



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:26 PM UTC

PDB ID : 7A0M / pdb_00007a0m
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	:	4-5-2 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

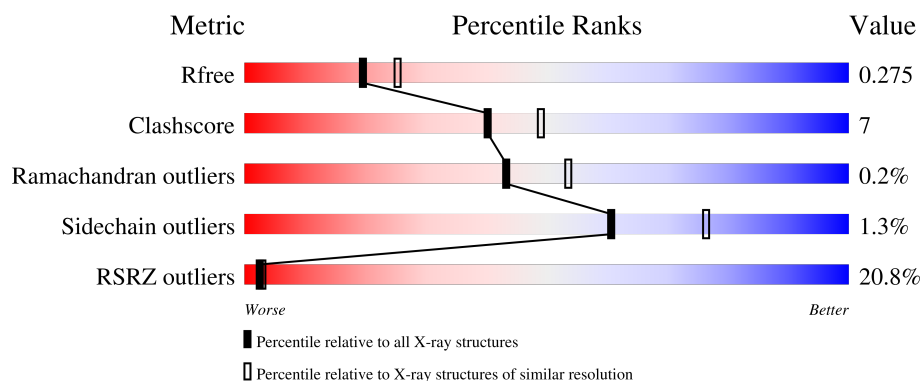
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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	14% 73% 12% • 14%
1	B	417	18% 70% 17% 13%
1	C	417	17% 73% 15% 12%
1	D	417	23% 71% 14% • 15%

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 (CCD ID: SO4) (formula: O₄S).



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

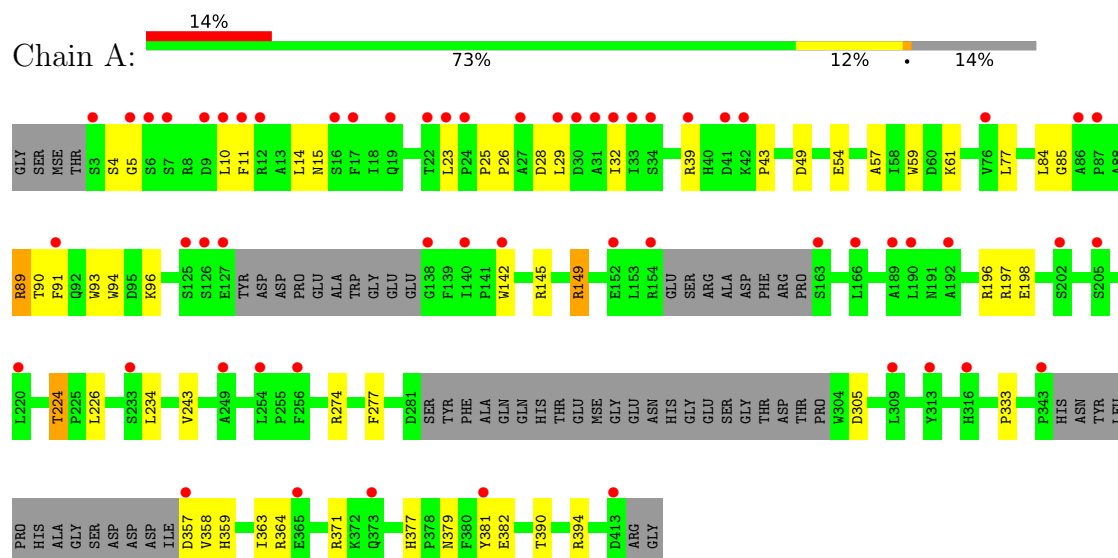
- Molecule 3 is water.

