



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:21 pm BST

PDB ID : 1Q8Z
Title : The apoenzyme structure of the yeast SR protein kinase, Sky1p
Authors : Nolen, B.; Ngo, J.; Chakrabarti, S.; Vu, D.; Adams, J.A.; Ghosh, G.
Deposited on : 2003-08-22
Resolution : 2.35 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 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 : 2.11
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) : 2.11

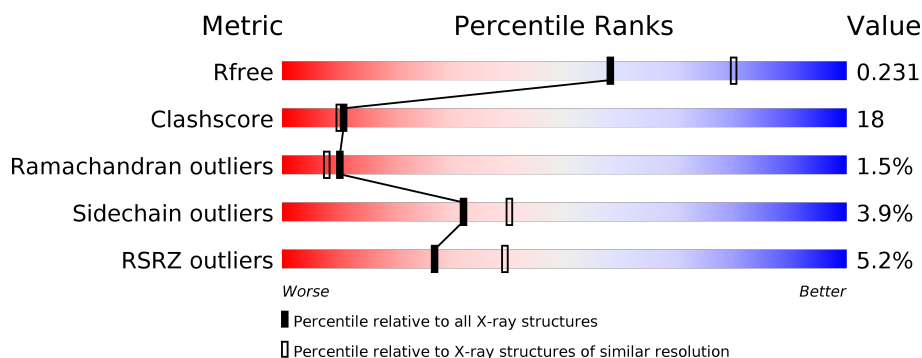
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on 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	373	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>30%</div> <div>• 5%</div> </div> </div>
1	B	373	<div> <div>6%</div> <div> <div></div> <div>62%</div> <div>32%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5943 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.

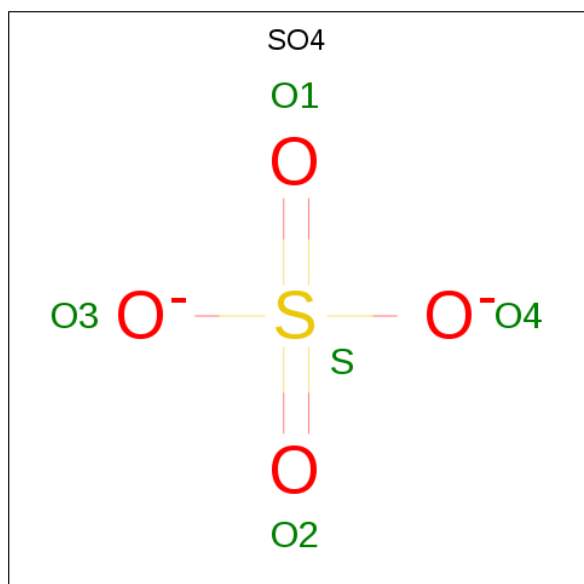
- Molecule 1 is a protein called SR Protein Kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2855	1835	486	522	12			
1	B	364	Total	C	N	O	S	0	0	0
			2933	1880	500	541	12			

There are 4 discrepancies between the modelled and reference sequences:

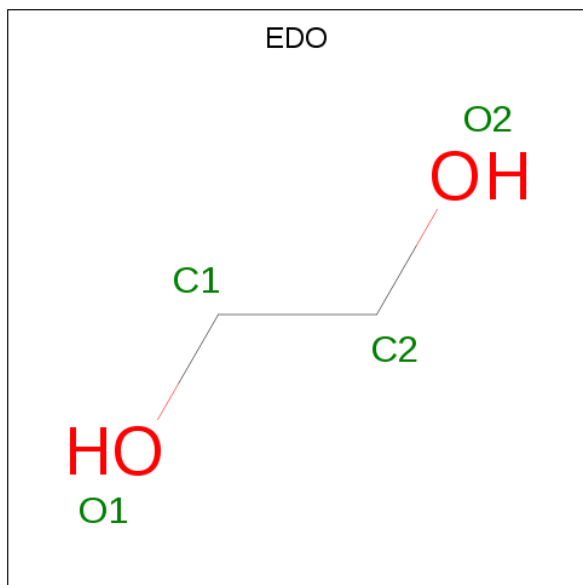
Chain	Residue	Modelled	Actual	Comment	Reference
A	305	VAL	-	SEE REMARK 999	UNP Q03656
A	306	ASP	-	SEE REMARK 999	UNP Q03656
B	305	VAL	-	SEE REMARK 999	UNP Q03656
B	306	ASP	-	SEE REMARK 999	UNP Q03656

