



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 04:34 pm BST

PDB ID : 2WJY
Title : Crystal structure of the complex between human nonsense mediated decay factors UPF1 and UPF2 Orthorhombic form
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 : 2.50 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

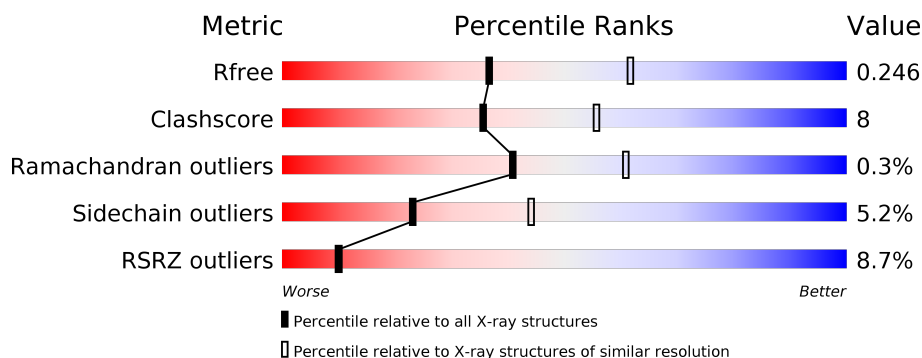
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	996	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6465 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	773	Total	C	N	O	S	0	7	0
			6168	3914	1084	1135	35			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

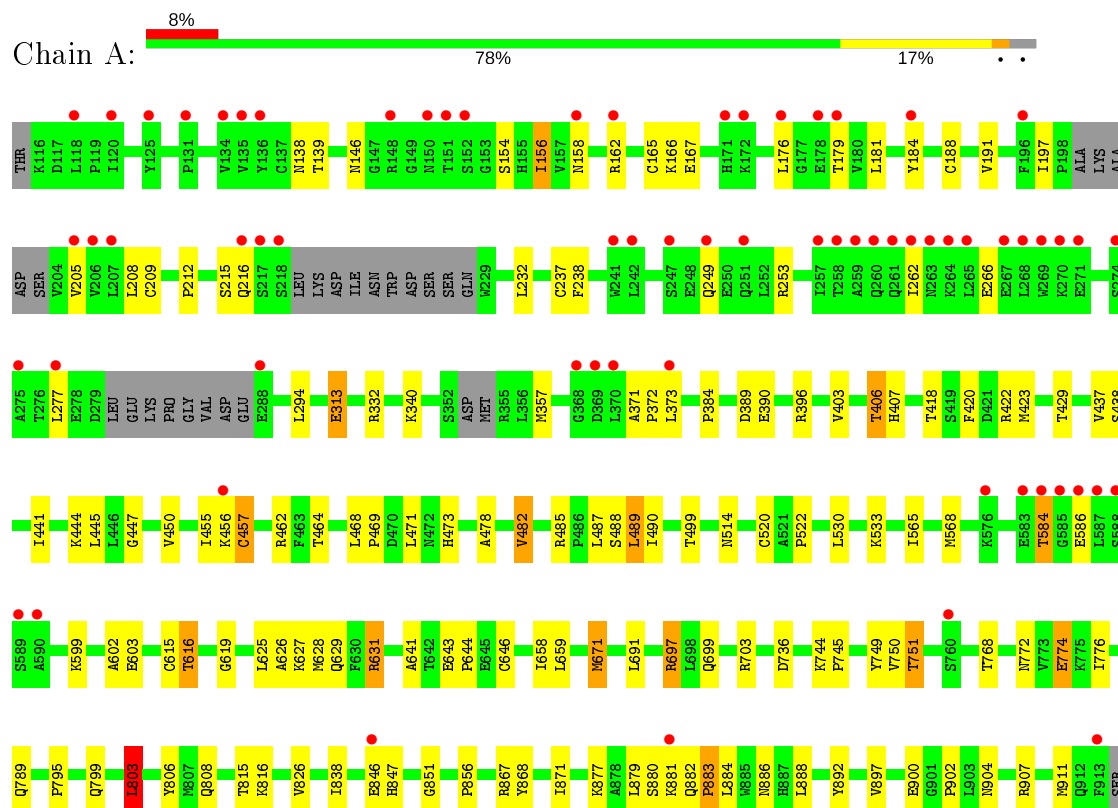
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	254	Total	O	0	0
			254	254		

3 Residue-property plots [i](#)

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	64.91Å 129.14Å 311.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 2.50 45.29 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.52-2.50) 98.4 (45.29-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.196 , 0.240 0.202 , 0.246	Depositor DCC
R_{free} test set	2266 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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	0.58	0/6293	0.68	1/8519 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	803	LEU	CA-CB-CG	5.25	127.36	115.30

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	6168	0	6217	100	0
2	A	3	0	0	0	0
3	A	40	0	0	3	0
4	A	254	0	0	10	0
All	All	6465	0	6217	100	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 8.

