



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 05:18 AM EDT

PDB ID : 7A0M
Title : TSC1 N-terminal domain
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Deposited on : 2020-08-10
Resolution : 2.32 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	:	2.37.1
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)	:	2.37.1

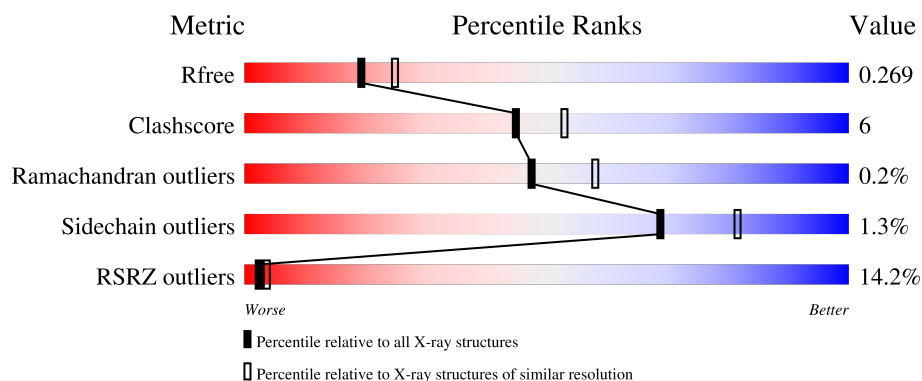
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	417	<div> <div>7%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>14%</div> </div> </div>
1	B	417	<div> <div>16%</div> <div> <div></div> <div>70%</div> <div>17%</div> <div>13%</div> </div> </div>
1	C	417	<div> <div>10%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>12%</div> </div> </div>
1	D	417	<div> <div>15%</div> <div> <div></div> <div>71%</div> <div>13%</div> <div>15%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11857 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 TSC1 N-terminal domain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	Se	0	0	0
			2923	1898	489	529	2	5			
1	B	364	Total	C	N	O	S	Se	0	0	0
			2976	1934	497	538	2	5			
1	C	368	Total	C	N	O	S	Se	0	0	0
			3001	1949	501	544	2	5			
1	D	355	Total	C	N	O	S	Se	0	0	0
			2918	1903	483	525	2	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP G0S5K3
A	0	SER	-	expression tag	UNP G0S5K3
B	-1	GLY	-	expression tag	UNP G0S5K3
B	0	SER	-	expression tag	UNP G0S5K3
C	-1	GLY	-	expression tag	UNP G0S5K3
C	0	SER	-	expression tag	UNP G0S5K3
D	-1	GLY	-	expression tag	UNP G0S5K3
D	0	SER	-	expression tag	UNP G0S5K3

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

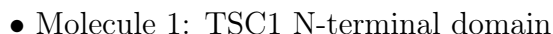
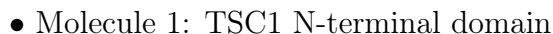


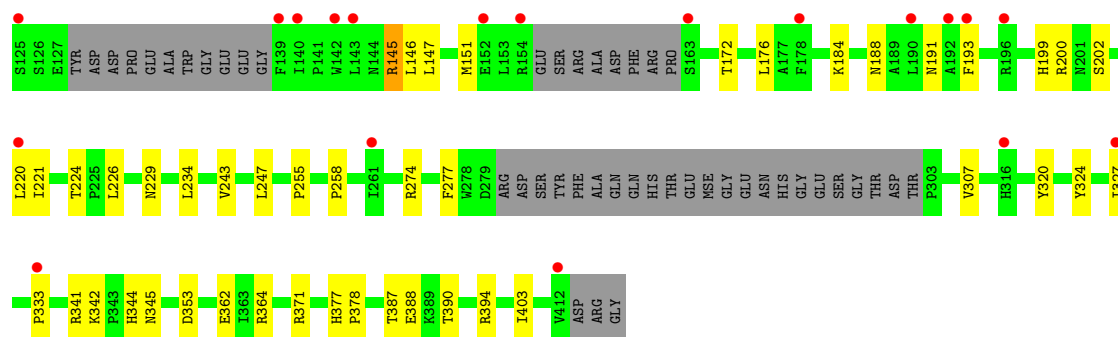
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

