



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:41 pm BST

PDB ID : 2WJV
Title : Crystal structure of the complex between human nonsense mediated decay factors UPF1 and UPF2
Authors : Clerici, M.; Mourao, A.; Gutsche, I.; Gehring, N.H.; Hentze, M.W.; Kulozik, A.; Kadlec, J.; Sattler, M.; Cusack, S.
Deposited on : 2009-06-01
Resolution : 2.85 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

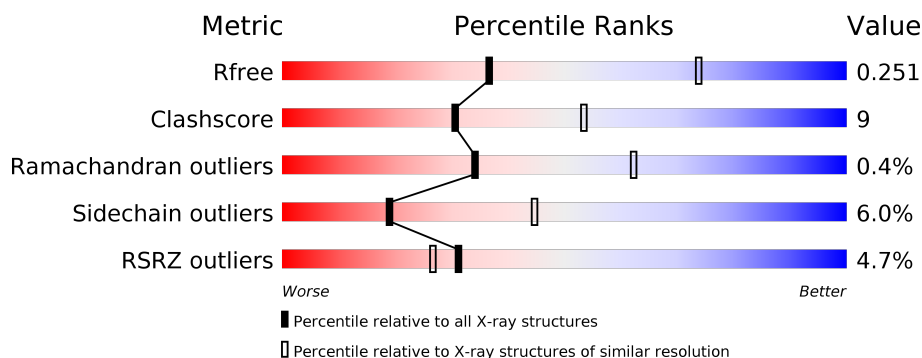
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	800	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	800	<div> <div>4%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
2	D	97	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>6%</div> <div>•</div> <div>44%</div> </div> </div>
2	E	97	<div> <div>9%</div> <div> <div></div> <div>43%</div> <div>15%</div> <div>•</div> <div>38%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	994	-	-	X	-
4	SO4	A	998	-	-	X	-
4	SO4	B	999	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13187 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 REGULATOR OF NONSENSE TRANSCRIPTS 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	0	0
			6094	3867	1067	1125	35			
1	B	768	Total	C	N	O	S	0	0	0
			6073	3858	1065	1115	35			

- Molecule 2 is a protein called REGULATOR OF NONSENSE TRANSCRIPTS 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	54	Total	C	N	O	S	0	0	0
			426	268	70	81	7			
2	E	60	Total	C	N	O	S	0	0	0
			473	295	82	89	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1102	ALA	-	expression tag	UNP Q9HAU5
D	1103	MET	-	expression tag	UNP Q9HAU5
D	1104	GLY	-	expression tag	UNP Q9HAU5
E	1102	ALA	-	expression tag	UNP Q9HAU5
E	1103	MET	-	expression tag	UNP Q9HAU5
E	1104	GLY	-	expression tag	UNP Q9HAU5

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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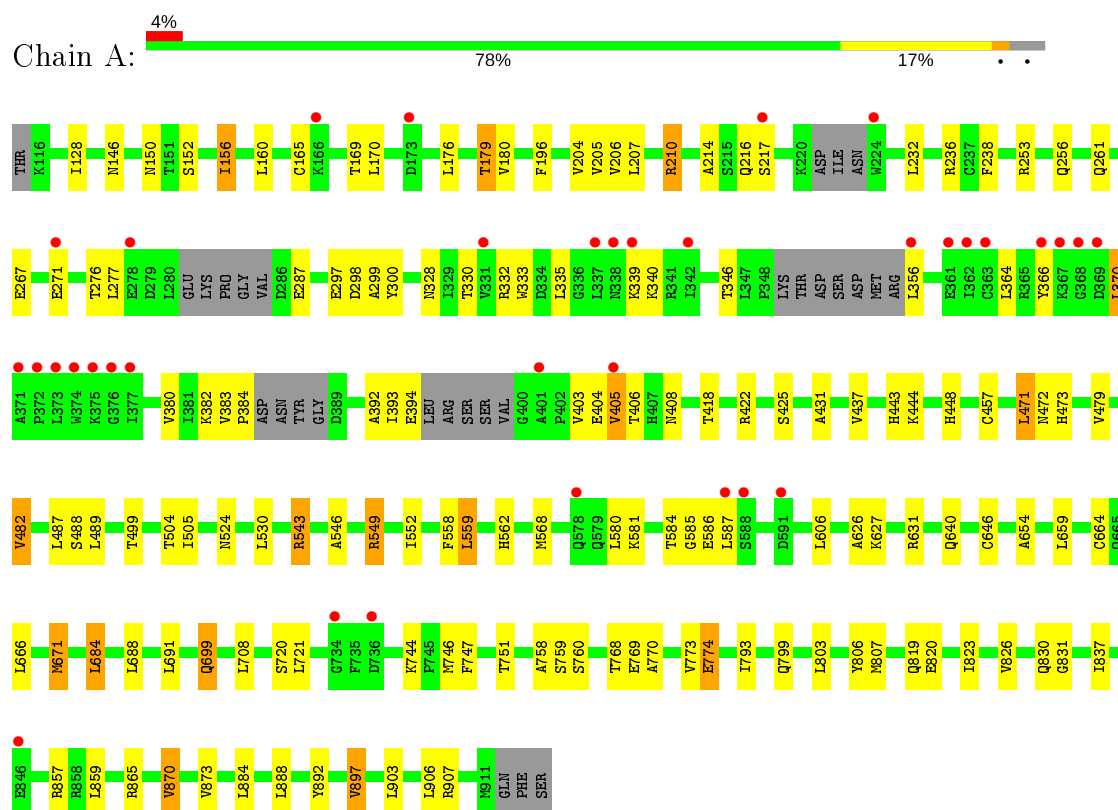
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0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