All (100) 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:881[B]:LYS:O	1:A:881[B]:LYS:HG2	1.38	1.18
1:A:616:THR:HG22	1:A:619:GLY:H	1.05	1.10
1:A:851:GLY:HA3	3:A:996:SO4:O4	1.69	0.90
1:A:881[B]:LYS:CG	1:A:881[B]:LYS:O	2.19	0.89
1:A:616:THR:HG22	1:A:619:GLY:N	1.90	0.85
1:A:357:MET:HG2	4:A:2037:HOH:O	1.80	0.80
1:A:599:LYS:O	1:A:603:GLU:HG3	1.82	0.79
1:A:625:LEU:HA	1:A:628:MET:HE3	1.66	0.77
1:A:816:LYS:HG2	4:A:2212:HOH:O	1.86	0.76
1:A:846:GLU:HG3	1:A:881[A]:LYS:HG3	1.69	0.74
1:A:154:SER:HB3	1:A:237:CYS:HB3	1.70	0.74
1:A:629:GLN:HG3	4:A:2143:HOH:O	1.87	0.73
1:A:749:TYR:HE2	1:A:772:ASN:ND2	1.88	0.71
1:A:499:THR:HG22	1:A:533:LYS:HG3	1.72	0.70
1:A:881[A]:LYS:O	1:A:882[A]:GLN:HG2	1.90	0.70
1:A:774:GLU:HG2	1:A:806:TYR:HE2	1.58	0.68
1:A:371:ALA:HB1	1:A:372:PRO:CD	2.25	0.66
1:A:616:THR:CG2	1:A:619:GLY:H	1.97	0.65
1:A:565:ILE:HD11	1:A:603:GLU:HG2	1.79	0.64
1:A:406:THR:HG22	1:A:407:HIS:ND1	2.12	0.64
1:A:907:ARG:HD2	4:A:2240:HOH:O	1.98	0.64
1:A:736:ASP:HB2	4:A:2186:HOH:O	1.99	0.62
1:A:749:TYR:CE2	1:A:772:ASN:ND2	2.68	0.61
1:A:166:LYS:O	1:A:191:VAL:HG23	2.00	0.61
1:A:826:VAL:HG12	3:A:996:SO4:O3	2.01	0.61
1:A:902:PRO:HB2	1:A:904:ASN:OD1	2.01	0.60
1:A:880[B]:SER:HB3	1:A:886[B]:ASN:HD22	1.68	0.59
1:A:568:MET:HE3	1:A:602:ALA:HB1	1.84	0.58
1:A:626:ALA:O	1:A:627:LYS:HB2	2.03	0.58
1:A:888:LEU:HD11	1:A:892:TYR:CE1	2.39	0.58
1:A:789:GLN:HA	4:A:2203:HOH:O	2.02	0.57
1:A:212:PRO:O	1:A:215:SER:HB3	2.04	0.56
1:A:856:PRO:HG3	1:A:883[B]:PRO:HB3	1.87	0.56
1:A:447:GLY:HA2	1:A:691:LEU:HD21	1.86	0.56
1:A:522:PRO:HG3	1:A:641:ALA:HB2	1.88	0.55
1:A:795:PRO:HB3	3:A:996:SO4:O4	2.06	0.55
1:A:703:ARG:HG3	1:A:867:ARG:HG2	1.89	0.54
1:A:482:VAL:HG13	1:A:658:ILE:HG12	1.89	0.54
1:A:799:GLN:HG3	1:A:803:LEU:HD22	1.89	0.54
1:A:478:ALA:O	1:A:482:VAL:HB	2.08	0.54
1:A:736:ASP:CB	4:A:2186:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883[A]:PRO:O	1:A:886[A]:ASN:HB3	2.09	0.53
1:A:462:ARG:HH21	1:A:464:THR:HB	1.73	0.53
1:A:154:SER:HB3	1:A:237:CYS:CB	2.36	0.53
1:A:888:LEU:CD1	1:A:892:TYR:CE1	2.92	0.52
1:A:438:SER:OG	1:A:441:ILE:HG12	2.10	0.51
1:A:181:LEU:HD13	1:A:232:LEU:HD21	1.92	0.51
1:A:625:LEU:HD23	1:A:628:MET:HE1	1.93	0.50
1:A:138:ASN:HA	4:A:2002:HOH:O	2.11	0.49
1:A:568:MET:CE	1:A:602:ALA:HB1	2.41	0.49
1:A:697:ARG:HD2	1:A:699:GLN:HE22	1.77	0.49
1:A:418:THR:O	1:A:422:ARG:HG3	2.12	0.49