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



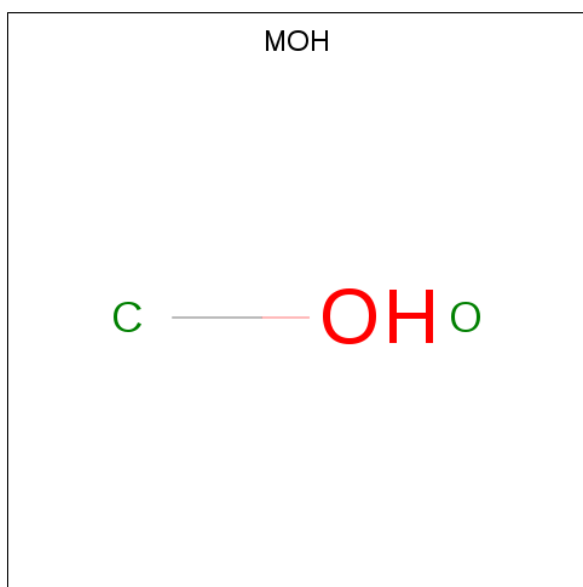
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is METHANOL (three-letter code: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			2	1	1		
4	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	70	Total	O	0	0
			70	70		
5	B	63	Total	O	0	0
			63	63		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.99 Å 88.70 Å 135.60 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 49.68 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.6 (20.00-2.35) 83.5 (49.68-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.34 Å)	Xtriage
Refinement program	CNS 1.0, XTALVIEW	Depositor
R, R_{free}	0.221 , 0.259 0.230 , 0.231	Depositor DCC
R_{free} test set	1551 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5943	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 82.25 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9174e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MOH, SO4, EDO

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	0.39	0/2923	0.60	0/3955
1	B	0.37	0/3005	0.60	0/4068
All	All	0.38	0/5928	0.60	0/8023

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	2855	0	2818	106	0
1	B	2933	0	2895	106	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	70	0	0	7	0
5	B	63	0	0	4	0
All	All	5943	0	5725	210	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 18.