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		

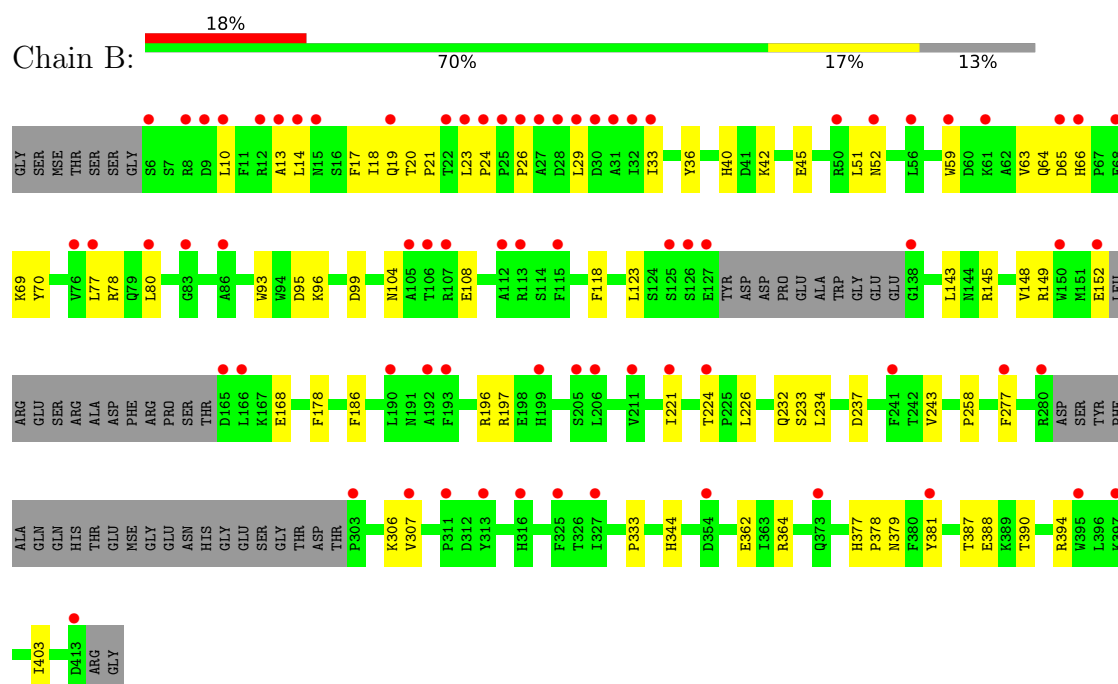
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