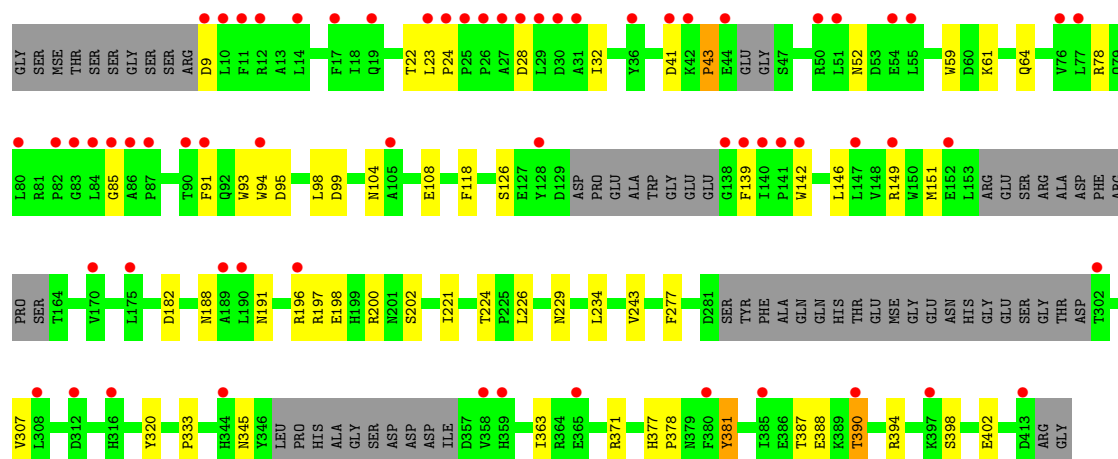
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	8	Total	O	0	0
			8	8		
3	C	6	Total	O	0	0
			6	6		
3	D	6	Total	O	0	0
			6	6		

- Molecule 1: TSC1 N-terminal domain





• Molecule 1: TSC1 N-terminal domain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.09Å 150.74Å 111.88Å 90.00° 108.47° 90.00°	Depositor
Resolution (Å)	44.90 – 2.32 44.90 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.90-2.32) 99.2 (44.90-2.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.32Å)	Xtriage
Refinement program	PHENIX (1.12rc1_2807: ???)	Depositor
R, R_{free}	0.240 , 0.270 0.240 , 0.269	Depositor DCC
R_{free} test set	2098 reflections (2.21%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.3	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	0.93	EDS
Total number of atoms	11857	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.76% 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: 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	0.24	0/2996	0.41	0/4065
1	B	0.25	0/3055	0.42	0/4150
1	C	0.25	0/3080	0.41	0/4184
1	D	0.26	0/2994	0.41	0/4067
All	All	0.25	0/12125	0.41	0/16466

