



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:23 AM UTC

PDB ID : 7KDF / pdb_00007kdf
Title : Structure of Stu2 Bound to dwarf Ndc80c
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Deposited on : 2020-10-08
Resolution : 2.72 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

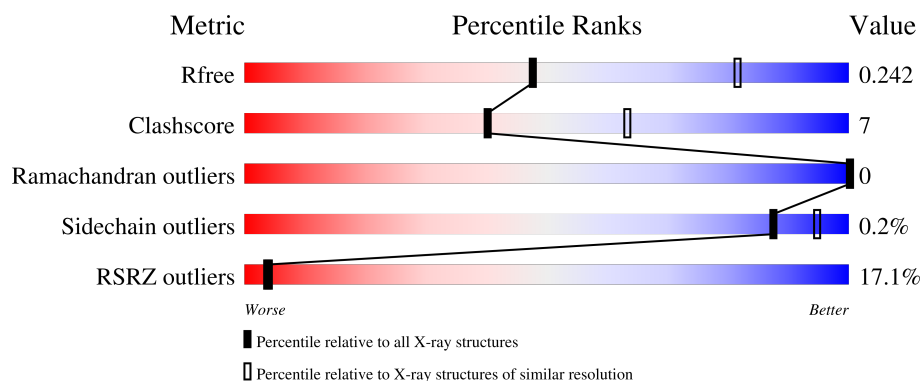
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	277	7% 84% 13% .
2	B	215	10% 88% 8% .
3	C	100	33% 72% 23% 5%
4	D	115	33% 79% 17% ..
5	E	33	30% 70% 15% 15%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5994 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 NDC80 isoform 1,NDC80 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	2	0
			2286	1469	384	427	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	SER	-	expression tag	UNP A0A6A5Q2M2
A	112	ASN	-	expression tag	UNP A0A6A5Q2M2
A	113	ALA	-	expression tag	UNP A0A6A5Q2M2

- Molecule 2 is a protein called NUF2 isoform 1,NUF2 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	207	Total	C	N	O	S	0	0	0
			1691	1070	273	336	12			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	SER	-	expression tag	UNP A0A6A5Q3C2
B	-16	ASN	-	expression tag	UNP A0A6A5Q3C2
B	-15	ALA	-	expression tag	UNP A0A6A5Q3C2
B	-14	SER	-	expression tag	UNP A0A6A5Q3C2
B	-13	ILE	-	expression tag	UNP A0A6A5Q3C2
B	-12	PHE	-	expression tag	UNP A0A6A5Q3C2
B	-11	LYS	-	expression tag	UNP A0A6A5Q3C2
B	-10	ASP	-	expression tag	UNP A0A6A5Q3C2
B	-9	LEU	-	expression tag	UNP A0A6A5Q3C2
B	-8	GLU	-	expression tag	UNP A0A6A5Q3C2
B	-7	ALA	-	expression tag	UNP A0A6A5Q3C2
B	-6	LEU	-	expression tag	UNP A0A6A5Q3C2
B	-5	SER	-	expression tag	UNP A0A6A5Q3C2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	PHE	-	expression tag	UNP A0A6A5Q3C2
B	-3	GLN	-	expression tag	UNP A0A6A5Q3C2
B	-2	SER	-	expression tag	UNP A0A6A5Q3C2
B	-1	ASN	-	expression tag	UNP A0A6A5Q3C2
B	0	ALA	-	expression tag	UNP A0A6A5Q3C2

- Molecule 3 is a protein called Spc24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	0	0	0
			793	499	137	156	1			

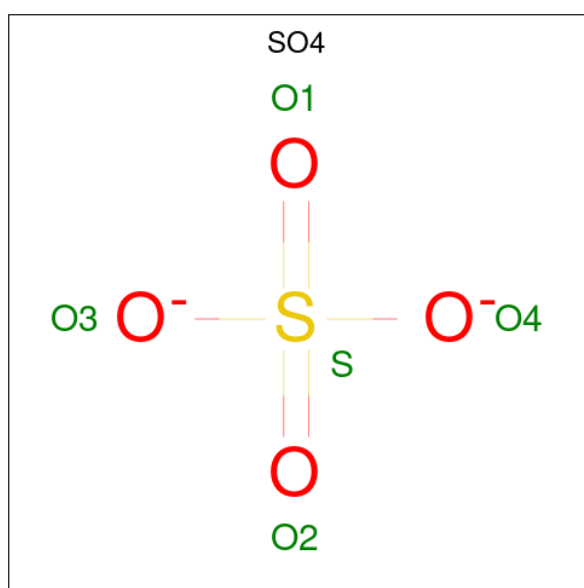
- Molecule 4 is a protein called SPC25 isoform 1,SPC25 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	113	Total	C	N	O	S	0	0	0
			883	553	163	163	4			