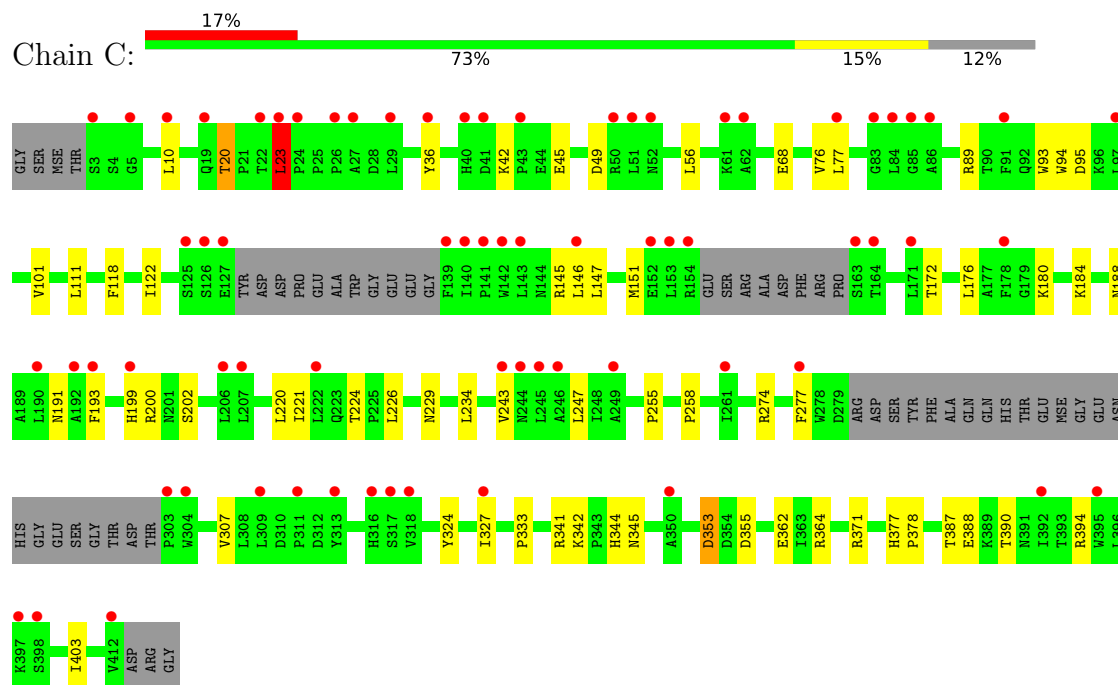
• Molecule 1: TSC1 N-terminal domain



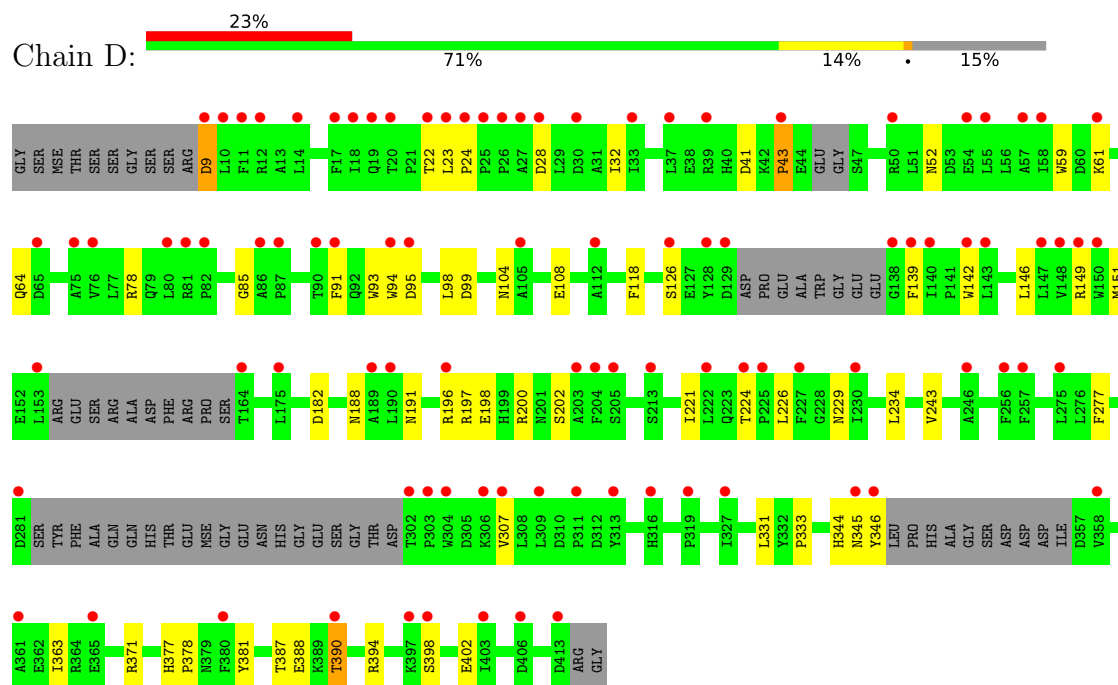
• Molecule 1: TSC1 N-terminal domain



• 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 0.243 , 0.275	Depositor DCC
R_{free} test set	2098 reflections (2.19%)	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)	0.31 , 51.5	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	0.12	0/2996	0.35	0/4065
1	B	0.14	0/3055	0.37	0/4150
1	C	0.13	0/3080	0.34	0/4184
1	D	0.14	0/2994	0.34	0/4067
All	All	0.13	0/12125	0.35	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	35	0
1	B	2976	0	2930	47	0
1	C	3001	0	2959	39	0
1	D	2918	0	2876	44	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	156	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 7.

All (156) 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:357:ASP:CG	1:A:358:VAL:H	2.16	0.53
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: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:B:19:GLN:C	1:B:21:PRO:HD3	2.35	0.51
1:B:42:LYS:HD3	1:B:45:GLU:CD	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:LYS:HD3	1:C:45:GLU:CD	2.37	0.49
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
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: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: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: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: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:68:GLU:H	1:C:68:GLU:CD	2.26	0.44
1:C:20:THR:O	1:C:20:THR:OG1	2.27	0.44
1:C:101:VAL:HG22	1:C:111:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:O	1:B:14:LEU:HG	2.18	0.44
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:B:233:SER:OG	1:B:237:ASP:OD2	2.35	0.42
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:D:344:HIS:C	1:D:346:TYR:H	2.28	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:49:ASP:CG	1:A:89:ARG:HH22	2.30	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