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	23	LEU	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	2923	0	2891	34	0
1	B	2976	0	2930	46	0
1	C	3001	0	2959	38	0
1	D	2918	0	2876	43	0
2	B	5	0	0	0	0
3	A	14	0	0	0	0
3	B	8	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	0	0
All	All	11857	0	11656	152	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 (152) 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:D:387:THR:HA	1:D:390:THR:HG22	1.60	0.84
1:B:64:GLN:O	1:B:70:TYR:OH	2.00	0.79
1:D:388:GLU:O	1:D:394:ARG:NH2	2.15	0.79
1:C:49:ASP:OD1	1:C:89:ARG:NH2	2.23	0.72
1:A:4:SER:O	1:A:39:ARG:NH1	2.24	0.71
1:D:59:TRP:NE1	1:D:64:GLN:OE1	2.23	0.71
1:D:91:PHE:HB3	1:D:142:TRP:HZ2	1.56	0.71
1:B:77:LEU:HD21	1:B:93:TRP:HB3	1.73	0.70
1:C:151:MSE:HE2	1:C:199:HIS:HB3	1.76	0.67
1:D:196:ARG:NH1	1:D:198:GLU:OE2	2.28	0.67
1:A:197:ARG:NH1	1:A:305:ASP:OD1	2.29	0.64
1:D:91:PHE:O	1:D:142:TRP:HH2	1.81	0.64
1:D:197:ARG:HG3	1:D:307:VAL:HG22	1.79	0.63
1:D:224:THR:HG23	1:D:226:LEU:H	1.63	0.63
1:B:388:GLU:O	1:B:394:ARG:NH2	2.31	0.63
1:C:224:THR:HG23	1:C:226:LEU:H	1.64	0.63
1:D:43:PRO:HB2	1:D:85:GLY:HA2	1.81	0.62
1:C:258:PRO:HG3	1:C:403:ILE:HD13	1.81	0.61
1:A:381:TYR:O	1:B:364:ARG:HD3	2.01	0.60
1:C:255:PRO:HD3	1:C:327:ILE:HD11	1.84	0.60
1:B:197:ARG:HG3	1:B:307:VAL:HG22	1.81	0.60
1:A:5:GLY:HA3	1:A:39:ARG:HD3	1.85	0.59
1:D:94:TRP:HH2	1:D:146:LEU:HD21	1.68	0.59
1:D:151:MSE:HE1	1:D:202:SER:HB2	1.84	0.59
1:B:224:THR:HG23	1:B:226:LEU:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ASN:OD1	1:C:224:THR:OG1	2.21	0.58
1:D:9:ASP:OD1	1:D:9:ASP:N	2.35	0.58
1:C:147:LEU:O	1:C:151:MSE:HG2	2.04	0.58
1:A:94:TRP:CD2	1:A:142:TRP:HZ3	2.23	0.57
1:B:59:TRP:HA	1:B:63:VAL:HB	1.87	0.57
1:A:91:PHE:HD1	1:A:142:TRP:CE2	2.23	0.56
1:C:333:PRO:HG3	1:C:377:HIS:CG	2.39	0.56
1:B:36:TYR:O	1:B:40:HIS:ND1	2.35	0.56
1:B:344:HIS:O	1:D:390:THR:HG21	2.06	0.56
1:B:23:LEU:HB2	1:B:24:PRO:HD3	1.87	0.55
1:D:23:LEU:HB2	1:D:24:PRO:HD3	1.88	0.55
1:B:258:PRO:HG3	1:B:403:ILE:HD13	1.88	0.55
1:C:77:LEU:HD21	1:C:93:TRP:HB3	1.89	0.55
1:A:379:ASN:HD21	1:A:394:ARG:NH1	2.05	0.55
1:A:94:TRP:CG	1:A:142:TRP:HZ3	2.24	0.55
1:B:52:ASN:HD22	1:B:93:TRP:HE1	1.53	0.55
1:B:333:PRO:HG3	1:B:377:HIS:CG	2.42	0.54
1:B:99:ASP:OD1	1:B:149:ARG:NE	2.40	0.54
1:A:364:ARG:HD3	1:B:381:TYR:O	2.08	0.53
1:D:95:ASP:HB2	1:D:142:TRP:CH2	2.43	0.53
1:C:20:THR:O	1:C:20:THR:OG1	2.27	0.52
1:B:277:PHE:HZ	1:B:362:GLU:HB3	1.75	0.52
1:A:91:PHE:HD1	1:A:142:TRP:CZ2	2.27	0.52
1:A:145:ARG:HH21	1:A:149:ARG:NH1	2.08	0.52
1:D:22:THR:OG1	1:D:24:PRO:O	2.23	0.51
1:C:277:PHE:HZ	1:C:362:GLU:HB3	1.76	0.51
1:D:94:TRP:CE3	1:D:142:TRP:HZ3	2.29	0.51