1:A:625:LEU:HD23	1:A:628:MET:CE	2.42	0.48
1:A:877:LYS:HG2	1:A:911:MET:CE	2.44	0.48
1:A:371:ALA:HB1	1:A:372:PRO:HD2	1.94	0.48
1:A:216:GLN:H	1:A:216:GLN:CD	2.17	0.48
1:A:138:ASN:HD22	1:A:167:GLU:HB3	1.79	0.48
1:A:313:GLU:HA	1:A:313:GLU:OE2	2.14	0.48
1:A:188:CYS:HB3	1:A:209:CYS:SG	2.54	0.47
1:A:197:ILE:HG12	1:A:208:LEU:HD12	1.96	0.47
1:A:357:MET:HG2	4:A:2010:HOH:O	2.14	0.47
1:A:879:LEU:C	1:A:881[A]:LYS:H	2.18	0.47
1:A:520:CYS:HA	1:A:615:CYS:O	2.14	0.47
1:A:462:ARG:HE	1:A:462:ARG:HB3	1.56	0.47
1:A:838:ILE:HA	1:A:871:ILE:O	2.14	0.46
1:A:146:ASN:HA	1:A:156:ILE:HD11	1.98	0.46
1:A:162:ARG:HB3	1:A:266:GLU:HG2	1.97	0.46
1:A:751:THR:HG21	1:A:768:THR:HG22	1.96	0.46
1:A:514:ASN:CB	1:A:631:ARG:HD3	2.45	0.46
1:A:482:VAL:HG21	1:A:490:ILE:HD11	1.97	0.46
1:A:745:PRO:HB2	1:A:868:TYR:O	2.15	0.46
1:A:846:GLU:CG	1:A:881[A]:LYS:HG3	2.44	0.46
1:A:165:CYS:C	1:A:166:LYS:HG3	2.37	0.45
1:A:750:VAL:HB	1:A:900:GLU:HG2	1.98	0.45
1:A:643:GLU:HB2	1:A:644:PRO:HD3	1.97	0.45
1:A:625:LEU:HA	1:A:628:MET:CE	2.43	0.45
1:A:473:HIS:CD2	4:A:2079:HOH:O	2.69	0.45
1:A:468:LEU:HB3	1:A:469:PRO:HD2	1.99	0.45
1:A:671:MET:HA	1:A:671:MET:CE	2.47	0.45
1:A:158:ASN:OD1	1:A:162:ARG:NH2	2.50	0.44
1:A:332:ARG:NH1	1:A:390:GLU:OE2	2.50	0.44
1:A:514:ASN:CG	1:A:631:ARG:HD3	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HH12	1:A:390:GLU:CD	2.21	0.44
1:A:774:GLU:HG2	1:A:806:TYR:CE2	2.44	0.44
1:A:847:HIS:CD2	1:A:882[B]:GLN:HE22	2.36	0.44
1:A:384:PRO:HB3	1:A:389:ASP:HA	2.00	0.43
1:A:584:THR:HB	1:A:586:GLU:H	1.84	0.43
1:A:156:ILE:HD13	1:A:238:PHE:CD1	2.55	0.42
1:A:441:ILE:HG22	1:A:445:LEU:CD1	2.50	0.42
1:A:455:ILE:HG13	1:A:485:ARG:C	2.39	0.42
1:A:444:LYS:HG2	1:A:487:LEU:HD23	2.01	0.42
1:A:456:LYS:O	1:A:457:CYS:HB3	2.20	0.41
1:A:420:PHE:HA	1:A:423:MET:HE3	2.03	0.41
1:A:877:LYS:HE2	1:A:911:MET:HE3	2.02	0.41
1:A:772:ASN:O	1:A:776:ILE:HG12	2.21	0.41
1:A:856:PRO:HB3	1:A:884[A]:LEU:HD22	2.03	0.41
1:A:162:ARG:HH12	1:A:262:ILE:HG22	1.86	0.40
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.91	0.40
1:A:482:VAL:HG22	1:A:488:SER:CB	2.50	0.40
1:A:489:LEU:HA	1:A:659:LEU:O	2.20	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	770/800 (96%)	737 (96%)	30 (4%)	3 (0%)	34 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	883[A]	PRO
1	A	883[B]	PRO
1	A	403	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	682/699 (98%)	647 (95%)	35 (5%)	24	45