- Molecule 5 is a protein called STU2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	28	Total	C	N	O	Se	0	0	0
			216	129	47	39	1			

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



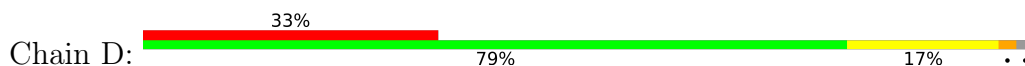
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	E	1	Total O S 5 4 1	0	0

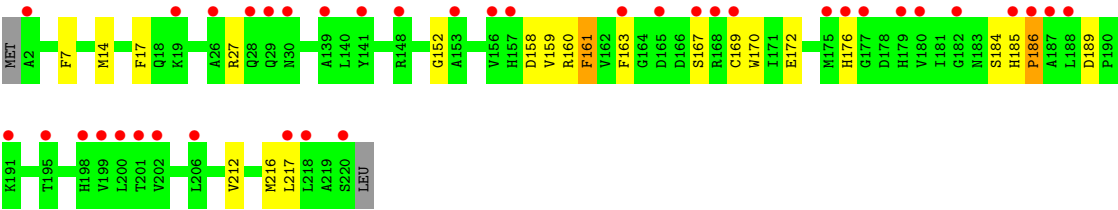
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	31	Total O 31 31	0	0
7	B	50	Total O 50 50	0	0
7	C	8	Total O 8 8	0	0
7	D	1	Total O 1 1	0	0
7	E	5	Total O 5 5	0	0

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- Molecule 1: NDC80 isoform 1,NDC80 isoform 1





● Molecule 5: STU2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	170.89Å 183.18Å 124.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.72 – 2.72 42.72 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.72-2.72) 95.2 (42.72-2.72)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.242 0.203 , 0.242	Depositor DCC
R_{free} test set	2015 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	58.2	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.0	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	5994	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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