1:D:333:PRO:HG3	1:D:377:HIS:CG	2.45	0.51
1:C:191:ASN:OD1	1:C:229:ASN:ND2	2.36	0.51
1:D:94:TRP:CE3	1:D:142:TRP:CZ3	2.99	0.51
1:D:188:ASN:OD1	1:D:224:THR:OG1	2.28	0.51
1:A:91:PHE:HA	1:A:142:TRP:CH2	2.45	0.51
1:A:43:PRO:HB2	1:A:85:GLY:HA2	1.93	0.50
1:B:10:LEU:HD22	1:B:36:TYR:CG	2.46	0.50
1:D:94:TRP:CZ3	1:D:98:LEU:HD22	2.45	0.50
1:B:59:TRP:CD1	1:B:96:LYS:HE3	2.47	0.50
1:D:28:ASP:O	1:D:32:ILE:HG13	2.12	0.50
1:D:41:ASP:O	1:D:43:PRO:HD3	2.11	0.50
1:A:333:PRO:HG3	1:A:377:HIS:CG	2.46	0.50
1:D:94:TRP:HZ3	1:D:98:LEU:HD22	1.76	0.49
1:C:151:MSE:HE1	1:C:202:SER:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:ARG:HB2	1:D:381:TYR:HA	1.94	0.49
1:C:184:LYS:HB2	1:C:220:LEU:HD13	1.94	0.49
1:A:357:ASP:CG	1:A:358:VAL:H	2.16	0.49
1:C:151:MSE:HG3	1:C:193:PHE:CD1	2.48	0.49
1:D:104:ASN:HB3	1:D:108:GLU:HG2	1.95	0.49
1:D:221:ILE:O	1:D:224:THR:HG22	2.13	0.48
1:A:234:LEU:HD23	1:A:243:VAL:HG13	1.95	0.48
1:D:91:PHE:O	1:D:142:TRP:CH2	2.65	0.48
1:A:196:ARG:NH1	1:A:198:GLU:OE2	2.43	0.48
1:D:234:LEU:HD23	1:D:243:VAL:HG13	1.96	0.48
1:C:200:ARG:NH1	1:C:307:VAL:HG23	2.28	0.48
1:C:234:LEU:O	1:C:274:ARG:NH1	2.42	0.48
1:C:378:PRO:HG3	1:D:371:ARG:CZ	2.44	0.48
1:B:17:PHE:CD1	1:B:29:LEU:HD11	2.49	0.48
1:C:56:LEU:HD12	1:C:93:TRP:CZ2	2.49	0.48
1:B:19:GLN:HG3	1:B:20:THR:HG23	1.96	0.47
1:B:148:VAL:O	1:B:152:GLU:HG3	2.15	0.47
1:A:26:PRO:HB2	1:A:28:ASP:OD1	2.14	0.47
1:B:51:LEU:HD11	1:B:80:LEU:HD13	1.96	0.47
1:B:59:TRP:O	1:B:64:GLN:N	2.46	0.47
1:D:99:ASP:OD1	1:D:149:ARG:NE	2.48	0.46
1:A:371:ARG:CZ	1:B:378:PRO:HG3	2.45	0.46
1:B:10:LEU:HD11	1:B:33:ILE:HG12	1.96	0.46
1:C:95:ASP:OD1	1:C:145:ARG:NH2	2.48	0.46
1:B:19:GLN:C	1:B:21:PRO:HD3	2.35	0.46
1:A:234:LEU:O	1:A:274:ARG:NH1	2.41	0.46
1:B:26:PRO:HD2	1:B:29:LEU:CD1	2.46	0.46
1:B:42:LYS:HD3	1:B:45:GLU:CD	2.36	0.46
1:A:145:ARG:HA	1:A:149:ARG:HH21	1.81	0.46
1:A:25:PRO:HB3	1:A:29:LEU:HD23	1.98	0.45
1:B:221:ILE:O	1:B:224:THR:HG22	2.15	0.45
1:B:234:LEU:HD23	1:B:243:VAL:HG13	1.99	0.45
1:C:42:LYS:HD3	1:C:45:GLU:CD	2.37	0.45
1:B:143:LEU:HD13	1:B:186:PHE:HA	1.99	0.45
1:D:52:ASN:ND2	1:D:93:TRP:HE1	2.15	0.45
1:A:11:PHE:CD1	1:A:54:GLU:HG2	2.52	0.45
1:D:191:ASN:OD1	1:D:229:ASN:ND2	2.38	0.45
1:D:200:ARG:NH1	1:D:307:VAL:HG23	2.32	0.45
1:B:123:LEU:HD21	1:B:178:PHE:CE1	2.52	0.44
1:C:101:VAL:HG22	1:C:111:LEU:HD11	2.00	0.44
1:B:10:LEU:O	1:B:14:LEU:HG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LYS:HD3	1:C:345:ASN:ND2	2.33	0.44
1:D:277:PHE:HE1	1:D:363:ILE:HG12	1.82	0.44
1:B:13:ALA:HB1	1:B:29:LEU:HD23	2.00	0.44
1:A:224:THR:CG2	1:A:226:LEU:H	2.31	0.43
1:C:94:TRP:HH2	1:C:146:LEU:HD21	1.83	0.43
1:A:28:ASP:O	1:A:32:ILE:HG12	2.19	0.43
1:D:94:TRP:CH2	1:D:98:LEU:HD13	2.53	0.43