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	348/417 (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%)	36	45
1	D	343/417 (82%)	334 (97%)	7 (2%)	2 (1%)	21	25
All	All	1407/1668 (84%)	1379 (98%)	25 (2%)	3 (0%)	43	53

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 ⓘ

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%)	55	72
1	B	323/359 (90%)	321 (99%)	2 (1%)	78	88
1	C	327/359 (91%)	321 (98%)	6 (2%)	51	69
1	D	317/359 (88%)	313 (99%)	4 (1%)	61	76
All	All	1285/1436 (90%)	1268 (99%)	17 (1%)	61	76

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	89	ARG
1	A	149	ARG
1	A	224	THR
1	A	382	GLU
1	B	65	ASP
1	B	168	GLU
1	C	20	THR
1	C	23	LEU
1	C	76	VAL
1	C	180	LYS
1	C	353	ASP
1	C	355	ASP
1	D	9	ASP
1	D	331	LEU
1	D	345	ASN
1	D	390	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	ASN
1	A	335	ASN

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Mol	Chain	Res	Type
1	A	359	HIS
1	B	15	ASN
1	B	19	GLN
1	B	52	ASN
1	B	92	GLN
1	B	188	ASN
1	B	359	HIS
1	C	52	ASN
1	C	144	ASN
1	D	52	ASN
1	D	79	GLN
1	D	104	ASN
1	D	169	GLN
1	D	212	ASN

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](#)