5.1 Standard geometry

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	0.19	0/2337	0.37	0/3146
2	B	0.20	0/1714	0.45	0/2307
3	C	0.24	0/803	0.50	0/1082
4	D	0.39	2/899 (0.2%)	0.53	1/1218 (0.1%)
5	E	0.27	0/214	0.48	0/280
All	All	0.24	2/5967 (0.0%)	0.44	1/8033 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	186	PRO	C-O	7.60	1.29	1.24
4	D	186	PRO	CA-C	-6.77	1.46	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	186	PRO	O-C-N	-6.10	118.40	122.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2286	0	2310	32	0
2	B	1691	0	1661	17	0
3	C	793	0	789	19	0
4	D	883	0	869	21	0
5	E	216	0	241	3	0
6	A	10	0	0	0	0
6	B	15	0	0	0	0
6	E	5	0	0	0	0
7	A	31	0	0	1	0
7	B	50	0	0	2	0
7	C	8	0	0	0	0
7	D	1	0	0	0	0
7	E	5	0	0	0	0
All	All	5994	0	5870	78	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 (78) 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:172:ARG:HE	1:A:229:ASN:HD21	1.27	0.82
1:A:180:THR:HG23	1:A:182:SER:H	1.50	0.77
1:A:203:ASN:ND2	1:A:205:SER:OG	2.22	0.73
4:D:152:GLY:N	4:D:158:ASP:O	2.26	0.68
5:E:873:ILE:HA	5:E:876:MSE:HE3	1.79	0.64
4:D:158:ASP:OD2	4:D:176:HIS:NE2	2.30	0.64
2:B:35:PRO:HB2	2:B:113:PRO:HB2	1.80	0.64
4:D:186:PRO:HD2	4:D:217:LEU:HD22	1.80	0.62
1:A:650:ILE:HD13	3:C:14:PHE:CD2	2.34	0.62
4:D:161:PHE:N	4:D:161:PHE:HD1	1.98	0.61
1:A:650:ILE:HG23	3:C:18:VAL:HG21	1.82	0.61
3:C:173:ASP:OD2	3:C:176:ASN:N	2.30	0.61
1:A:246:GLN:HG2	1:A:249:GLN:HE21	1.67	0.59
1:A:246:GLN:HA	1:A:249:GLN:HG3	1.85	0.58
3:C:178:GLN:HG3	3:C:191:ILE:HD12	1.85	0.58
1:A:283:PHE:HE1	2:B:135:ARG:HB2	1.66	0.58
1:A:206:GLN:HG3	1:A:214:ASN:HD22	1.68	0.58
4:D:161:PHE:N	4:D:161:PHE:CD1	2.72	0.57
2:B:442:MET:HE2	4:D:17:PHE:HB3	1.87	0.56
1:A:195:ARG:HG2	1:A:195:ARG:HH21	1.71	0.56
1:A:264:GLN:HG2	1:A:267:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:NH2	7:A:802:HOH:O	2.39	0.55
2:B:83:THR:O	2:B:86:VAL:HG12	2.07	0.55
1:A:647:ILE:HD11	3:C:8:LEU:HD21	1.88	0.54
1:A:157:PRO:HG3	1:A:215:TRP:CZ2	2.43	0.54
1:A:261:LEU:HD23	2:B:414:LYS:HE3	1.89	0.53
4:D:169:CYS:HB3	4:D:217:LEU:HB3	1.91	0.53
4:D:184:SER:OG	4:D:217:LEU:HD21	2.09	0.53
1:A:630:GLU:OE2	1:A:630:GLU:HA	2.08	0.53
1:A:643:HIS:O	1:A:647:ILE:HG12	2.09	0.53
2:B:86:VAL:HG23	2:B:111:TYR:CZ	2.44	0.53
1:A:274:MET:HE3	1:A:311:PHE:HB2	1.90	0.52
1:A:246:GLN:HG2	1:A:249:GLN:NE2	2.24	0.52
1:A:180:THR:HG22	1:A:186:GLU:OE2	2.11	0.52
1:A:195:ARG:HG2	1:A:195:ARG:NH2	2.25	0.50
4:D:159:VAL:HG12	4:D:161:PHE:CE1	2.46	0.50
1:A:634:ASP:OD2	1:A:638:LYS:HE2	2.12	0.49
3:C:172:LEU:CD1	3:C:179:VAL:HG22	2.43	0.48
3:C:172:LEU:HD13	3:C:179:VAL:HG22	1.96	0.48
1:A:172:ARG:NE	1:A:229:ASN:HD21	2.04	0.48
4:D:160:ARG:HB2	4:D:172:GLU:HG2	1.95	0.48
3:C:210:ARG:C	3:C:211:LEU:HD12	2.39	0.47
3:C:176:ASN:O	3:C:178:GLN:HG2	2.14	0.47
4:D:212:VAL:O	4:D:216:MET:HG3	2.14	0.47
3:C:192:LEU:HD12	3:C:193:PRO:HD2	1.97	0.47
1:A:152:LYS:O	1:A:155:LYS:HB2	2.16	0.46
1:A:206:GLN:HG3	1:A:214:ASN:ND2	2.29	0.46
4:D:170:TRP:NE1	4:D:185:HIS:HB2	2.30	0.46
2:B:31:ASN:ND2	7:B:604:HOH:O	2.49	0.45
2:B:442:MET:O	2:B:446:LEU:HD23	2.17	0.45
2:B:91:LYS:NZ	7:B:603:HOH:O	2.47	0.45
4:D:185:HIS:HB3	4:D:186:PRO:HD3	1.97	0.45
3:C:199:SER:HB3	3:C:203:LYS:NZ	2.30	0.45
3:C:14:PHE:HE1	5:E:866:THR:HG23	1.82	0.44
1:A:652:ILE:HD11	4:D:7:PHE:CZ	2.52	0.44
4:D:189:ASP:N	4:D:189:ASP:OD1	2.49	0.44
2:B:442:MET:HE2	4:D:17:PHE:CB	2.48	0.43
1:A:670:GLU:OE2	4:D:27:ARG:HG3	2.18	0.43
1:A:639:ARG:HB2	2:B:420:PHE:HE2	1.83	0.43
3:C:179:VAL:HG23	3:C:194:LEU:HD21	1.99	0.43
2:B:442:MET:CE	4:D:14:MET:HA	2.48	0.43
2:B:134:GLU:OE1	2:B:135:ARG:NH1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:162:LEU:HD23	3:C:162:LEU:HA	1.87	0.42
3:C:199:SER:HB3	3:C:203:LYS:HZ3	1.83	0.42
1:A:121:ASP:O	1:A:125:GLN:HG3	2.19	0.42
2:B:107:MET:HE3	2:B:107:MET:HB3	1.72	0.42
4:D:163:PHE:HB2	4:D:169:CYS:HB2	2.00	0.42
4:D:167:SER:O	4:D:167:SER:OG	2.30	0.42
2:B:84:LEU:HD23	2:B:84:LEU:HA	1.92	0.42
1:A:252:THR:O	1:A:256:GLN:HG2	2.20	0.42
3:C:30:ALA:O	3:C:34:ILE:HG13	2.20	0.42
3:C:204:THR:HG22	3:C:208:TRP:HD1	1.86	0.41
4:D:160:ARG:C	4:D:161:PHE:HD1	2.28	0.41
5:E:879:LYS:O	5:E:882:ARG:HG2	2.21	0.41
1:A:279:LEU:HB3	2:B:132:ARG:HH12	1.86	0.41
2:B:441:TYR:HD1	3:C:24:ILE:HG12	1.86	0.41
1:A:172:ARG:HE	1:A:229:ASN:ND2	2.08	0.40
3:C:184:LYS:NZ	3:C:210:ARG:O	2.54	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	270/277 (98%)	268 (99%)	2 (1%)	0	100	100
2	B	203/215 (94%)	199 (98%)	4 (2%)	0	100	100
3	C	93/100 (93%)	88 (95%)	5 (5%)	0	100	100
4	D	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
5	E	26/33 (79%)	24 (92%)	2 (8%)	0	100	100
All	All	703/740 (95%)	686 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	261/266 (98%)	261 (100%)	0	100	100
2	B	194/201 (96%)	194 (100%)	0	100	100
3	C	90/95 (95%)	90 (100%)	0	100	100
4	D	94/96 (98%)	93 (99%)	1 (1%)	65	84
5	E	22/26 (85%)	22 (100%)	0	100	100
All	All	661/684 (97%)	660 (100%)	1 (0%)	87	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	161	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	214	ASN
1	A	229	ASN
1	A	645	GLN
2	B	50	ASN
2	B	76	ASN
2	B	116	GLN
2	B	417	GLN
2	B	439	ASN
3	C	26	GLN
3	C	197	ASN
4	D	18	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	SO4	B	501	-	4,4,4	0.21	0	6,6,6	0.16	0
6	SO4	B	503	-	4,4,4	0.25	0	6,6,6	0.14	0
6	SO4	B	502	-	4,4,4	0.24	0	6,6,6	0.10	0
6	SO4	A	701	-	4,4,4	0.25	0	6,6,6	0.10	0
6	SO4	E	901	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	A	702	-	4,4,4	0.24	0	6,6,6	0.06	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