All (210) 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:249:LEU:HD11	1:B:547:LYS:HD2	1.44	0.99
1:A:655:LYS:HD3	1:A:657:LYS:HE3	1.53	0.88
1:A:623:ILE:CD1	1:A:629:LEU:HD13	2.10	0.80
1:A:144:TYR:HB2	1:A:190:ARG:HG3	1.63	0.79
1:A:249:LEU:HD22	1:A:547:LYS:HD2	1.66	0.77
1:B:297:PRO:HD3	1:B:593:LEU:HD13	1.65	0.77
1:A:297:PRO:HD3	1:A:593:LEU:HD13	1.68	0.76
1:A:562:THR:HG22	1:A:564:SER:H	1.50	0.76
1:A:272:GLN:HE22	1:A:543:LEU:HA	1.51	0.75
1:B:306:ASP:OD2	1:B:540:PRO:HD2	1.87	0.75
1:A:568:ARG:HH12	1:A:614:LYS:CB	2.00	0.74
1:A:623:ILE:HD13	1:A:629:LEU:HD13	1.69	0.74
1:B:565:ILE:HG13	1:B:566:GLN:HG3	1.69	0.73
1:B:641:ARG:HE	1:B:641:ARG:HA	1.54	0.73
1:B:180:ASN:O	1:B:182:THR:HG23	1.89	0.72
1:A:176:LYS:HD3	1:A:178:MET:HE1	1.71	0.71
1:A:249:LEU:CD2	1:A:547:LYS:HD2	2.21	0.71
1:A:249:LEU:HD23	1:A:301:LEU:HB2	1.73	0.71
1:A:624:GLU:HG3	1:A:657:LYS:O	1.90	0.71
1:B:302:MET:HB3	1:B:546:ILE:HG22	1.73	0.70
1:A:249:LEU:HG	1:A:303:GLU:OE2	1.91	0.70
1:B:170:SER:OG	1:B:187:LYS:HG3	1.93	0.69
1:B:272:GLN:HE22	1:B:543:LEU:HA	1.56	0.69
1:A:180:ASN:O	1:A:182:THR:HG23	1.93	0.68
1:A:203:ILE:O	1:A:207:GLN:HG3	1.94	0.68
1:B:641:ARG:NE	1:B:641:ARG:HA	2.08	0.68
1:A:302:MET:HB2	1:A:546:ILE:HG22	1.75	0.67
1:B:238:ASN:H	1:B:238:ASN:ND2	1.93	0.66
1:B:216:LYS:HB2	1:B:216:LYS:NZ	2.09	0.66
1:B:696:ASP:O	1:B:700:LEU:HD12	1.96	0.66
1:B:169:PHE:HB3	1:B:195:TYR:CD2	2.31	0.65
1:B:660:PRO:O	1:B:664:VAL:HG23	1.95	0.65
1:A:252:ASN:OD1	1:A:254:LEU:HB2	1.98	0.64
1:B:169:PHE:HB3	1:B:195:TYR:HD2	1.62	0.64
1:B:630:PRO:HD2	1:B:633:LEU:HD12	1.79	0.64
1:A:542:ASN:HA	5:A:57:HOH:O	1.98	0.64
1:B:272:GLN:HE22	1:B:544:ILE:H	1.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLN:NE2	1:B:544:ILE:H	1.97	0.63
1:A:623:ILE:HD11	1:A:629:LEU:HD13	1.80	0.61
1:A:655:LYS:HE2	1:B:659:TRP:CH2	2.36	0.61
1:A:644:PHE:HA	1:A:649:LEU:O	2.01	0.60
1:A:306:ASP:OD2	1:A:540:PRO:HD2	2.02	0.59
1:A:170:SER:OG	1:A:187:LYS:HE3	2.03	0.59
1:A:304:ILE:N	1:A:304:ILE:HD12	2.17	0.59
1:B:572:SER:HB2	1:B:573:PRO:HD2	1.84	0.58
1:A:147:ALA:HB1	1:A:160:LEU:CD1	2.33	0.58
1:A:615:ASP:HB3	1:A:643:PHE:HE2	1.68	0.58
1:B:660:PRO:HD2	1:B:663:ASP:OD2	2.04	0.57
1:A:247:GLU:OE2	1:A:547:LYS:HE3	2.04	0.57
1:A:645:ASN:HD22	1:A:645:ASN:C	2.05	0.57
1:B:286:ARG:HB3	1:B:287:ARG:HE	1.69	0.57
1:B:147:ALA:HB1	1:B:160:LEU:CD1	2.34	0.57
1:A:565:ILE:HG13	1:A:566:GLN:HG3	1.85	0.57