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	0.23	0	6,6,6	0.07	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%)	1.10	57 (16%) 4 5	34, 57, 106, 143	0
1	B	359/417 (86%)	1.35	73 (20%) 3 3	37, 67, 133, 156	0
1	C	363/417 (87%)	1.32	71 (19%) 3 3	41, 67, 107, 124	0
1	D	350/417 (83%)	1.50	96 (27%) 1 1	43, 75, 130, 161	0
All	All	1425/1668 (85%)	1.32	297 (20%) 2 3	34, 67, 121, 161	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	12.2
1	A	11	PHE	7.8
1	C	23	LEU	7.5
1	D	11	PHE	7.1
1	A	142	TRP	7.0
1	B	23	LEU	6.5
1	D	23	LEU	6.3
1	D	10	LEU	6.2
1	D	91	PHE	5.9
1	C	303	PRO	5.8
1	B	106	THR	5.7
1	B	166	LEU	5.4
1	B	313	TYR	5.1
1	D	26	PRO	4.7
1	D	303	PRO	4.7
1	D	346	TYR	4.7
1	B	6	SER	4.6
1	C	36	TYR	4.6
1	B	8	ARG	4.5
1	B	126	SER	4.4
1	B	76	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	94	TRP	4.3
1	A	86	ALA	4.3
1	A	189	ALA	4.3
1	D	142	TRP	4.2
1	C	327	ILE	4.2
1	B	241	PHE	4.2
1	D	316	HIS	4.1
1	C	316	HIS	4.0
1	D	27	ALA	4.0
1	B	80	LEU	4.0
1	C	154	ARG	4.0
1	C	249	ALA	4.0
1	C	412	VAL	4.0
1	A	24	PRO	3.9
1	C	24	PRO	3.9
1	C	142	TRP	3.9
1	B	138	GLY	3.9
1	B	280	ARG	3.9
1	D	190	LEU	3.9
1	A	413	ASP	3.8
1	D	138	GLY	3.8
1	B	192	ALA	3.8
1	C	140	ILE	3.8
1	B	29	LEU	3.7
1	A	138	GLY	3.7
1	A	313	TYR	3.7
1	A	16	SER	3.7
1	D	20	THR	3.6
1	B	413	ASP	3.6
1	C	143	LEU	3.6
1	D	25	PRO	3.6
1	D	12	ARG	3.6
1	D	164	THR	3.6
1	D	24	PRO	3.6
1	A	22	THR	3.5
1	A	27	ALA	3.5
1	B	19	GLN	3.5
1	B	10	LEU	3.5
1	D	413	ASP	3.5
1	B	277	PHE	3.4
1	D	397	LYS	3.4
1	D	9	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	3	SER	3.4
1	A	140	ILE	3.3
1	B	24	PRO	3.3
1	C	26	PRO	3.3
1	B	68	GLU	3.3
1	B	316	HIS	3.3
1	B	125	SER	3.3
1	D	19	GLN	3.3
1	D	105	ALA	3.3
1	A	126	SER	3.3
1	B	381	TYR	3.3
1	B	83	GLY	3.2
1	A	32	ILE	3.2
1	C	152	GLU	3.2
1	C	27	ALA	3.2
1	C	192	ALA	3.2
1	D	30	ASP	3.2
1	C	91	PHE	3.2
1	B	9	ASP	3.2
1	D	128	TYR	3.2
1	C	22	THR	3.2
1	D	227	PHE	3.1
1	A	357	ASP	3.1
1	C	5	GLY	3.1
1	B	105	ALA	3.1
1	D	86	ALA	3.1
1	C	61	LYS	3.1
1	B	27	ALA	3.1
1	B	303	PRO	3.1
1	D	140	ILE	3.1
1	B	66	HIS	3.1
1	B	12	ARG	3.1
1	B	26	PRO	3.1
1	D	306	LYS	3.1
1	D	153	LEU	3.1
1	A	91	PHE	3.0
1	C	126	SER	3.0
1	D	39	ARG	3.0
1	B	127	GLU	3.0
1	D	143	LEU	3.0
1	D	302	THR	3.0
1	C	83	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	365	GLU	3.0
1	A	17	PHE	2.9
1	C	139	PHE	2.9
1	B	14	LEU	2.9
1	C	141	PRO	2.9
1	B	113	ARG	2.9
1	D	203	ALA	2.9
1	D	311	PRO	2.9
1	A	249	ALA	2.9
1	D	189	ALA	2.9
1	A	163	SER	2.8
1	A	19	GLN	2.8
1	C	245	LEU	2.8
1	D	150	TRP	2.8
1	C	85	GLY	2.8
1	A	87	PRO	2.8
1	A	166	LEU	2.8
1	C	51	LEU	2.8
1	C	97	LEU	2.8
1	D	147	LEU	2.8
1	B	31	ALA	2.8
1	D	406	ASP	2.8
1	C	317	SER	2.8
1	A	309	LEU	2.8
1	C	77	LEU	2.8
1	D	224	THR	2.7
1	A	5	GLY	2.7
1	C	311	PRO	2.7
1	A	192	ALA	2.7
1	B	150	TRP	2.7
1	D	14	LEU	2.7
1	A	316	HIS	2.7
1	A	256	PHE	2.7
1	B	115	PHE	2.7
1	D	17	PHE	2.7
1	D	76	VAL	2.7