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	270/277 (97%)	0.35	20 (7%)	20	18	31, 71, 120, 171	2 (0%)
2	B	207/215 (96%)	0.40	21 (10%)	12	11	38, 62, 134, 190	0
3	C	95/100 (95%)	1.50	33 (34%)	1	1	59, 124, 215, 232	0
4	D	113/115 (98%)	1.76	38 (33%)	1	1	77, 124, 170, 206	0
5	E	27/33 (81%)	2.11	10 (37%)	1	1	78, 96, 140, 161	0
All	All	712/740 (96%)	0.81	122 (17%)	4	4	31, 78, 170, 232	2 (0%)

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	157	HIS	8.4
5	E	863	ALA	7.0
4	D	156	VAL	7.0
2	B	-13	ILE	7.0
3	C	212	GLY	6.5
5	E	888	THR	5.8
3	C	201	PHE	5.8
1	A	113	ALA	5.6
5	E	885	THR	5.5
3	C	198	LEU	5.5
2	B	-15	ALA	5.4
3	C	189	ILE	5.3
2	B	67	THR	5.2
5	E	884	GLY	5.1
4	D	28	GLN	4.9
2	B	-12	PHE	4.5
4	D	167	SER	4.5
5	E	861	ARG	4.5
4	D	198	HIS	4.2
5	E	883	GLU	4.2