1:B:170:SER:OG	1:B:187:LYS:HE3	2.04	0.57
1:B:216:LYS:HB2	1:B:216:LYS:HZ2	1.69	0.57
1:B:282:ASP:OD1	1:B:286:ARG:HD3	2.05	0.57
1:A:722:LEU:O	1:A:723:TYR:HB2	2.04	0.56
1:B:284:MET:HE2	1:B:290:ILE:HG22	1.87	0.56
1:A:145:HIS:HB2	1:A:241:HIS:NE2	2.20	0.56
1:B:604:PHE:O	1:B:606:PRO:HD3	2.05	0.56
1:A:645:ASN:ND2	1:A:646:SER:N	2.53	0.56
1:B:578:GLY:HA3	1:B:639:TYR:CE1	2.41	0.56
1:B:238:ASN:N	1:B:238:ASN:ND2	2.54	0.55
1:B:663:ASP:HB3	1:B:667:GLU:OE1	2.07	0.55
1:A:568:ARG:HH22	1:A:615:ASP:N	2.04	0.55
1:A:615:ASP:HB3	1:A:643:PHE:CE2	2.41	0.55
1:A:145:HIS:HB2	1:A:241:HIS:CD2	2.42	0.55
1:A:688:GLN:HE21	1:A:690:ASP:H	1.53	0.55
1:A:253:LEU:O	1:A:257:ILE:HG13	2.07	0.54
1:A:663:ASP:O	1:A:667:GLU:HB2	2.07	0.54
1:B:253:LEU:O	1:B:257:ILE:HG13	2.07	0.54
1:B:643:PHE:O	1:B:651:ARG:HG2	2.08	0.54
1:B:702:ASN:OD1	1:B:716:ARG:HB2	2.08	0.54
1:A:287:ARG:HG3	1:A:287:ARG:HH11	1.72	0.54
1:A:562:THR:HG22	1:A:563:ASN:N	2.23	0.54
1:A:170:SER:HB3	1:A:189:VAL:HA	1.91	0.53
1:A:639:TYR:N	1:A:639:TYR:CD1	2.76	0.53
1:B:583:CYS:HB2	1:B:732:TRP:CE3	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:624:GLU:HG2	1:B:657:LYS:O	2.08	0.53
1:A:638:LYS:HB2	1:A:639:TYR:CE1	2.43	0.53
1:A:143:GLY:N	1:A:190:ARG:HH21	2.07	0.53
1:A:638:LYS:HE3	5:A:121:HOH:O	2.07	0.53
1:A:143:GLY:HA3	1:A:166:TRP:HZ3	1.74	0.52
1:B:584:GLY:HA3	5:B:22:HOH:O	2.08	0.52
1:A:144:TYR:HD2	1:A:190:ARG:CG	2.22	0.52
1:B:253:LEU:HD22	1:B:300:VAL:HB	1.91	0.52
1:A:568:ARG:NH2	1:A:615:ASP:HA	2.24	0.52
1:B:285:HIS:HE1	1:B:586:ASP:OD2	1.93	0.52
1:B:203:ILE:O	1:B:207:GLN:HG3	2.10	0.51
1:B:145:HIS:HE1	1:B:151:GLU:OE2	1.94	0.51
1:B:238:ASN:N	1:B:238:ASN:HD22	2.07	0.51
1:A:587:ILE:HG13	1:A:732:TRP:HH2	1.75	0.51
1:B:287:ARG:HH11	1:B:287:ARG:HG3	1.75	0.51
1:B:546:ILE:C	1:B:546:ILE:HD12	2.31	0.51
1:A:297:PRO:HD3	1:A:593:LEU:CD1	2.38	0.51
1:A:254:LEU:O	1:A:258:LYS:HG3	2.10	0.51
1:A:644:PHE:O	1:A:651:ARG:HD2	2.09	0.51
1:B:224:HIS:HD2	1:B:546:ILE:O	1.94	0.51
1:B:292:HIS:C	1:B:293:THR:HG23	2.31	0.50
1:B:651:ARG:NH1	1:B:651:ARG:HB3	2.27	0.50
1:A:702:ASN:OD1	1:A:716:ARG:HB2	2.11	0.50
1:B:541:GLU:O	1:B:542:ASN:HB2	2.12	0.50
1:B:595:PHE:CD1	1:B:603:LEU:HD13	2.46	0.50
1:A:541:GLU:O	1:A:542:ASN:HB2	2.11	0.50
1:B:238:ASN:HD22	1:B:239:GLY:H	1.58	0.50
1:B:615:ASP:HB3	1:B:643:PHE:CE2	2.47	0.49
1:A:660:PRO:O	1:A:664:VAL:HG23	2.13	0.49
1:A:275:LYS:HD2	1:A:706:LEU:HB3	1.94	0.49