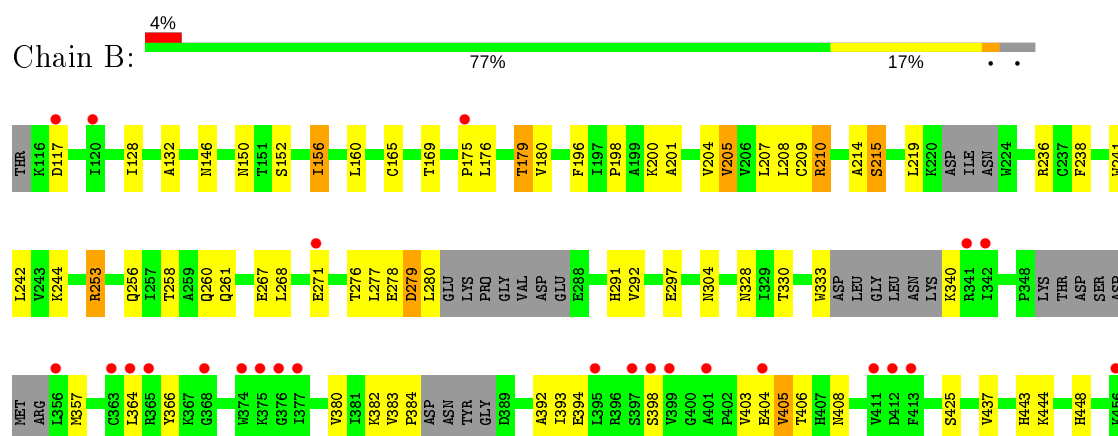
3 Residue-property plots

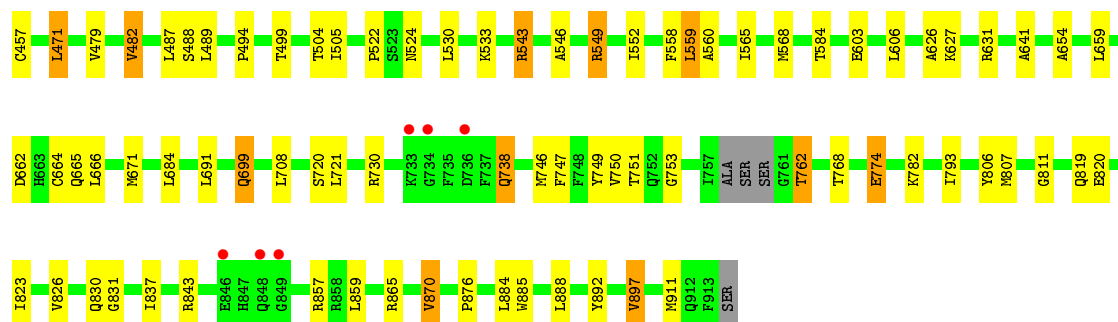
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: REGULATOR OF NONSENSE TRANSCRIPTS 1

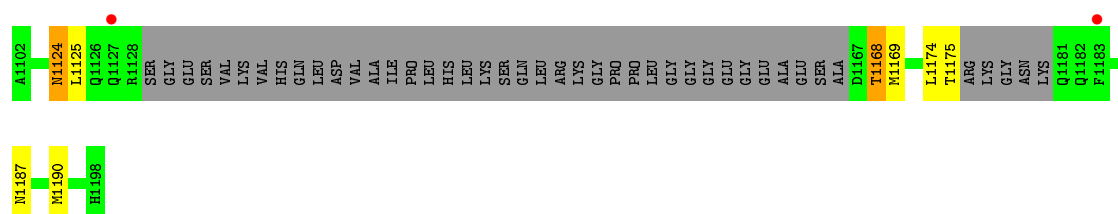


• Molecule 1: REGULATOR OF NONSENSE TRANSCRIPTS 1

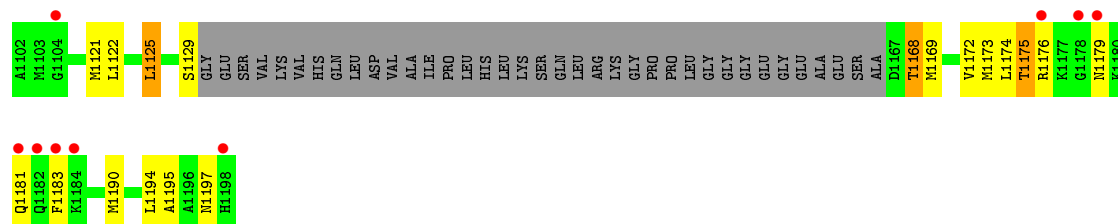
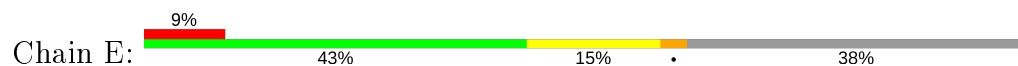




• Molecule 2: REGULATOR OF NONSENSE TRANSCRIPTS 2



• Molecule 2: REGULATOR OF NONSENSE TRANSCRIPTS 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.41 Å 97.29 Å 124.60 Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	48.79 – 2.85 48.77 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.9 (48.79-2.85) 96.9 (48.77-2.85)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.86 Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.200 , 0.248 0.206 , 0.251	Depositor DCC
R_{free} test set	2463 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	64.9	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13187	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.78% 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: ZN, 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	0.53	1/6215 (0.0%)	0.61	0/8412
1	B	0.54	1/6194 (0.0%)	0.62	0/8382
2	D	0.45	0/430	0.59	0/576
2	E	0.51	0/478	0.65	0/639
All	All	0.53	2/13317 (0.0%)	0.62	0/18009

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	664	CYS	CB-SG	-5.58	1.72	1.81
1	A	664	CYS	CB-SG	-5.45	1.73	1.81

There are no bond angle outliers.

