



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 1Z3I / pdb_00001z3i
Title : Structure of the SWI2/SNF2 chromatin remodeling domain of eukaryotic Rad54
Authors : Thoma, N.H.; Czyzewski, B.K.; Alexeev, A.A.; Mazin, A.V.; Kowalczykowski, S.C.; Pavletich, N.P.
Deposited on : 2005-03-12
Resolution : 3.00 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

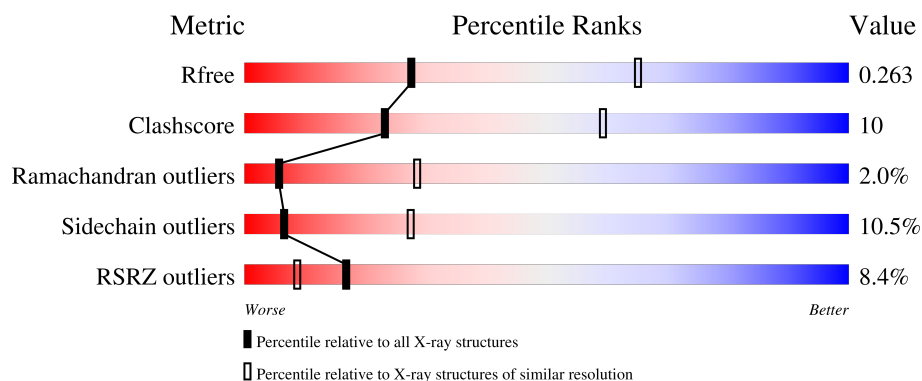
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	X	644	8% 73% 22% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 5098 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 similar to RAD54-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	644	Total	C	N	O	S	0	0	0
			5052	3190	906	928	28			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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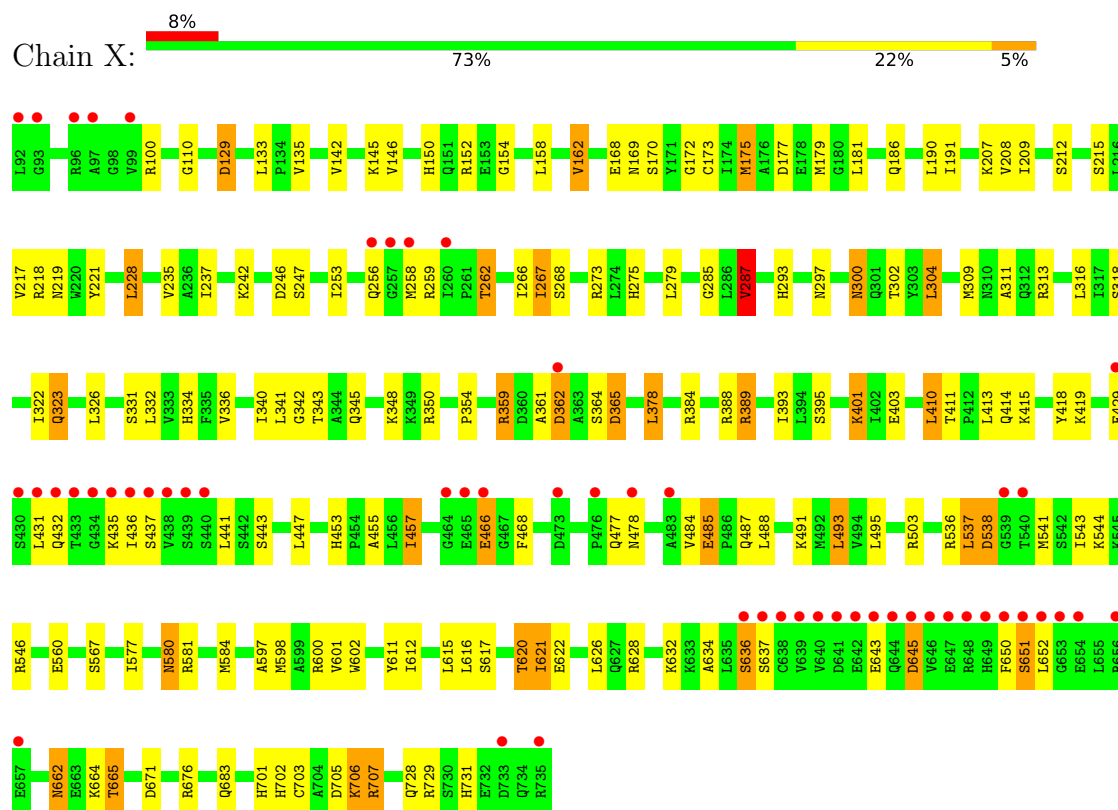
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		
3	X	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

