2.2
1	A	81	PHE	2.2
1	A	231	THR	2.2
1	A	253	TYR	2.2
1	B	340	VAL	2.2
1	A	84	CYS	2.2
1	A	194	GLN	2.2
1	A	216	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	52	ALA	2.2
1	A	158	LEU	2.2
1	A	256	LEU	2.2
1	A	172	PRO	2.2
1	A	337	ARG	2.1
1	A	14	LEU	2.1
1	A	195	ILE	2.1
1	A	317	LEU	2.1
1	B	203	GLY	2.1
1	A	351	THR	2.1
1	A	298	TYR	2.1
1	A	20	ILE	2.1
1	A	130	LEU	2.1
1	A	295	LEU	2.1
1	A	297	LEU	2.1
1	A	29	CYS	2.1
1	B	214	THR	2.1
1	B	151	ILE	2.1
1	B	216	THR	2.1
1	A	395	HIS	2.1
1	B	35	ILE	2.1
1	A	181	VAL	2.1
1	A	232	VAL	2.1
1	B	5	CYS	2.0
1	A	364	PRO	2.0
1	A	237	ALA	2.0
1	B	9	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
4	MPO	A	706	13/13	0.87	0.14	58,70,79,82	13
4	MPO	B	706	13/13	0.93	0.11	52,60,66,68	13
3	PO4	A	705	5/5	0.97	0.06	39,47,49,56	0
3	PO4	B	704	5/5	0.97	0.06	40,46,52,54	0
3	PO4	B	705	5/5	0.97	0.06	45,45,49,51	0
2	ZN	B	702	1/1	0.97	0.04	70,70,70,70	0
3	PO4	A	704	5/5	0.97	0.06	43,46,49,52	0
2	ZN	A	703	1/1	0.98	0.06	110,110,110,110	0
2	ZN	A	702	1/1	0.98	0.04	66,66,66,66	0
2	ZN	B	703	1/1	0.98	0.05	76,76,76,76	0
2	ZN	A	701	1/1	0.99	0.03	64,64,64,64	0
2	ZN	B	701	1/1	1.00	0.04	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.