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	6094	0	6140	107	0
1	B	6073	0	6126	119	0
2	D	426	0	421	18	0
2	E	473	0	475	11	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
4	A	65	0	0	8	0
4	B	50	0	0	4	0
All	All	13187	0	13162	243	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 9.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:CG1	2:D:1174:LEU:HD12	1.94	0.98
1:B:364:LEU:HD22	1:B:393:ILE:HD11	1.46	0.97
1:A:364:LEU:HD22	1:A:393:ILE:HD11	1.49	0.91
1:B:524:ASN:HD22	1:B:543:ARG:HH22	1.15	0.91
1:A:584:THR:HG22	1:A:585:GLY:O	1.71	0.89
1:B:762:THR:O	1:B:762:THR:CG2	2.26	0.84
1:B:268:LEU:HD22	1:B:280:LEU:HD21	1.63	0.81
1:A:524:ASN:HD22	1:A:543:ARG:HH22	1.26	0.80
1:B:196:PHE:CD2	1:B:205:VAL:HG13	2.18	0.78
1:B:762:THR:HG22	1:B:762:THR:O	1.83	0.77
1:A:580:LEU:HD23	1:A:587:LEU:HD22	1.67	0.77
1:A:473:HIS:ND1	4:A:994:SO4:O1	2.16	0.76
2:D:1168:THR:HG23	2:D:1169:MET:N	2.01	0.76
1:A:207:LEU:HD11	1:A:232:LEU:HD13	1.67	0.74
1:A:253:ARG:NH2	1:A:437:VAL:O	2.21	0.74
1:B:382:LYS:HB3	1:B:392:ALA:HB3	1.69	0.73
1:B:443:HIS:HD2	1:B:448:HIS:ND1	1.86	0.73
1:A:382:LYS:HB3	1:A:392:ALA:HB3	1.70	0.73
1:A:482:VAL:HG22	1:A:488:SER:CB	2.19	0.72
1:A:499:THR:HG23	1:A:530:LEU:HD13	1.71	0.72
2:D:1168:THR:CG2	2:D:1169:MET:N	2.55	0.69
1:B:482:VAL:HG22	1:B:488:SER:CB	2.24	0.68
1:B:708:LEU:HD22	1:B:870:VAL:HG13	1.75	0.68
1:A:482:VAL:HG22	1:A:488:SER:HB2	1.75	0.67
1:A:793:ILE:HG21	1:A:826:VAL:HG12	1.77	0.67
1:B:666:LEU:HD12	1:B:830:GLN:CG	2.25	0.67
2:E:1168:THR:CG2	2:E:1169:MET:N	2.56	0.67
1:A:907:ARG:NH2	4:A:988:SO4:O2	2.28	0.66
2:D:1175:THR:O	2:D:1175:THR:HG22	1.95	0.66
1:B:253:ARG:NH2	1:B:437:VAL:O	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1168:THR:HG21	2:D:1187:ASN:HB3	1.78	0.66
1:B:499:THR:HG23	1:B:530:LEU:HD13	1.77	0.65
1:B:558:PHE:CE1	1:B:559:LEU:HD13	2.33	0.64
1:A:443:HIS:HD2	1:A:448:HIS:ND1	1.95	0.64
2:D:1124:ASN:HD22	2:D:1124:ASN:N	1.95	0.64
1:A:330:THR:HG23	1:A:406:THR:CG2	2.29	0.63
2:D:1169:MET:HB2	2:D:1190:MET:HE1	1.80	0.63
2:E:1168:THR:HG23	2:E:1169:MET:N	2.14	0.63
1:B:207:LEU:O	1:B:208:LEU:HD23	1.99	0.63
1:B:826:VAL:HG22	4:B:996:SO4:O3	1.97	0.63
1:B:383:VAL:HG12	1:B:384:PRO:HD2	1.81	0.63
1:A:330:THR:HG23	1:A:406:THR:HG23	1.81	0.62
1:A:146:ASN:HD22	1:A:156:ILE:HD11	1.65	0.62
1:B:278:GLU:HG2	1:B:304:ASN:HD21	1.65	0.62
1:B:750:VAL:HG11	1:B:911:MET:HE1	1.82	0.62
1:A:333:TRP:CB	1:A:403:VAL:HG13	2.30	0.61
2:D:1190:MET:HA	2:D:1190:MET:HE2	1.81	0.61
1:A:549:ARG:HA	1:A:552:ILE:HD13	1.82	0.61
1:B:330:THR:HG23	1:B:406:THR:CG2	2.31	0.61
1:B:383:VAL:HG12	1:B:384:PRO:CD	2.31	0.60
1:A:568:MET:HE3	1:A:606:LEU:HD21	1.82	0.60
1:A:383:VAL:HG12	1:A:384:PRO:HD2	1.83	0.60
1:B:699:GLN:HE21	1:B:720:SER:HB2	1.67	0.59
1:B:333:TRP:CB	1:B:403:VAL:HG13	2.33	0.59
1:A:558:PHE:CE1	1:A:559:LEU:HD13	2.37	0.59
1:A:146:ASN:HD22	1:A:156:ILE:CD1	2.14	0.59
1:B:843:ARG:NH1	4:B:991:SO4:O2	2.34	0.59
1:B:210:ARG:O	1:B:214:ALA:HB3	2.03	0.59