1:A:298:GLU:H	1:A:298:GLU:CD	2.16	0.48
1:A:559:GLU:HA	1:A:735:GLU:OE2	2.13	0.48
1:A:569:GLU:HG2	1:A:602:PHE:CE2	2.49	0.48
1:A:645:ASN:O	1:A:646:SER:HB2	2.14	0.48
1:B:623:ILE:HA	1:B:627:GLY:O	2.14	0.48
1:A:297:PRO:CD	1:A:593:LEU:HD13	2.43	0.47
1:B:177:ASP:OD2	1:B:180:ASN:ND2	2.47	0.47
1:A:192:ASP:OD1	1:A:194:VAL:HG23	2.15	0.47
1:A:546:ILE:C	1:A:546:ILE:HD12	2.35	0.47
1:B:578:GLY:HA3	1:B:639:TYR:CD1	2.50	0.47
1:B:254:LEU:O	1:B:258:LYS:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LEU:HD23	1:B:551:LEU:HD12	1.97	0.47
1:A:224:HIS:HD2	1:A:546:ILE:O	1.98	0.46
1:B:284:MET:CE	1:B:290:ILE:HG22	2.46	0.46
1:A:144:TYR:HD2	1:A:190:ARG:HG3	1.80	0.46
1:B:539:SER:HB3	1:B:540:PRO:HD3	1.96	0.46
1:A:655:LYS:HG3	1:B:659:TRP:CZ2	2.51	0.46
1:B:561:TYR:CE1	3:B:1003:EDO:H21	2.51	0.46
1:B:192:ASP:OD2	1:B:194:VAL:HB	2.16	0.46
1:A:696:ASP:CG	1:A:720:ARG:HH21	2.18	0.46
1:B:171:THR:HG23	1:B:188:ILE:HB	1.98	0.45
1:B:692:ARG:HG2	1:B:733:PHE:CG	2.51	0.45
1:B:722:LEU:O	1:B:723:TYR:HB2	2.15	0.45
1:A:292:HIS:C	1:A:293:THR:HG23	2.37	0.45
1:A:578:GLY:HA3	1:A:639:TYR:CE1	2.52	0.45
1:A:660:PRO:HD2	1:A:663:ASP:OD2	2.16	0.45
1:B:256:LEU:HD13	1:B:265:ILE:HD13	1.98	0.45
1:B:688:GLN:HE21	1:B:690:ASP:H	1.65	0.45
1:A:304:ILE:N	1:A:304:ILE:CD1	2.80	0.45
1:A:643:PHE:O	1:A:650:LEU:HA	2.16	0.45
1:B:277:LEU:HD13	1:B:590:THR:HG23	1.98	0.45
1:B:651:ARG:HH11	1:B:651:ARG:CB	2.30	0.45
1:A:250:GLY:HA3	1:A:302:MET:O	2.16	0.45
1:B:561:TYR:CD1	3:B:1003:EDO:H21	2.52	0.44
1:B:256:LEU:HD22	1:B:265:ILE:CD1	2.48	0.44
1:A:285:HIS:HD2	5:A:2:HOH:O	1.99	0.44
1:A:277:LEU:CD1	1:A:590:THR:HG23	2.47	0.44
1:B:606:PRO:HA	1:B:617:ASP:OD2	2.17	0.44
1:A:645:ASN:ND2	1:A:645:ASN:C	2.70	0.44
1:B:268:ILE:HG23	5:B:35:HOH:O	2.16	0.44
1:A:579:ALA:HB1	1:A:580:PRO:HD2	2.00	0.44
1:B:287:ARG:NH1	1:B:287:ARG:HG3	2.33	0.44
1:B:145:HIS:HB2	1:B:241:HIS:NE2	2.33	0.44
1:A:170:SER:HB2	1:A:188:ILE:O	2.18	0.44
1:A:287:ARG:HG3	1:A:287:ARG:NH1	2.32	0.44
1:B:272:GLN:HE22	1:B:544:ILE:N	2.15	0.43
1:B:287:ARG:NE	1:B:287:ARG:N	2.66	0.43
1:A:684:SER:HB2	1:A:685:PRO:HD3	2.00	0.43
1:B:157:ARG:HH21	1:B:180:ASN:ND2	2.15	0.43
1:A:645:ASN:HD22	1:A:646:SER:N	2.16	0.43
1:B:712:MET:HA	1:B:715:ILE:HD12	2.00	0.43
1:B:731:GLY:HA2	1:B:734:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:O	1:B:546:ILE:HA	2.18	0.43
1:A:282:ASP:OD1	1:A:286:ARG:HD3	2.18	0.43
1:A:569:GLU:H	1:A:569:GLU:CD	2.22	0.43