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Mol	Chain	Res	Type	RSRZ
4	D	29	GLN	4.1
1	A	262	ASP	4.1
5	E	862	ALA	4.1
4	D	202	VAL	4.0
2	B	-14	SER	3.9
2	B	69	ASP	3.9
3	C	183	ARG	3.9
3	C	191	ILE	3.9
5	E	864	ALA	3.8
3	C	200	ASP	3.8
4	D	175	MET	3.8
3	C	181	ILE	3.8
1	A	260	THR	3.7
3	C	184	LYS	3.7
1	A	156	GLN	3.7
3	C	202	TYR	3.6
4	D	168	ARG	3.5
4	D	179	HIS	3.5
4	D	177	GLY	3.5
5	E	887	ARG	3.5
4	D	218	LEU	3.4
3	C	180	LEU	3.4
4	D	199	VAL	3.3
3	C	171	ILE	3.3
2	B	-10	ASP	3.3
3	C	199	SER	3.2
1	A	181	LYS	3.1
1	A	206	GLN	3.1
2	B	76	ASN	3.1
4	D	165	ASP	3.1
2	B	-9	LEU	3.1
2	B	26	LEU	3.1
1	A	264	GLN	3.1
3	C	192	LEU	3.0
3	C	203	LYS	3.0
2	B	38	ASP	3.0
5	E	886	THR	2.9
4	D	186	PRO	2.9
1	A	202	ILE	2.9
3	C	182	ASN	2.9
4	D	187	ALA	2.9
4	D	188	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	210	ARG	2.9
3	C	190	ASP	2.9
2	B	450	GLN	2.8
3	C	211	LEU	2.8
2	B	-11	LYS	2.8
4	D	220	SER	2.7
4	D	176	HIS	2.7
4	D	185	HIS	2.7
1	A	265	ASP	2.7
4	D	206	LEU	2.7
1	A	160	LYS	2.7
2	B	-6	LEU	2.6
1	A	261	LEU	2.6
3	C	172	LEU	2.6
3	C	169	GLY	2.6
4	D	26	ALA	2.6
4	D	30	ASN	2.6
2	B	68	GLY	2.6
4	D	182	GLY	2.6
4	D	180	VAL	2.6
1	A	180	THR	2.5
3	C	206	TYR	2.5
4	D	2	ALA	2.5
1	A	203	ASN	2.5
2	B	-5	SER	2.5
3	C	187	GLY	2.5
4	D	139	ALA	2.5
4	D	191	LYS	2.4
2	B	135	ARG	2.4
2	B	78	ASN	2.4
3	C	194	LEU	2.4
4	D	169	CYS	2.4
2	B	77	GLU	2.4
3	C	209	GLU	2.4
1	A	259	LYS	2.4
4	D	163	PHE	2.4
3	C	178	GLN	2.3
4	D	141	TYR	2.3
4	D	195	THR	2.3
3	C	5	ASP	2.3
3	C	193	PRO	2.3
3	C	174	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	153	ALA	2.3
3	C	205	LYS	2.3
4	D	148	ARG	2.3
2	B	-2	SER	2.2
1	A	145	THR	2.2
2	B	-3	GLN	2.2
4	D	200	LEU	2.2
1	A	142	ASP	2.2
3	C	188	ASN	2.1
4	D	19	LYS	2.1
4	D	217	LEU	2.1
1	A	144	GLU	2.1
1	A	114	ARG	2.1
3	C	35	ARG	2.1
3	C	204	THR	2.1
4	D	201	THR	2.1
1	A	249	GLN	2.0
1	A	148	PRO	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(Å ²)	Q<0.9
6	SO4	A	702	5/5	0.69	0.09	146,162,169,176	0
6	SO4	E	901	5/5	0.79	0.10	91,106,142,143	0
6	SO4	A	701	5/5	0.83	0.11	98,108,137,157	0
6	SO4	B	501	5/5	0.92	0.10	64,74,85,91	1
6	SO4	B	503	5/5	0.98	0.06	51,52,56,63	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	502	5/5	0.98	0.09	43,46,47,48	5

6.5 Other polymers [i](#)

There are no such residues in this entry.