1:B:18:ILE:O	1:B:69:LYS:HD3	2.18	0.43
1:B:196:ARG:NH1	1:B:196:ARG:HA	2.34	0.43
1:A:57:ALA:O	1:A:61:LYS:HG2	2.19	0.43
1:A:277:PHE:HE1	1:A:363:ILE:HG12	1.83	0.43
1:B:59:TRP:NE1	1:B:96:LYS:HE3	2.34	0.43
1:B:78:ARG:HG2	1:B:118:PHE:CD1	2.54	0.43
1:C:247:LEU:HD11	1:C:324:TYR:CG	2.53	0.43
1:C:221:ILE:O	1:C:224:THR:HG22	2.19	0.43
1:C:364:ARG:HD3	1:D:381:TYR:O	2.19	0.42
1:C:234:LEU:HD23	1:C:243:VAL:HG13	2.01	0.42
1:C:387:THR:HA	1:C:390:THR:HB	2.01	0.42
1:A:10:LEU:O	1:A:14:LEU:HG	2.19	0.42
1:A:59:TRP:CD1	1:A:96:LYS:HE3	2.55	0.42
1:A:390:THR:HG21	1:C:344:HIS:O	2.19	0.42
1:C:388:GLU:O	1:C:394:ARG:NH2	2.44	0.42
1:A:84:LEU:HD12	1:A:90:THR:HG22	2.02	0.42
1:B:232:GLN:HE21	1:B:232:GLN:HB2	1.64	0.42
1:C:371:ARG:NH1	1:D:378:PRO:HD3	2.35	0.42
1:B:66:HIS:HB3	1:B:69:LYS:HE2	2.00	0.42
1:B:95:ASP:OD1	1:B:145:ARG:NE	2.50	0.42
1:D:94:TRP:CH2	1:D:146:LEU:HD21	2.52	0.42
1:A:11:PHE:O	1:A:15:ASN:ND2	2.51	0.42
1:B:13:ALA:HB1	1:B:29:LEU:CD2	2.51	0.41
1:D:139:PHE:HD2	1:D:182:ASP:HB2	1.85	0.41
1:C:353:ASP:OD1	1:C:353:ASP:N	2.54	0.41
1:C:94:TRP:CH2	1:C:146:LEU:HD21	2.55	0.41
1:C:118:PHE:CZ	1:C:122:ILE:HD11	2.55	0.41
1:B:197:ARG:HD3	1:B:306:LYS:O	2.21	0.41
1:C:172:THR:O	1:C:176:LEU:HD13	2.20	0.41
1:D:398:SER:HA	1:D:402:GLU:OE2	2.21	0.41
1:B:379:ASN:HD21	1:B:394:ARG:NH1	2.20	0.40
1:C:10:LEU:HD22	1:C:36:TYR:CG	2.56	0.40
1:D:61:LYS:HA	1:D:61:LYS:HD2	1.79	0.40
1:B:104:ASN:HB3	1:B:108:GLU:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:A:93:TRP:HB3	2.03	0.40
1:A:359:HIS:CE1	1:A:363:ILE:HD11	2.57	0.40
1:D:78:ARG:HG2	1:D:118:PHE:CD1	2.57	0.40
1:B:387:THR:HA	1:B:390:THR:HB	2.03	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	348/417 (84%)	342 (98%)	6 (2%)	0	100	100
1	B	356/417 (85%)	349 (98%)	7 (2%)	0	100	100
1	C	360/417 (86%)	354 (98%)	5 (1%)	1 (0%)	41	50
1	D	343/417 (82%)	334 (97%)	7 (2%)	2 (1%)	25	30
All	All	1407/1668 (84%)	1379 (98%)	25 (2%)	3 (0%)	47	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	126	SER
1	C	23	LEU
1	D	43	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	318/359 (89%)	313 (98%)	5 (2%)	62	77
1	B	323/359 (90%)	318 (98%)	5 (2%)	65	79
1	C	327/359 (91%)	324 (99%)	3 (1%)	78	89
1	D	317/359 (88%)	313 (99%)	4 (1%)	69	81
All	All	1285/1436 (90%)	1268 (99%)	17 (1%)	69	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	149	ARG
1	A	224	THR
1	A	320	TYR
1	A	382	GLU
1	B	65	ASP
1	B	168	GLU
1	B	196	ARG
1	B	320	TYR
1	B	355	ASP
1	C	23	LEU
1	C	145	ARG
1	C	320	TYR
1	D	320	TYR
1	D	345	ASN
1	D	381	TYR
1	D	390	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	359	HIS
1	A	379	ASN
1	B	19	GLN
1	B	52	ASN
1	C	52	ASN
1	C	79	GLN
1	D	52	ASN
1	D	79	GLN