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: similar to RAD54-like



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	205.05Å 205.05Å 189.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 99.6 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.198 , 0.234 0.232 , 0.263	Depositor DCC
R_{free} test set	1545 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 22.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5098	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 3.80% 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	X	0.54	0/5148	0.88	3/6959 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	287	VAL	CB-CA-C	-6.62	100.75	110.81
1	X	228	LEU	N-CA-C	5.95	120.14	112.41
1	X	580	ASN	N-CA-C	-5.71	106.94	114.31

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	X	5052	0	5073	105	0
2	X	1	0	0	0	0
3	X	45	0	0	1	0
All	All	5098	0	5073	105	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 10.

All (105) 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:X:683:GLN:NE2	1:X:702:HIS:H	1.64	0.94
1:X:453:HIS:HD2	1:X:455:ALA:H	1.15	0.90
1:X:262:THR:O	1:X:262:THR:HG22	1.75	0.86
1:X:620:THR:HG22	1:X:622:GLU:H	1.40	0.84
1:X:253:ILE:HD11	1:X:279:LEU:HD23	1.60	0.84
1:X:343:THR:HG22	1:X:345:GLN:H	1.47	0.79
1:X:209:ILE:CG2	1:X:267:ILE:HD11	2.14	0.77
1:X:538:ASP:H	1:X:541:MET:HE2	1.49	0.76
1:X:162:VAL:HG22	1:X:313:ARG:HB2	1.70	0.74
1:X:617:SER:O	1:X:620:THR:HB	1.88	0.73
1:X:728:GLN:HE21	1:X:729:ARG:H	1.37	0.72
1:X:262:THR:O	1:X:262:THR:CG2	2.38	0.72
1:X:287:VAL:HG22	1:X:311:ALA:HB3	1.72	0.72
1:X:209:ILE:HG23	1:X:267:ILE:HD11	1.73	0.70
1:X:150:HIS:O	1:X:389:ARG:NH2	2.24	0.70
1:X:287:VAL:HG13	1:X:309:MET:HE1	1.73	0.69
1:X:584:MET:HE1	1:X:597:ALA:HB3	1.74	0.68
1:X:683:GLN:HE22	1:X:702:HIS:H	1.42	0.68
1:X:411:THR:HG22	1:X:413:LEU:H	1.60	0.67
1:X:177:ASP:OD2	1:X:389:ARG:NH1	2.27	0.67
1:X:665:THR:HG23	1:X:671:ASP:OD2	1.96	0.66
1:X:287:VAL:CG1	1:X:309:MET:HE1	2.26	0.66
1:X:491:LYS:HG2	1:X:615:LEU:HB3	1.79	0.64
1:X:110:GLY:O	1:X:152:ARG:NH2	2.31	0.64
1:X:395:SER:HB2	1:X:731:HIS:ND1	2.14	0.63
1:X:410:LEU:HG	1:X:414:GLN:HB3	1.81	0.62
1:X:158:LEU:HD21	1:X:175:MET:HG3	1.82	0.61
1:X:219:ASN:OD1	1:X:546:ARG:NH1	2.33	0.61
1:X:620:THR:HG22	1:X:622:GLU:N	2.14	0.60
1:X:620:THR:CG2	1:X:622:GLU:H	2.12	0.60
1:X:297:ASN:HD21	1:X:331:SER:H	1.50	0.59
1:X:410:LEU:HD13	1:X:617:SER:HB3	1.84	0.59
1:X:191:ILE:HG23	1:X:208:VAL:HG21	1.85	0.59
1:X:401:LYS:HE3	1:X:602:TRP:CE3	2.38	0.58
1:X:297:ASN:ND2	1:X:331:SER:H	2.02	0.57
1:X:100:ARG:NH1	1:X:133:LEU:O	2.37	0.57
1:X:705:ASP:C	1:X:707:ARG:H	2.13	0.57
1:X:665:THR:CG2	1:X:671:ASP:OD2	2.53	0.56
1:X:418:TYR:OH	1:X:621:ILE:HG13	2.05	0.56
1:X:581:ARG:HG2	1:X:611:TYR:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:300:ASN:H	1:X:300:ASN:HD22	1.54	0.54
1:X:343:THR:HG22	1:X:345:GLN:N	2.18	0.54
1:X:537:LEU:HA	1:X:541:MET:CE	2.37	0.54
1:X:453:HIS:CD2	1:X:455:ALA:H	2.08	0.54