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	THR
1	A	156	ILE
1	A	176	LEU
1	A	179	THR
1	A	184	TYR
1	A	205	VAL
1	A	249	GLN
1	A	253	ARG
1	A	277	LEU
1	A	313	GLU
1	A	340	LYS
1	A	373	LEU
1	A	396	ARG
1	A	406	THR
1	A	429	THR
1	A	437	VAL
1	A	450	VAL
1	A	457	CYS
1	A	471	LEU
1	A	482	VAL
1	A	489	LEU
1	A	530	LEU
1	A	584	THR
1	A	616	THR
1	A	631	ARG
1	A	646	CYS
1	A	671	MET
1	A	697	ARG
1	A	744	LYS
1	A	751	THR

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Mol	Chain	Res	Type
1	A	774	GLU
1	A	803	LEU
1	A	808	GLN
1	A	815	THR
1	A	897	VAL

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

Mol	Chain	Res	Type
1	A	138	ASN
1	A	473	HIS
1	A	484	GLN
1	A	699	GLN
1	A	772	ASN
1	A	808	GLN
1	A	848	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\# Z > 2$
3	SO4	A	994	-	4,4,4	0.21	0	6,6,6	0.38	0
3	SO4	A	990	-	4,4,4	0.27	0	6,6,6	0.30	0
3	SO4	A	991	-	4,4,4	0.13	0	6,6,6	0.43	0
3	SO4	A	996	-	4,4,4	0.14	0	6,6,6	0.52	0
3	SO4	A	992	-	4,4,4	0.17	0	6,6,6	0.16	0
3	SO4	A	995	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	A	997	-	4,4,4	0.11	0	6,6,6	0.20	0
3	SO4	A	993	-	4,4,4	0.32	0	6,6,6	0.41	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	996	SO4	3	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	773/800 (96%)	0.37	67 (8%) 10 10	7, 20, 34, 50	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	179	THR	4.7
1	A	268	LEU	4.5
1	A	184	TYR	4.5
1	A	587	LEU	4.3
1	A	373	LEU	4.3
1	A	274	SER	4.1
1	A	270	LYS	3.8
1	A	217	SER	3.8
1	A	136	TYR	3.8
1	A	152	SER	3.7
1	A	148	ARG	3.6
1	A	585	GLY	3.6
1	A	176	LEU	3.6
1	A	249	GLN	3.5
1	A	369	ASP	3.5
1	A	125	TYR	3.4
1	A	134	VAL	3.3
1	A	216	GLN	3.3
1	A	271	GLU	3.3
1	A	196	PHE	3.2
1	A	267	GLU	3.2
1	A	131	PRO	3.0
1	A	158	ASN	3.0
1	A	257	ILE	3.0
1	A	205	VAL	2.9
1	A	171	HIS	2.9
1	A	275	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	258	THR	2.9
1	A	269	TRP	2.9
1	A	265	LEU	2.8
1	A	241	TRP	2.8
1	A	588	SER	2.8
1	A	590	ALA	2.8
1	A	259	ALA	2.8
1	A	207	LEU	2.8
1	A	263	ASN	2.7
1	A	913	PHE	2.7
1	A	584	THR	2.7
1	A	589	SER	2.6
1	A	120	ILE	2.6
1	A	251	GLN	2.6
1	A	586	GLU	2.6
1	A	247	SER	2.6
1	A	135	VAL	2.6
1	A	264	LYS	2.5
1	A	172	LYS	2.5
1	A	368	GLY	2.5
1	A	260	GLN	2.5
1	A	151	THR	2.4
1	A	118	LEU	2.4
1	A	277	LEU	2.4
1	A	288	GLU	2.4
1	A	150	ASN	2.4
1	A	261	GLN	2.4
1	A	760	SER	2.4
1	A	218	SER	2.3
1	A	206	VAL	2.3
1	A	846	GLU	2.3
1	A	456	LYS	2.3
1	A	881[A]	LYS	2.3
1	A	178	GLU	2.3
1	A	242	LEU	2.2
1	A	583	GLU	2.2
1	A	370	LEU	2.2
1	A	576	LYS	2.1
1	A	162	ARG	2.1
1	A	262	ILE	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(\AA^2)	Q<0.9
3	SO4	A	997	5/5	0.91	0.28	79,79,79,80	5
3	SO4	A	992	5/5	0.93	0.24	91,92,92,93	0
2	ZN	A	3	1/1	0.94	0.09	79,79,79,79	0
3	SO4	A	994	5/5	0.95	0.17	51,52,53,55	0
3	SO4	A	996	5/5	0.97	0.26	49,51,54,54	0
2	ZN	A	2	1/1	0.98	0.13	111,111,111,111	1
3	SO4	A	991	5/5	0.98	0.12	53,53,54,54	0
2	ZN	A	1	1/1	0.99	0.08	58,58,58,58	0
3	SO4	A	995	5/5	0.99	0.12	36,38,40,41	0
3	SO4	A	993	5/5	0.99	0.17	36,37,40,40	0
3	SO4	A	990	5/5	1.00	0.19	14,18,22,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.