1	C	127	GLU	2.7
1	B	56	LEU	2.7
1	B	325	PHE	2.7
1	B	33	ILE	2.7
1	A	202	SER	2.7
1	D	398	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	80	LEU	2.7
1	D	75	ALA	2.6
1	D	204	PHE	2.6
1	B	28	ASP	2.6
1	C	246	ALA	2.6
1	A	381	TYR	2.6
1	B	30	ASP	2.6
1	C	244	ASN	2.6
1	D	139	PHE	2.6
1	D	90	THR	2.6
1	C	206	LEU	2.6
1	D	304	TRP	2.6
1	D	313	TYR	2.6
1	C	163	SER	2.6
1	A	39	ARG	2.6
1	B	395	TRP	2.6
1	A	9	ASP	2.5
1	D	28	ASP	2.5
1	B	221	ILE	2.5
1	C	40	HIS	2.5
1	A	127	GLU	2.5
1	D	54	GLU	2.5
1	C	146	LEU	2.5
1	A	76	VAL	2.5
1	C	261	ILE	2.5
1	C	313	TYR	2.5
1	C	153	LEU	2.5
1	C	62	ALA	2.5
1	B	107	ARG	2.5
1	A	205	SER	2.4
1	A	10	LEU	2.4
1	C	43	PRO	2.4
1	C	3	SER	2.4
1	D	126	SER	2.4
1	D	205	SER	2.4
1	C	178	PHE	2.4
1	C	392	ILE	2.4
1	C	395	TRP	2.4
1	C	190	LEU	2.4
1	D	345	ASN	2.4
1	B	224	THR	2.4
1	A	233	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	380	PHE	2.4
1	B	59	TRP	2.4
1	B	50	ARG	2.4
1	A	365	GLU	2.4
1	B	165	ASP	2.4
1	D	225	PRO	2.4
1	D	246	ALA	2.4
1	C	193	PHE	2.4
1	D	257	PHE	2.4
1	D	37	LEU	2.4
1	D	22	THR	2.3
1	C	398	SER	2.3
1	C	29	LEU	2.3
1	D	55	LEU	2.3
1	D	95	ASP	2.3
1	D	281	ASP	2.3
1	B	112	ALA	2.3
1	C	164	THR	2.3
1	D	230	ILE	2.3
1	A	220	LEU	2.3
1	D	175	LEU	2.3
1	B	61	LYS	2.3
1	C	50	ARG	2.3
1	B	373	GLN	2.3
1	D	403	ILE	2.3
1	C	277	PHE	2.3
1	B	52	ASN	2.3
1	B	13	ALA	2.3
1	B	86	ALA	2.3
1	D	361	ALA	2.3
1	A	29	LEU	2.2
1	A	30	ASP	2.2
1	C	52	ASN	2.2
1	D	129	ASP	2.2
1	D	87	PRO	2.2
1	D	196	ARG	2.2
1	B	327	ILE	2.2
1	B	307	VAL	2.2
1	C	318	VAL	2.2
1	D	275	LEU	2.2
1	D	256	PHE	2.2
1	D	358	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	43	PRO	2.2
1	D	57	ALA	2.2
1	D	61	LYS	2.2
1	C	171	LEU	2.2
1	C	309	LEU	2.2
1	B	211	VAL	2.2
1	D	148	VAL	2.2
1	D	65	ASP	2.2
1	B	311	PRO	2.2
1	A	373	GLN	2.2
1	C	19	GLN	2.2
1	C	397	LYS	2.2
1	A	6	SER	2.2
1	D	390	THR	2.2
1	C	304	TRP	2.2
1	A	154	ARG	2.2
1	A	190	LEU	2.2
1	D	50	ARG	2.2
1	B	65	ASP	2.2
1	B	354	ASP	2.2
1	A	152	GLU	2.2
1	A	254	LEU	2.1
1	C	10	LEU	2.1
1	D	58	ILE	2.1
1	D	327	ILE	2.1
1	B	193	PHE	2.1
1	A	7	SER	2.1
1	A	125	SER	2.1
1	B	22	THR	2.1
1	B	205	SER	2.1
1	C	86	ALA	2.1
1	C	350	ALA	2.1
1	A	33	ILE	2.1
1	B	190	LEU	2.1
1	C	41	ASP	2.1
1	A	12	ARG	2.1
1	D	81	ARG	2.1
1	D	149	ARG	2.1
1	A	34	SER	2.1
1	B	397	LYS	2.1
1	D	222	LEU	2.1
1	A	41	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	25	PRO	2.1
1	D	307	VAL	2.1
1	D	319	PRO	2.1
1	C	84	LEU	2.1
1	C	207	LEU	2.1
1	B	32	ILE	2.1
1	D	82	PRO	2.1
1	C	243	VAL	2.1
1	C	125	SER	2.0
1	B	152	GLU	2.0
1	B	15	ASN	2.0
1	B	77	LEU	2.0
1	D	309	LEU	2.0
1	D	18	ILE	2.0
1	D	33	ILE	2.0
1	D	213	SER	2.0
1	A	31	ALA	2.0
1	D	112	ALA	2.0
1	B	199	HIS	2.0
1	C	199	HIS	2.0
1	B	206	LEU	2.0
1	C	222	LEU	2.0
1	A	343	PRO	2.0
1	A	42	LYS	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($\text{\AA}^2$)	Q<0.9
2	SO4	B	501	5/5	0.91	0.12	70,77,82,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.