1:X:617:SER:HB2	1:X:620:THR:HG21	1.90	0.53
1:X:580:ASN:ND2	1:X:581:ARG:HG3	2.23	0.52
1:X:628:ARG:HD3	1:X:632:LYS:HE3	1.90	0.52
1:X:334:HIS:HE1	1:X:342:GLY:O	1.93	0.52
1:X:683:GLN:HE22	1:X:701:HIS:HA	1.74	0.52
1:X:218:ARG:HG2	1:X:543:ILE:HG12	1.93	0.51
1:X:536:ARG:O	1:X:541:MET:HE1	2.10	0.51
1:X:487:GLN:HA	1:X:493:LEU:HG	1.92	0.50
1:X:650:PHE:O	1:X:651:SER:HB2	2.12	0.50
1:X:485:GLU:HB3	1:X:488:LEU:HG	1.94	0.50
1:X:616:LEU:HD11	1:X:626:LEU:HG	1.94	0.50
1:X:287:VAL:CG2	1:X:311:ALA:HB3	2.41	0.49
1:X:703:CYS:SG	1:X:705:ASP:O	2.70	0.49
1:X:285:GLY:O	1:X:313:ARG:HG2	2.13	0.49
1:X:597:ALA:O	1:X:600:ARG:HG2	2.12	0.49
1:X:177:ASP:CG	1:X:389:ARG:HH11	2.22	0.48
1:X:168:GLU:O	1:X:169:ASN:HB2	2.13	0.48
1:X:273:ARG:NH1	1:X:302:THR:OG1	2.37	0.48
1:X:293:HIS:HB3	1:X:318:SER:HB2	1.96	0.48
1:X:411:THR:HG22	1:X:413:LEU:N	2.27	0.48
1:X:172:GLY:HA3	1:X:336:VAL:O	2.13	0.48
1:X:154:GLY:HA3	1:X:186:GLN:OE1	2.13	0.48
1:X:453:HIS:HE1	1:X:485:GLU:O	1.97	0.47
1:X:477:GLN:H	1:X:477:GLN:CD	2.23	0.47
1:X:457:ILE:HD12	1:X:457:ILE:HA	1.77	0.47
1:X:158:LEU:HD23	1:X:173:CYS:SG	2.55	0.46
1:X:580:ASN:HD22	1:X:581:ARG:HG3	1.81	0.46
1:X:598:MET:HE3	1:X:612:ILE:HG21	1.97	0.46
1:X:584:MET:HE3	1:X:598:MET:HG3	1.98	0.46
1:X:350:ARG:O	1:X:354:PRO:HG2	2.15	0.46
1:X:388:ARG:HD3	3:X:736:SO4:O4	2.16	0.45
1:X:341:LEU:HD23	1:X:341:LEU:HA	1.83	0.45
1:X:441:LEU:HD12	1:X:645:ASP:HA	1.99	0.45
1:X:662:ASN:HD22	1:X:664:LYS:H	1.64	0.44
1:X:212:SER:O	1:X:268:SER:HA	2.16	0.44
1:X:246:ASP:OD1	1:X:275:HIS:HD2	2.00	0.44
1:X:361:ALA:O	1:X:362:ASP:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:364:SER:O	1:X:365:ASP:CB	2.66	0.44
1:X:142:VAL:HA	1:X:145:LYS:HE2	2.00	0.44
1:X:401:LYS:HD3	1:X:403:GLU:CG	2.48	0.44
1:X:332:LEU:C	1:X:332:LEU:HD23	2.42	0.43
1:X:323:GLN:NE2	1:X:323:GLN:H	2.16	0.43
1:X:287:VAL:HG22	1:X:311:ALA:CB	2.46	0.43
1:X:304:LEU:HD12	1:X:304:LEU:HA	1.71	0.43
1:X:457:ILE:HG13	1:X:468:PHE:CE2	2.53	0.43
1:X:705:ASP:O	1:X:707:ARG:N	2.52	0.43
1:X:359:ARG:HH11	1:X:359:ARG:HB2	1.84	0.43
1:X:150:HIS:HB3	1:X:393:ILE:HD12	2.01	0.42
1:X:170:SER:HB2	1:X:340:ILE:HG23	2.01	0.42
1:X:466:GLU:H	1:X:466:GLU:HG2	1.52	0.42
1:X:378:LEU:HD23	1:X:378:LEU:HA	1.89	0.42
1:X:634:ALA:C	1:X:636:SER:H	2.28	0.41
1:X:217:VAL:HG13	1:X:266:ILE:HG22	2.01	0.41
1:X:221:TYR:CD2	1:X:543:ILE:HG21	2.56	0.41
1:X:447:LEU:HB3	1:X:621:ILE:HD11	2.03	0.41
1:X:237:ILE:HB	1:X:267:ILE:HG23	2.03	0.41
1:X:364:SER:O	1:X:365:ASP:HB2	2.21	0.40
1:X:410:LEU:HB3	1:X:415:LYS:HG3	2.03	0.40
1:X:316:LEU:HD21	1:X:332:LEU:HD11	2.02	0.40
1:X:129:ASP:OD2	1:X:129:ASP:N	2.42	0.40
1:X:620:THR:CG2	1:X:621:ILE:N	2.83	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	X	642/644 (100%)	591 (92%)	38 (6%)	13 (2%)	6 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	362	ASP
1	X	435	LYS
1	X	437	SER
1	X	636	SER
1	X	256	GLN
1	X	436	ILE
1	X	637	SER
1	X	645	ASP
1	X	706	LYS
1	X	258	MET
1	X	643	GLU
1	X	651	SER
1	X	538	ASP