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Mol	Chain	Res	Type
1	D	169	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	B	501	-	4,4,4	0.14	0	6,6,6	0.04	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.

No monomer is involved in short contacts.

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	353/417 (84%)	0.75	28 (7%) 12 17	34, 57, 106, 143	0
1	B	359/417 (86%)	1.20	68 (18%) 1 1	37, 67, 133, 156	0
1	C	363/417 (87%)	0.86	42 (11%) 4 7	41, 67, 107, 124	0
1	D	350/417 (83%)	1.20	64 (18%) 1 1	43, 75, 130, 161	0
All	All	1425/1668 (85%)	1.00	202 (14%) 2 4	34, 67, 121, 161	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	LEU	12.2
1	B	29	LEU	9.6
1	B	8	ARG	9.1
1	A	23	LEU	8.9
1	A	142	TRP	8.9
1	B	10	LEU	8.6
1	D	10	LEU	8.4
1	D	11	PHE	8.1
1	D	91	PHE	7.9
1	B	76	VAL	7.8
1	D	142	TRP	7.2
1	C	23	LEU	7.1
1	D	12	ARG	7.0
1	B	106	THR	6.9
1	B	48	GLY	6.9
1	D	26	PRO	6.9
1	B	28	ASP	6.8
1	D	94	TRP	6.1
1	B	14	LEU	6.0
1	B	31	ALA	5.5
1	D	413	ASP	5.5