1:A:418:THR:HG23	4:A:998:SO4:O3	2.03	0.58
1:B:666:LEU:HD12	1:B:830:GLN:HG2	1.85	0.58
1:A:383:VAL:HG12	1:A:384:PRO:CD	2.33	0.58
1:B:482:VAL:HG22	1:B:488:SER:HB2	1.86	0.58
1:B:793:ILE:HG21	1:B:826:VAL:HG12	1.85	0.58
1:B:549:ARG:HA	1:B:552:ILE:HD13	1.85	0.57
1:A:584:THR:CG2	1:A:585:GLY:N	2.68	0.57
1:A:332:ARG:NH2	1:B:811:GLY:O	2.37	0.57
1:B:330:THR:HG23	1:B:406:THR:HG23	1.86	0.57
1:A:699:GLN:HE21	1:A:720:SER:HB2	1.69	0.57
1:B:146:ASN:HD22	1:B:156:ILE:HD11	1.69	0.57
1:B:626:ALA:O	1:B:627:LYS:HB2	2.05	0.57
1:B:494:PRO:HA	4:B:999:SO4:O2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:LEU:HD12	1:B:830:GLN:CD	2.26	0.56
1:A:333:TRP:CG	1:A:403:VAL:HG13	2.41	0.56
1:B:671:MET:HA	1:B:671:MET:CE	2.36	0.56
1:B:708:LEU:HD22	1:B:870:VAL:CG1	2.36	0.55
2:D:1169:MET:HB2	2:D:1190:MET:CE	2.37	0.55
1:A:626:ALA:O	1:A:627:LYS:HB2	2.05	0.55
1:A:897:VAL:HG13	1:A:897:VAL:O	2.06	0.55
1:A:146:ASN:HD21	1:A:238:PHE:H	1.55	0.55
1:A:333:TRP:CE3	1:A:403:VAL:HG22	2.41	0.55
1:A:584:THR:HG22	1:A:585:GLY:N	2.22	0.55
1:A:206:VAL:HG13	2:D:1174:LEU:HD12	1.84	0.54
1:B:888:LEU:HD11	1:B:892:TYR:CE1	2.42	0.54
1:A:671:MET:CE	1:A:671:MET:HA	2.38	0.54
1:B:774:GLU:HG2	1:B:806:TYR:HE2	1.71	0.54
1:B:859:LEU:HD23	1:B:884:LEU:CD2	2.38	0.54
1:B:750:VAL:CG1	1:B:911:MET:HE1	2.37	0.54
1:A:479:VAL:HG22	1:A:505:ILE:HG13	1.89	0.54
1:B:444:LYS:HG2	1:B:487:LEU:HD13	1.89	0.54
1:B:807:MET:HE1	1:B:823:ILE:HD11	1.88	0.54
1:A:774:GLU:HG2	1:A:806:TYR:HE2	1.73	0.53
1:B:558:PHE:CD1	1:B:559:LEU:HD13	2.44	0.53
1:A:206:VAL:HG11	2:D:1174:LEU:HD12	1.86	0.53
1:A:888:LEU:HD11	1:A:892:TYR:CE1	2.44	0.53
1:B:437:VAL:HG12	1:B:654:ALA:HB3	1.91	0.53
1:A:403:VAL:O	1:A:403:VAL:HG12	2.09	0.53
1:A:580:LEU:CD2	1:A:587:LEU:HD22	2.38	0.53
1:A:206:VAL:HG12	2:D:1174:LEU:HD12	1.85	0.52
1:A:546:ALA:HB3	1:A:549:ARG:HG3	1.91	0.51
1:B:196:PHE:HD2	1:B:205:VAL:HG13	1.71	0.51
1:B:366:TYR:OH	1:B:405:VAL:HG11	2.10	0.51
2:D:1168:THR:HG23	2:D:1169:MET:H	1.73	0.51
1:B:179:THR:HG21	2:E:1175:THR:HG21	1.93	0.51
1:B:487:LEU:HD23	1:B:487:LEU:C	2.31	0.51
1:B:831:GLY:HA2	4:B:999:SO4:O3	2.10	0.51
1:A:487:LEU:C	1:A:487:LEU:HD23	2.31	0.51
1:B:443:HIS:CD2	1:B:448:HIS:ND1	2.74	0.51
1:A:799:GLN:O	1:A:803:LEU:HB2	2.10	0.51
1:B:146:ASN:HD21	1:B:238:PHE:H	1.59	0.51
1:B:333:TRP:CG	1:B:403:VAL:HG13	2.46	0.51
1:B:750:VAL:HG11	1:B:911:MET:CE	2.40	0.51
1:B:487:LEU:HD23	1:B:488:SER:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HA	1:A:214:ALA:HB3	1.92	0.51
1:A:558:PHE:CD1	1:A:559:LEU:HD13	2.46	0.51
1:B:524:ASN:HD22	1:B:543:ARG:NH2	1.97	0.51
1:A:640:GLN:NE2	1:A:830:GLN:OE1	2.44	0.50
1:B:546:ALA:HB3	1:B:549:ARG:HG3	1.92	0.50
1:A:666:LEU:HD12	1:A:830:GLN:CG	2.42	0.50
1:B:568:MET:HE3	1:B:606:LEU:HD21	1.91	0.50
2:D:1190:MET:HE2	2:D:1190:MET:CA	2.42	0.50
1:A:366:TYR:OH	1:A:405:VAL:HG11	2.11	0.50
1:B:169:THR:OG1	1:B:180:VAL:HG22	2.12	0.50
1:B:479:VAL:HG22	1:B:505:ILE:HG13	1.93	0.49
1:B:897:VAL:HG13	1:B:897:VAL:O	2.12	0.49
1:A:562:HIS:ND1	4:A:999:SO4:O4	2.38	0.49