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	X	553/574 (96%)	495 (90%)	58 (10%)	6 27

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	129	ASP
1	X	135	VAL
1	X	146	VAL
1	X	162	VAL
1	X	175	MET
1	X	179	MET
1	X	181	LEU
1	X	190	LEU
1	X	207	LYS
1	X	215	SER
1	X	228	LEU
1	X	235	VAL

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Mol	Chain	Res	Type
1	X	242	LYS
1	X	247	SER
1	X	259	ARG
1	X	262	THR
1	X	267	ILE
1	X	287	VAL
1	X	300	ASN
1	X	304	LEU
1	X	322	ILE
1	X	323	GLN
1	X	326	LEU
1	X	348	LYS
1	X	359	ARG
1	X	365	ASP
1	X	378	LEU
1	X	384	ARG
1	X	389	ARG
1	X	401	LYS
1	X	410	LEU
1	X	419	LYS
1	X	429	GLU
1	X	431	LEU
1	X	432	GLN
1	X	443	SER
1	X	457	ILE
1	X	466	GLU
1	X	478	ASN
1	X	484	VAL
1	X	485	GLU
1	X	493	LEU
1	X	495	LEU
1	X	503	ARG
1	X	537	LEU
1	X	544	LYS
1	X	560	GLU
1	X	567	SER
1	X	577	ILE
1	X	601	VAL
1	X	620	THR
1	X	621	ILE
1	X	652	LEU
1	X	662	ASN