1:B:645:ASN:HA	1:B:651:ARG:NH2	2.33	0.43
1:A:238:ASN:ND2	1:A:238:ASN:H	2.17	0.43
1:B:147:ALA:HA	1:B:151:GLU:OE1	2.19	0.43
1:A:272:GLN:NE2	1:A:544:ILE:H	2.17	0.43
1:A:268:ILE:HG23	5:A:26:HOH:O	2.19	0.42
1:A:555:CYS:HB2	1:A:559:GLU:O	2.19	0.42
1:A:695:ALA:HB1	5:A:95:HOH:O	2.18	0.42
1:B:287:ARG:NE	1:B:287:ARG:CA	2.81	0.42
1:A:569:GLU:HG2	1:A:602:PHE:CD2	2.53	0.42
1:B:546:ILE:O	1:B:546:ILE:HD12	2.19	0.42
1:A:287:ARG:HA	1:A:287:ARG:CZ	2.49	0.42
1:A:249:LEU:HD11	1:A:303:GLU:OE1	2.19	0.42
1:A:166:TRP:CZ3	1:A:171:THR:HG22	2.54	0.42
1:B:696:ASP:HA	1:B:732:TRP:CH2	2.54	0.42
1:A:145:HIS:CE1	1:A:234:HIS:HE1	2.38	0.42
1:B:145:HIS:HB2	1:B:241:HIS:CD2	2.55	0.42
1:A:576:LEU:HD11	1:A:618:HIS:CD2	2.55	0.42
1:A:696:ASP:HB2	5:A:23:HOH:O	2.19	0.42
1:B:298:GLU:N	1:B:298:GLU:OE1	2.48	0.42
1:A:198:ALA:O	1:A:201:ASP:HB2	2.20	0.41
1:A:568:ARG:HB2	5:A:68:HOH:O	2.20	0.41
1:B:230:ASP:OD1	1:B:231:HIS:N	2.51	0.41
1:B:249:LEU:HD12	1:B:301:LEU:HD12	2.02	0.41
1:B:249:LEU:O	1:B:250:GLY:O	2.38	0.41
1:B:650:LEU:HD23	1:B:653:ILE:HB	2.02	0.41
1:B:247:GLU:OE2	1:B:547:LYS:HE3	2.19	0.41
1:B:651:ARG:NH1	1:B:651:ARG:CB	2.83	0.41
1:A:249:LEU:HD23	1:A:301:LEU:CB	2.46	0.41
1:B:555:CYS:HB2	1:B:559:GLU:O	2.20	0.41
1:B:574:GLU:HG2	1:B:691:PRO:HG3	2.02	0.41
1:B:726:GLY:HA3	1:B:732:TRP:CE2	2.55	0.41
1:B:286:ARG:HD2	1:B:720:ARG:HD3	2.03	0.41
1:B:560:HIS:HE1	5:B:92:HOH:O	2.04	0.41
1:B:215:THR:O	1:B:218:ASP:HB2	2.21	0.41
1:B:250:GLY:HA3	1:B:302:MET:O	2.20	0.41
1:A:144:TYR:CD2	1:A:190:ARG:HG3	2.55	0.41
1:B:649:LEU:N	1:B:649:LEU:HD12	2.36	0.41
1:A:192:ASP:HB3	1:A:195:TYR:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:ARG:CD	1:B:737:ARG:H	2.34	0.40
1:A:615:ASP:O	1:A:619:ILE:HG13	2.21	0.40
1:B:296:LYS:HE2	1:B:299:ASN:ND2	2.35	0.40
1:A:196:THR:O	1:A:200:GLU:HG2	2.22	0.40
1:B:151:GLU:OE2	1:B:234:HIS:HE1	2.04	0.40
1:A:274:SER:O	1:A:278:LEU:HG	2.22	0.40
1:A:298:GLU:CD	1:A:298:GLU:N	2.75	0.40
1:A:630:PRO:HD2	1:A:633:LEU:HD12	2.03	0.40
1:B:568:ARG:HD2	5:B:27:HOH:O	2.20	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	348/373 (93%)	316 (91%)	27 (8%)	5 (1%)	11	9
1	B	362/373 (97%)	332 (92%)	24 (7%)	6 (2%)	9	7
All	All	710/746 (95%)	648 (91%)	51 (7%)	11 (2%)	10	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	TYR
1	A	250	GLY
1	A	262	HIS
1	B	250	GLY
1	B	261	GLU
1	B	568	ARG
1	B	566	GLN
1	B	654	SER
1	A	651	ARG