1:B:146:ASN:HD22	1:B:156:ILE:CD1	2.26	0.49
1:B:489:LEU:HD22	1:B:659:LEU:HB2	1.94	0.49
1:A:206:VAL:HG12	2:D:1174:LEU:HB2	1.94	0.49
1:A:146:ASN:ND2	1:A:156:ILE:HD11	2.28	0.48
1:A:747:PHE:HA	1:A:897:VAL:HG13	1.95	0.48
1:B:565:ILE:HD11	1:B:603:GLU:HG3	1.94	0.48
1:A:328:ASN:ND2	1:A:408:ASN:HD22	2.11	0.48
1:A:380:VAL:HA	1:A:393:ILE:HG22	1.95	0.48
1:B:156:ILE:HD12	1:B:156:ILE:H	1.79	0.48
1:B:291:HIS:HD2	1:B:292:VAL:O	1.96	0.48
1:A:770:ALA:HB1	1:A:803:LEU:HD13	1.96	0.48
1:A:152:SER:O	1:A:236:ARG:NH1	2.46	0.48
1:B:403:VAL:O	1:B:403:VAL:HG12	2.13	0.48
1:A:903:LEU:HA	1:A:906:LEU:HG	1.96	0.48
1:A:487:LEU:HD23	1:A:488:SER:N	2.29	0.47
1:A:150:ASN:HD21	1:A:256:GLN:HB3	1.79	0.47
2:D:1175:THR:CG2	2:D:1175:THR:O	2.61	0.47
1:A:708:LEU:HD22	1:A:870:VAL:HG13	1.96	0.47
1:B:210:ARG:HG2	2:E:1125:LEU:HD21	1.97	0.47
1:A:437:VAL:HG12	1:A:654:ALA:HB3	1.96	0.47
1:B:747:PHE:HA	1:B:897:VAL:HG13	1.95	0.47
1:A:169:THR:OG1	1:A:180:VAL:HG22	2.15	0.47
1:A:769:GLU:O	1:A:773:VAL:HG23	2.15	0.47
1:B:662:ASP:HB3	1:B:665:GLN:HE21	1.79	0.47
1:B:333:TRP:CE3	1:B:403:VAL:HG22	2.50	0.47
1:A:333:TRP:CD2	1:A:403:VAL:HG22	2.49	0.47
1:B:152:SER:O	1:B:236:ARG:NH1	2.48	0.47
1:B:366:TYR:CZ	1:B:405:VAL:HG11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:LYS:O	1:B:201:ALA:HB3	2.14	0.46
1:A:335:LEU:HD22	1:B:782:LYS:HA	1.97	0.46
1:B:150:ASN:HD21	1:B:256:GLN:HB3	1.81	0.46
1:B:297:GLU:HA	1:B:297:GLU:OE1	2.16	0.46
1:B:380:VAL:HA	1:B:393:ILE:HG22	1.97	0.46
1:A:156:ILE:H	1:A:156:ILE:HD12	1.80	0.46
1:A:333:TRP:HB2	1:A:403:VAL:HG13	1.98	0.46
1:B:366:TYR:CE1	1:B:405:VAL:HG11	2.51	0.46
1:A:684:LEU:HD22	1:A:688:LEU:CD1	2.46	0.46
1:A:769:GLU:HG3	1:A:873:VAL:HG12	1.98	0.46
1:B:198:PRO:HB3	2:E:1194:LEU:HD11	1.98	0.45
1:A:444:LYS:HG2	1:A:487:LEU:HD13	1.98	0.45
1:B:471:LEU:HD21	1:B:504:THR:HG21	1.98	0.45
1:A:422:ARG:NE	4:A:998:SO4:O3	2.47	0.45
1:A:160:LEU:HD23	1:A:165:CYS:HB2	1.99	0.45
1:A:684:LEU:HD22	1:A:688:LEU:HD11	1.98	0.45
2:E:1176:ARG:HA	2:E:1181:GLN:HA	1.99	0.45
1:B:662:ASP:CB	1:B:665:GLN:HE21	2.29	0.45
1:A:472:ASN:HB2	4:A:994:SO4:O1	2.17	0.45
1:B:176:LEU:HD23	1:B:179:THR:OG1	2.17	0.45
1:A:340:LYS:HD2	1:A:394:GLU:OE2	2.17	0.45
1:B:837:ILE:HG13	1:B:865:ARG:HB2	1.99	0.45
1:B:261:GLN:OE1	1:B:277:LEU:HD21	2.17	0.45
1:B:146:ASN:ND2	1:B:156:ILE:HD11	2.31	0.44
1:B:219:LEU:HD23	1:B:219:LEU:O	2.18	0.44
1:A:403:VAL:CG1	1:A:403:VAL:O	2.66	0.44
1:B:543:ARG:O	1:B:560:ALA:HA	2.18	0.44
2:E:1174:LEU:HD23	2:E:1183:PHE:CD2	2.52	0.44
1:B:738:GLN:HE21	1:B:738:GLN:HA	1.82	0.44
2:D:1124:ASN:N	2:D:1124:ASN:ND2	2.65	0.44
1:A:489:LEU:HD22	1:A:659:LEU:HB2	1.99	0.44
1:A:758:ALA:O	1:A:760:SER:N	2.50	0.44
1:B:132:ALA:HB1	1:B:244:LYS:HG3	1.98	0.44
1:B:328:ASN:ND2	1:B:408:ASN:HD22	2.16	0.44
1:B:205:VAL:HG12	2:E:1173:MET:HG3	2.00	0.44
1:B:333:TRP:HB2	1:B:403:VAL:HG13	1.99	0.43
1:B:522:PRO:HG3	1:B:641:ALA:HB2	1.99	0.43
1:A:366:TYR:CE1	1:A:405:VAL:HG11	2.53	0.43
1:A:366:TYR:CZ	1:A:405:VAL:HG11	2.53	0.43