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Mol	Chain	Res	Type
1	X	665	THR
1	X	676	ARG
1	X	706	LYS
1	X	707	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	104	HIS
1	X	136	HIS
1	X	222	ASN
1	X	233	GLN
1	X	255	GLN
1	X	275	HIS
1	X	297	ASN
1	X	300	ASN
1	X	323	GLN
1	X	334	HIS
1	X	404	GLN
1	X	453	HIS
1	X	478	ASN
1	X	596	GLN
1	X	627	GLN
1	X	662	ASN
1	X	683	GLN
1	X	701	HIS
1	X	728	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 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	X	740	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	X	736	-	4,4,4	0.25	0	6,6,6	0.17	0
3	SO4	X	738	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	X	739	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	X	901	-	4,4,4	0.24	0	6,6,6	0.22	0
3	SO4	X	742	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	X	902	-	4,4,4	0.27	0	6,6,6	0.28	0
3	SO4	X	737	-	4,4,4	0.27	0	6,6,6	0.29	0
3	SO4	X	903	-	4,4,4	0.29	0	6,6,6	0.09	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 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	736	SO4	1	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	X	644/644 (100%)	0.49	54 (8%) 17 9	54, 70, 96, 132	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	433	THR	8.7
1	X	637	SER	7.2
1	X	436	ILE	6.3
1	X	437	SER	5.9
1	X	641	ASP	5.8
1	X	642	GLU	5.7
1	X	645	ASP	5.7
1	X	435	LYS	5.4
1	X	636	SER	5.3
1	X	640	VAL	5.2
1	X	643	GLU	5.1
1	X	466	GLU	4.9
1	X	438	VAL	4.6
1	X	644	GLN	4.5
1	X	638	CYS	4.5
1	X	652	LEU	4.3
1	X	92	LEU	4.3
1	X	97	ALA	4.3
1	X	430	SER	4.2
1	X	431	LEU	4.2
1	X	434	GLY	4.1
1	X	432	GLN	4.0
1	X	439	SER	3.9
1	X	733	ASP	3.6
1	X	440	SER	3.6
1	X	93	GLY	3.5
1	X	429	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	X	647	GLU	3.3
1	X	639	VAL	3.3
1	X	478	ASN	3.2
1	X	464	GLY	3.1
1	X	735	ARG	3.1
1	X	96	ARG	3.0
1	X	657	GLU	2.9
1	X	649	HIS	2.9
1	X	540	THR	2.9
1	X	99	VAL	2.8
1	X	646	VAL	2.8
1	X	256	GLN	2.7
1	X	651	SER	2.7
1	X	650	PHE	2.6
1	X	258	MET	2.6
1	X	648	ARG	2.5
1	X	654	GLU	2.5
1	X	260	ILE	2.4
1	X	465	GLU	2.4
1	X	539	GLY	2.3
1	X	476	PRO	2.3
1	X	473	ASP	2.3
1	X	257	GLY	2.2
1	X	656	ARG	2.2
1	X	483	ALA	2.2
1	X	362	ASP	2.1
1	X	653	GLY	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
3	SO4	X	740	5/5	0.75	0.15	125,126,127,127	0
3	SO4	X	738	5/5	0.82	0.15	103,103,104,104	0
3	SO4	X	742	5/5	0.88	0.17	129,130,131,131	0
3	SO4	X	737	5/5	0.90	0.17	96,97,97,97	0
3	SO4	X	736	5/5	0.91	0.13	93,95,96,96	0
3	SO4	X	739	5/5	0.91	0.20	109,109,110,110	0
3	SO4	X	903	5/5	0.94	0.12	79,79,81,81	0
3	SO4	X	902	5/5	0.97	0.09	63,65,67,67	0
3	SO4	X	901	5/5	0.97	0.14	78,78,80,80	0
2	ZN	X	900	1/1	0.99	0.06	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.