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Mol	Chain	Res	Type	RSRZ
1	B	23	LEU	5.2
1	B	166	LEU	5.2
1	A	138	GLY	5.2
1	B	26	PRO	5.1
1	D	358	VAL	5.1
1	D	42	LYS	5.0
1	B	84	LEU	4.9
1	D	86	ALA	4.9
1	A	27	ALA	4.9
1	B	413	ASP	4.9
1	A	413	ASP	4.9
1	B	80	LEU	4.9
1	D	27	ALA	4.8
1	D	14	LEU	4.8
1	D	138	GLY	4.6
1	C	142	TRP	4.5
1	D	139	PHE	4.5
1	D	147	LEU	4.5
1	C	84	LEU	4.4
1	A	17	PHE	4.4
1	C	316	HIS	4.3
1	C	36	TYR	4.3
1	B	192	ALA	4.3
1	C	51	LEU	4.2
1	D	189	ALA	4.2
1	B	19	GLN	4.2
1	D	17	PHE	4.2
1	C	192	ALA	4.1
1	B	45	GLU	4.0
1	C	5	GLY	4.0
1	C	154	ARG	3.9
1	D	308	LEU	3.9
1	C	196	ARG	3.9
1	D	87	PRO	3.9
1	A	11	PHE	3.8
1	D	344	HIS	3.8
1	B	33	ILE	3.8
1	B	83	GLY	3.7
1	B	397	LYS	3.7
1	B	105	ALA	3.7
1	B	13	ALA	3.7
1	C	27	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	24	PRO	3.6
1	C	140	ILE	3.6
1	B	55	LEU	3.6
1	C	10	LEU	3.6
1	B	27	ALA	3.5
1	D	312	ASP	3.5
1	C	122	ILE	3.5
1	B	51	LEU	3.5
1	B	57	ALA	3.5
1	B	165	ASP	3.5
1	B	15	ASN	3.5
1	A	10	LEU	3.5
1	B	30	ASP	3.4
1	C	91	PHE	3.4
1	B	68	GLU	3.4
1	C	178	PHE	3.4
1	B	24	PRO	3.4
1	D	85	GLY	3.4
1	D	76	VAL	3.3
1	B	37	LEU	3.3
1	C	143	LEU	3.3
1	A	150	TRP	3.2
1	B	316	HIS	3.2
1	C	89	ARG	3.2
1	C	152	GLU	3.2
1	C	139	PHE	3.2
1	C	24	PRO	3.2
1	B	16	SER	3.1
1	A	14	LEU	3.1
1	A	24	PRO	3.1
1	D	29	LEU	3.1
1	D	19	GLN	3.0
1	A	32	ILE	3.0
1	C	77	LEU	3.0
1	B	313	TYR	3.0
1	D	84	LEU	3.0
1	D	44	GLU	3.0
1	D	302	THR	3.0
1	B	102	LEU	3.0
1	B	277	PHE	2.9
1	D	196	ARG	2.9
1	B	85	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	18	ILE	2.9
1	A	39	ARG	2.9
1	B	303	PRO	2.9
1	B	381	TYR	2.9
1	C	40	HIS	2.9
1	D	365	GLU	2.9
1	D	90	THR	2.9
1	A	146	LEU	2.9
1	B	36	TYR	2.9
1	B	12	ARG	2.8
1	B	22	THR	2.8
1	D	83	GLY	2.8
1	D	36	TYR	2.8
1	B	6	SER	2.8
1	D	28	ASP	2.7
1	A	85	GLY	2.7
1	A	76	VAL	2.7
1	C	193	PHE	2.7
1	B	58	ILE	2.7
1	D	105	ALA	2.7
1	D	385	ILE	2.7
1	D	359	HIS	2.7
1	B	396	LEU	2.7
1	D	140	ILE	2.6
1	D	55	LEU	2.6
1	D	41	ASP	2.6
1	B	280	ARG	2.6
1	C	412	VAL	2.6
1	D	82	PRO	2.6
1	D	152	GLU	2.6
1	D	390	THR	2.5
1	C	25	PRO	2.5
1	D	80	LEU	2.5
1	B	9	ASP	2.5
1	A	381	TYR	2.5
1	D	149	ARG	2.5
1	B	32	ILE	2.5
1	C	90	THR	2.5
1	C	327	ILE	2.5
1	D	25	PRO	2.5
1	A	358	VAL	2.5
1	D	316	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	190	LEU	2.5
1	D	51	LEU	2.4
1	B	43	PRO	2.4
1	B	139	PHE	2.4
1	B	107	ARG	2.4
1	D	9	ASP	2.4
1	D	31	ALA	2.4
1	B	89	ARG	2.4
1	A	220	LEU	2.4
1	B	167	LYS	2.3
1	C	26	PRO	2.3
1	C	22	THR	2.3
1	C	42	LYS	2.3
1	A	33	ILE	2.3
1	B	221	ILE	2.3
1	D	50	ARG	2.3
1	C	13	ALA	2.3
1	B	11	PHE	2.3
1	C	190	LEU	2.2
1	D	141	PRO	2.2
1	C	261	ILE	2.2
1	C	163	SER	2.2
1	C	88	ALA	2.2
1	D	128	TYR	2.2
1	D	175	LEU	2.2
1	B	44	GLU	2.2
1	B	66	HIS	2.1
1	A	86	ALA	2.1
1	A	16	SER	2.1
1	A	22	THR	2.1
1	A	385	ILE	2.1
1	C	125	SER	2.1
1	C	333	PRO	2.1
1	B	52	ASN	2.1
1	A	5	GLY	2.1
1	D	77	LEU	2.1
1	B	112	ALA	2.1
1	B	138	GLY	2.1
1	C	123	LEU	2.1
1	A	45	GLU	2.1
1	B	113	ARG	2.1
1	A	189	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	163	SER	2.1
1	B	59	TRP	2.1
1	C	29	LEU	2.0
1	B	17	PHE	2.0
1	B	65	ASP	2.0
1	D	380	PHE	2.0
1	D	54	GLU	2.0
1	B	50	ARG	2.0
1	D	170	VAL	2.0
1	D	397	LYS	2.0
1	C	220	LEU	2.0
1	C	6	SER	2.0
1	D	30	ASP	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, 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	SO4	B	501	5/5	0.94	0.22	70,77,82,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.