1:A:471:LEU:HD21	1:A:504:THR:HG21	2.00	0.43
1:A:204:VAL:O	1:A:205:VAL:HG23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:MET:O	1:A:897:VAL:HG21	2.18	0.43
1:B:258:THR:O	1:B:261:GLN:N	2.49	0.43
1:A:837:ILE:HG13	1:A:865:ARG:HB2	1.99	0.43
1:B:160:LEU:HD23	1:B:165:CYS:HB2	1.99	0.43
1:A:196:PHE:CD2	1:A:205:VAL:CG1	3.02	0.43
1:B:888:LEU:CD1	1:B:892:TYR:CE1	3.02	0.43
1:A:826:VAL:HG22	4:A:996:SO4:O2	2.18	0.43
2:E:1174:LEU:HD23	2:E:1183:PHE:HD2	1.84	0.43
1:A:196:PHE:HA	1:A:206:VAL:O	2.19	0.42
1:B:196:PHE:CD2	1:B:205:VAL:CG1	2.96	0.42
1:B:204:VAL:HG22	2:E:1172:VAL:HB	2.01	0.42
1:B:750:VAL:HG21	1:B:911:MET:CE	2.49	0.42
1:A:176:LEU:HD23	1:A:179:THR:OG1	2.19	0.42
1:A:297:GLU:HA	1:A:297:GLU:OE1	2.19	0.42
1:A:831:GLY:HA2	4:A:990:SO4:O3	2.18	0.42
1:A:807:MET:HE1	1:A:823:ILE:HD11	2.01	0.42
1:B:746:MET:O	1:B:897:VAL:CG2	2.67	0.42
1:A:366:TYR:OH	1:A:370:LEU:HB2	2.19	0.42
1:A:770:ALA:CB	1:A:803:LEU:HD13	2.50	0.42
1:B:499:THR:HG22	1:B:533:LYS:HG3	2.01	0.42
1:B:753:GLY:HA3	1:B:768:THR:HB	2.00	0.42
1:B:242:LEU:HA	1:B:242:LEU:HD12	1.86	0.41
1:B:330:THR:HG23	1:B:406:THR:HG22	2.02	0.41
1:B:279:ASP:O	1:B:280:LEU:HD23	2.20	0.41
1:A:747:PHE:HB3	1:A:897:VAL:HG22	2.02	0.41
1:B:258:THR:HG23	1:B:261:GLN:HE21	1.86	0.41
1:A:169:THR:HG22	1:A:170:LEU:O	2.21	0.41
1:B:885:TRP:CZ3	1:B:888:LEU:HD23	2.56	0.41
1:B:876:PRO:HG2	1:B:911:MET:HE1	2.02	0.41
1:B:762:THR:HG23	1:B:762:THR:O	2.12	0.41
1:A:751:THR:CG2	1:A:768:THR:HG22	2.51	0.41
1:B:333:TRP:CD2	1:B:403:VAL:HG22	2.56	0.41
1:B:807:MET:CE	1:B:823:ILE:HD11	2.51	0.41
2:E:1190:MET:HA	2:E:1195:ALA:HB1	2.03	0.41
1:A:859:LEU:HD23	1:A:884:LEU:CD2	2.51	0.41
1:B:876:PRO:HG2	1:B:911:MET:CE	2.51	0.41
1:A:888:LEU:CD1	1:A:892:TYR:CE1	3.04	0.41
1:B:340:LYS:HD2	1:B:394:GLU:OE2	2.20	0.41
1:B:751:THR:HG23	1:B:768:THR:HG22	2.03	0.41
1:A:299:ALA:HB3	1:A:431:ALA:HA	2.02	0.41
1:B:204:VAL:HG12	1:B:205:VAL:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:565:ILE:HD11	1:B:603:GLU:CG	2.51	0.41
1:A:581:LYS:O	1:A:584:THR:O	2.39	0.40
1:B:403:VAL:CG1	1:B:403:VAL:O	2.68	0.40
1:A:261:GLN:OE1	1:A:277:LEU:HD21	2.22	0.40
2:D:1169:MET:CB	2:D:1190:MET:HE1	2.49	0.40
1:A:298:ASP:OD2	1:A:300:TYR:HB2	2.22	0.40
1:A:580:LEU:O	1:A:584:THR:HB	2.21	0.40
1:B:364:LEU:HD12	1:B:364:LEU:HA	1.85	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	760/800 (95%)	728 (96%)	27 (4%)	5 (1%)	22	50
1	B	754/800 (94%)	720 (96%)	32 (4%)	2 (0%)	41	68
2	D	48/97 (50%)	42 (88%)	6 (12%)	0	100	100
2	E	56/97 (58%)	53 (95%)	3 (5%)	0	100	100
All	All	1618/1794 (90%)	1543 (95%)	68 (4%)	7 (0%)	34	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	SER
1	B	215	SER
1	A	216	GLN
1	A	339	LYS
1	A	287	GLU
1	A	586	GLU
1	B	175	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	673/699 (96%)	639 (95%)	34 (5%)	24	52
1	B	671/699 (96%)	629 (94%)	42 (6%)	18	42
2	D	49/82 (60%)	46 (94%)	3 (6%)	18	43
2	E	54/82 (66%)	46 (85%)	8 (15%)	3	8
All	All	1447/1562 (93%)	1360 (94%)	87 (6%)	19	45