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Mol	Chain	Res	Type
1	B	192	ASP
1	A	652	ASN

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	306/327 (94%)	297 (97%)	9 (3%)	42	52
1	B	316/327 (97%)	301 (95%)	15 (5%)	26	31
All	All	622/654 (95%)	598 (96%)	24 (4%)	32	40

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	TYR
1	A	238	ASN
1	A	277	LEU
1	A	287	ARG
1	A	568	ARG
1	A	617	ASP
1	A	629	LEU
1	A	639	TYR
1	A	645	ASN
1	B	169	PHE
1	B	171	THR
1	B	208	ARG
1	B	238	ASN
1	B	256	LEU
1	B	277	LEU
1	B	287	ARG
1	B	293	THR
1	B	303	GLU
1	B	560	HIS
1	B	608	GLU
1	B	618	HIS

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Mol	Chain	Res	Type
1	B	641	ARG
1	B	714	GLU
1	B	737	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	HIS
1	A	224	HIS
1	A	234	HIS
1	A	238	ASN
1	A	272	GLN
1	A	285	HIS
1	A	618	HIS
1	A	645	ASN
1	A	688	GLN
1	B	145	HIS
1	B	168	HIS
1	B	180	ASN
1	B	224	HIS
1	B	234	HIS
1	B	238	ASN
1	B	272	GLN
1	B	285	HIS
1	B	560	HIS
1	B	621	GLN
1	B	636	ASN
1	B	688	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

6 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
2	SO4	A	801	-	4,4,4	0.31	0	6,6,6	0.10	0
3	EDO	B	1003	-	3,3,3	1.07	0	2,2,2	0.46	0
4	MOH	B	2389	4	1,1,1	0.46	0	-		
2	SO4	B	802	-	4,4,4	0.30	0	6,6,6	0.11	0
3	EDO	A	1000	-	3,3,3	0.96	0	2,2,2	0.49	0
4	MOH	A	2390	4	1,1,1	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
3	EDO	B	1003	-	-	1/1/1/1	-
3	EDO	A	1000	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1003	EDO	O1-C1-C2-O2
3	A	1000	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	EDO	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	354/373 (94%)	0.15	16 (4%) 33 46	18, 34, 60, 80	0
1	B	364/373 (97%)	0.24	21 (5%) 23 33	17, 34, 64, 76	0
All	All	718/746 (96%)	0.20	37 (5%) 27 39	17, 34, 62, 80	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	648	GLY	6.4
1	A	641	ARG	6.1
1	B	609	GLY	4.9
1	B	649	LEU	4.7
1	B	610	HIS	4.3
1	B	646	SER	4.2
1	B	611	SER	4.1
1	B	641	ARG	3.8
1	A	613	THR	3.6
1	B	577	LEU	3.4
1	A	262	HIS	3.2
1	B	607	ASP	3.2
1	A	654	SER	3.0
1	B	633	LEU	3.0
1	A	658	PHE	3.0
1	B	654	SER	2.9
1	A	645	ASN	2.9
1	A	144	TYR	2.8
1	A	644	PHE	2.8
1	B	613	THR	2.8
1	A	651	ARG	2.8
1	B	263	ARG	2.8
1	B	644	PHE	2.7
1	B	737	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	612	TYR	2.7
1	B	645	ASN	2.7
1	B	262	HIS	2.6
1	B	647	ARG	2.5
1	A	575	VAL	2.5
1	B	634	LEU	2.5
1	A	249	LEU	2.4
1	A	143	GLY	2.2
1	A	263	ARG	2.2
1	A	653	ILE	2.2
1	B	608	GLU	2.2
1	A	646	SER	2.1
1	A	737	ARG	2.1

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 carbohydrates 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
4	MOH	B	2389	2/2	0.76	0.17	51,51,51,52	0
3	EDO	A	1000	4/4	0.84	0.25	34,34,35,37	0
2	SO4	B	802	5/5	0.88	0.18	81,81,82,83	0
4	MOH	A	2390	2/2	0.88	0.12	45,45,45,47	0
3	EDO	B	1003	4/4	0.91	0.18	37,38,38,38	0
2	SO4	A	801	5/5	0.97	0.10	57,58,59,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.