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	ILE
1	A	156	ILE
1	A	179	THR
1	A	210	ARG
1	A	217	SER
1	A	267	GLU
1	A	271	GLU
1	A	276	THR
1	A	346	THR
1	A	356	LEU
1	A	370	LEU
1	A	404	GLU
1	A	405	VAL
1	A	425	SER
1	A	457	CYS
1	A	471	LEU
1	A	482	VAL
1	A	543	ARG
1	A	549	ARG
1	A	559	LEU
1	A	631	ARG
1	A	646	CYS
1	A	671	MET
1	A	684	LEU

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Mol	Chain	Res	Type
1	A	691	LEU
1	A	699	GLN
1	A	721	LEU
1	A	744	LYS
1	A	774	GLU
1	A	819	GLN
1	A	820	GLU
1	A	857	ARG
1	A	870	VAL
1	A	897	VAL
1	B	117	ASP
1	B	128	ILE
1	B	156	ILE
1	B	179	THR
1	B	205	VAL
1	B	209	CYS
1	B	210	ARG
1	B	215	SER
1	B	241	TRP
1	B	253	ARG
1	B	260	GLN
1	B	267	GLU
1	B	271	GLU
1	B	276	THR
1	B	279	ASP
1	B	357	MET
1	B	398	SER
1	B	404	GLU
1	B	405	VAL
1	B	425	SER
1	B	457	CYS
1	B	471	LEU
1	B	482	VAL
1	B	543	ARG
1	B	549	ARG
1	B	559	LEU
1	B	584	THR
1	B	631	ARG
1	B	684	LEU
1	B	691	LEU
1	B	699	GLN
1	B	721	LEU

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Mol	Chain	Res	Type
1	B	730	ARG
1	B	738	GLN
1	B	749	TYR
1	B	762	THR
1	B	774	GLU
1	B	819	GLN
1	B	820	GLU
1	B	857	ARG
1	B	870	VAL
1	B	897	VAL
2	D	1124	ASN
2	D	1125	LEU
2	D	1168	THR
2	E	1121	MET
2	E	1122	LEU
2	E	1125	LEU
2	E	1129	SER
2	E	1168	THR
2	E	1175	THR
2	E	1179	ASN
2	E	1197	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	A	146	ASN
1	A	150	ASN
1	A	185	ASN
1	A	304	ASN
1	A	328	ASN
1	A	408	ASN
1	A	443	HIS
1	A	458	GLN
1	A	524	ASN
1	A	629	GLN
1	A	665	GLN
1	A	699	GLN
1	A	722	GLN
1	A	741	GLN
1	A	860	ASN
1	A	886	ASN

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Mol	Chain	Res	Type
1	B	138	ASN
1	B	146	ASN
1	B	150	ASN
1	B	185	ASN
1	B	228	GLN
1	B	291	HIS
1	B	304	ASN
1	B	328	ASN
1	B	408	ASN
1	B	443	HIS
1	B	458	GLN
1	B	524	ASN
1	B	629	GLN
1	B	665	GLN
1	B	699	GLN
1	B	722	GLN
1	B	738	GLN
1	B	741	GLN
1	B	752	GLN
1	B	860	ASN
1	B	886	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 6 are monoatomic - leaving 23 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	SO4	B	993	-	4,4,4	0.13	0	6,6,6	0.11	0
4	SO4	A	992	-	4,4,4	0.20	0	6,6,6	0.49	0
4	SO4	A	999	-	4,4,4	0.15	0	6,6,6	0.22	0
4	SO4	A	989	-	4,4,4	0.16	0	6,6,6	0.37	0
4	SO4	B	999	-	4,4,4	0.15	0	6,6,6	0.58	0
4	SO4	B	995	-	4,4,4	0.19	0	6,6,6	0.38	0
4	SO4	A	988	-	4,4,4	0.12	0	6,6,6	0.18	0
4	SO4	B	991	-	4,4,4	0.12	0	6,6,6	0.17	0
4	SO4	B	998	-	4,4,4	0.14	0	6,6,6	0.24	0
4	SO4	A	987	-	4,4,4	0.17	0	6,6,6	0.14	0
4	SO4	B	996	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	A	994	-	4,4,4	0.15	0	6,6,6	0.26	0
4	SO4	B	997	-	4,4,4	0.12	0	6,6,6	0.11	0
4	SO4	B	990	-	4,4,4	0.14	0	6,6,6	0.27	0
4	SO4	A	995	-	4,4,4	0.21	0	6,6,6	0.17	0
4	SO4	A	991	-	4,4,4	0.14	0	6,6,6	0.16	0
4	SO4	A	996	-	4,4,4	0.14	0	6,6,6	0.25	0
4	SO4	B	992	-	4,4,4	0.15	0	6,6,6	0.18	0
4	SO4	A	990	-	4,4,4	0.34	0	6,6,6	0.78	0
4	SO4	A	997	-	4,4,4	0.14	0	6,6,6	0.13	0
4	SO4	A	993	-	4,4,4	0.13	0	6,6,6	0.26	0
4	SO4	A	998	-	4,4,4	0.19	0	6,6,6	0.20	0
4	SO4	B	989	-	4,4,4	0.10	0	6,6,6	0.36	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.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	SO4	1	0
4	B	999	SO4	2	0
4	A	988	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	991	SO4	1	0
4	B	996	SO4	1	0
4	A	994	SO4	2	0
4	A	996	SO4	1	0
4	A	990	SO4	1	0
4	A	998	SO4	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	772/800 (96%)	0.20	35 (4%) 33 28	9, 20, 33, 44	0
1	B	768/800 (96%)	0.14	31 (4%) 38 32	8, 20, 34, 46	0
2	D	54/97 (55%)	0.33	2 (3%) 41 36	9, 29, 45, 47	0
2	E	60/97 (61%)	0.62	9 (15%) 2 1	9, 34, 49, 52	0
All	All	1654/1794 (92%)	0.20	77 (4%) 31 27	8, 20, 38, 52	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	1179	ASN	6.1
1	A	377	ILE	5.2
1	A	337	LEU	5.0
1	A	373	LEU	4.5
1	A	368	GLY	4.5
2	E	1104	GLY	4.5
1	A	587	LEU	4.0
1	A	401	ALA	3.9
1	B	736	ASP	3.9
1	B	363	CYS	3.8
2	E	1181	GLN	3.7
1	B	399	VAL	3.6
2	E	1183	PHE	3.5
1	B	401	ALA	3.5
1	B	368	GLY	3.4
1	A	278	GLU	3.4
1	A	734	GLY	3.4
1	B	404	GLU	3.4
1	B	733	LYS	3.4
1	A	338	ASN	3.2
1	B	456	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	217	SER	3.1
1	A	339	LYS	3.0
2	E	1178	GLY	3.0
2	E	1182	GLN	3.0
1	A	736	ASP	3.0
1	A	372	PRO	3.0
1	B	398	SER	2.9
1	B	734	GLY	2.9
1	B	846	GLU	2.8
1	B	120	ILE	2.8
1	B	376	GLY	2.8
1	A	361	GLU	2.8
1	B	375	LYS	2.8
1	A	846	GLU	2.7
1	A	374	TRP	2.7
1	B	365	ARG	2.7
1	B	395	LEU	2.6
1	A	331	VAL	2.6
1	A	369	ASP	2.6
1	A	405	VAL	2.6
1	B	411	VAL	2.6
1	A	376	GLY	2.5
1	B	377	ILE	2.5
1	B	271	GLU	2.5
1	B	374	TRP	2.5
1	B	412	ASP	2.5
1	B	341	ARG	2.5
1	B	364	LEU	2.5
1	A	578	GLN	2.5
1	B	848	GLN	2.5
1	A	271	GLU	2.5
1	A	591	ASP	2.4
1	A	224	TRP	2.4
1	A	166	LYS	2.4
1	A	375	LYS	2.4
2	D	1183	PHE	2.4
2	E	1198	HIS	2.3
1	A	366	TYR	2.3
1	B	117	ASP	2.3
1	B	397	SER	2.3
1	A	367	LYS	2.3
1	A	362	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	413	PHE	2.2
2	E	1176	ARG	2.1
1	B	175	PRO	2.1
1	A	356	LEU	2.1
2	D	1127	GLN	2.1
1	A	371	ALA	2.1
1	A	363	CYS	2.1
1	A	173	ASP	2.1
1	A	342	ILE	2.1
1	B	849	GLY	2.1
1	B	356	LEU	2.1
1	B	342	ILE	2.0
2	E	1184	LYS	2.0
1	A	588	SER	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 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(Å ²)	Q<0.9
4	SO4	A	987	5/5	0.73	0.27	127,127,127,128	0
4	SO4	B	989	5/5	0.75	0.24	118,118,119,119	0
4	SO4	B	992	5/5	0.77	0.25	129,129,129,129	0
4	SO4	A	988	5/5	0.79	0.22	141,141,142,142	0
4	SO4	A	996	5/5	0.81	0.32	138,138,138,138	0
4	SO4	B	990	5/5	0.82	0.31	110,111,111,112	0
4	SO4	A	992	5/5	0.83	0.21	96,97,97,97	0
4	SO4	A	994	5/5	0.85	0.16	126,126,126,127	0
4	SO4	A	998	5/5	0.86	0.19	119,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	993	5/5	0.87	0.14	113,113,113,113	0
4	SO4	B	998	5/5	0.87	0.18	104,104,105,105	0
4	SO4	B	999	5/5	0.87	0.22	73,75,76,76	0
4	SO4	B	991	5/5	0.88	0.20	151,151,152,152	0
4	SO4	B	996	5/5	0.89	0.32	152,152,153,153	0
4	SO4	A	989	5/5	0.89	0.18	113,114,114,114	0
4	SO4	B	997	5/5	0.89	0.24	131,131,131,131	0
4	SO4	A	997	5/5	0.91	0.35	133,133,133,133	0
4	SO4	A	991	5/5	0.92	0.10	117,118,118,118	0
4	SO4	A	999	5/5	0.93	0.41	135,135,135,136	0
4	SO4	B	993	5/5	0.94	0.13	106,107,107,108	0
4	SO4	A	990	5/5	0.94	0.17	71,72,73,73	0
4	SO4	B	995	5/5	0.95	0.13	79,80,81,82	0
4	SO4	A	995	5/5	0.96	0.13	96,96,97,97	0
3	ZN	A	3	1/1	0.98	0.10	19,19,19,19	0
3	ZN	B	1	1/1	0.99	0.12	10,10,10,10	0
3	ZN	B	2	1/1	0.99	0.08	24,24,24,24	1
3	ZN	B	3	1/1	0.99	0.13	13,13,13,13	0
3	ZN	A	2	1/1	0.99	0.06	20,20,20,20	1
3	ZN	A	1	1/1	1.00	0.10	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.