



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 12:45 AM UTC

PDB ID : 7CSO / pdb_00007cso
Title : Structure of Ephexin4 DH-PH-SH3
Authors : Zhang, M.; Lin, L.; Wang, C.; Zhu, J.
Deposited on : 2020-08-15
Resolution : 2.39 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

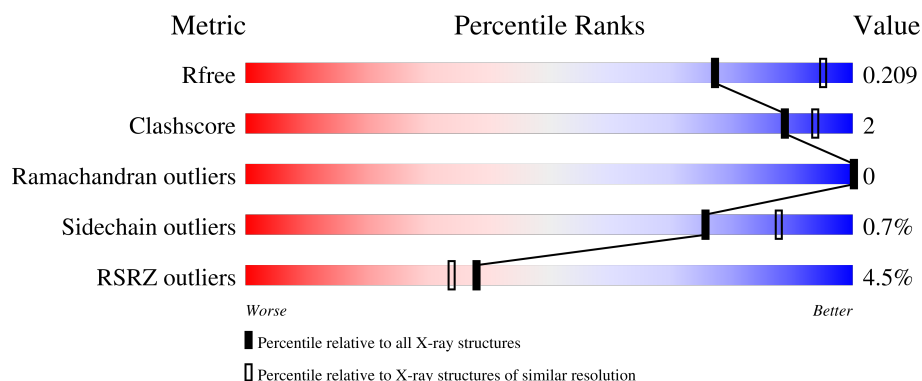
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	459	5% 89% 5% 6%
1	B	459	4% 89% 5% 6%
1	C	459	4% 90% 5% 5%
1	D	459	4% 88% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14658 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 Rho guanine nucleotide exchange factor 16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	0
			3468	2198	603	654	13			
1	B	433	Total	C	N	O	S	0	0	0
			3501	2218	611	659	13			
1	C	437	Total	C	N	O	S	0	0	0
			3501	2216	609	663	13			
1	D	434	Total	C	N	O	S	0	0	0
			3510	2222	615	660	13			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLY	-	expression tag	UNP Q3U5C8
A	256	PRO	-	expression tag	UNP Q3U5C8
A	257	GLY	-	expression tag	UNP Q3U5C8
A	258	SER	-	expression tag	UNP Q3U5C8
A	259	GLY	-	expression tag	UNP Q3U5C8
A	260	PRO	-	expression tag	UNP Q3U5C8
B	255	GLY	-	expression tag	UNP Q3U5C8
B	256	PRO	-	expression tag	UNP Q3U5C8
B	257	GLY	-	expression tag	UNP Q3U5C8
B	258	SER	-	expression tag	UNP Q3U5C8
B	259	GLY	-	expression tag	UNP Q3U5C8
B	260	PRO	-	expression tag	UNP Q3U5C8
C	255	GLY	-	expression tag	UNP Q3U5C8
C	256	PRO	-	expression tag	UNP Q3U5C8
C	257	GLY	-	expression tag	UNP Q3U5C8
C	258	SER	-	expression tag	UNP Q3U5C8
C	259	GLY	-	expression tag	UNP Q3U5C8
C	260	PRO	-	expression tag	UNP Q3U5C8
D	255	GLY	-	expression tag	UNP Q3U5C8
D	256	PRO	-	expression tag	UNP Q3U5C8
D	257	GLY	-	expression tag	UNP Q3U5C8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	258	SER	-	expression tag	UNP Q3U5C8
D	259	GLY	-	expression tag	UNP Q3U5C8
D	260	PRO	-	expression tag	UNP Q3U5C8

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

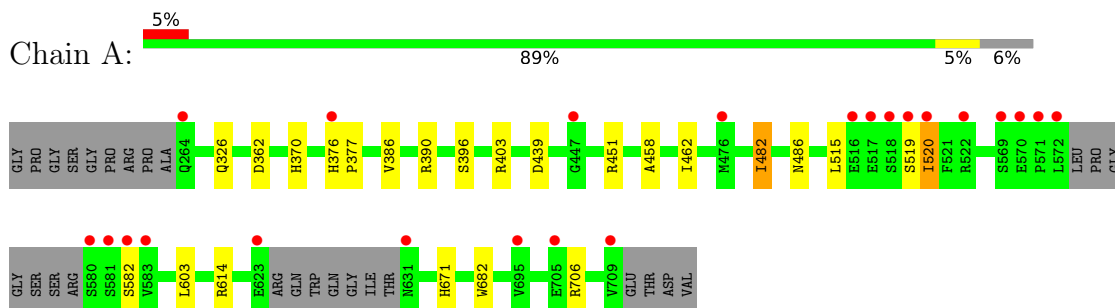
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	152	Total	O	0	0
			152	152		
3	B	132	Total	O	0	0
			132	132		
3	C	139	Total	O	0	0
			139	139		
3	D	190	Total	O	0	0
			190	190		

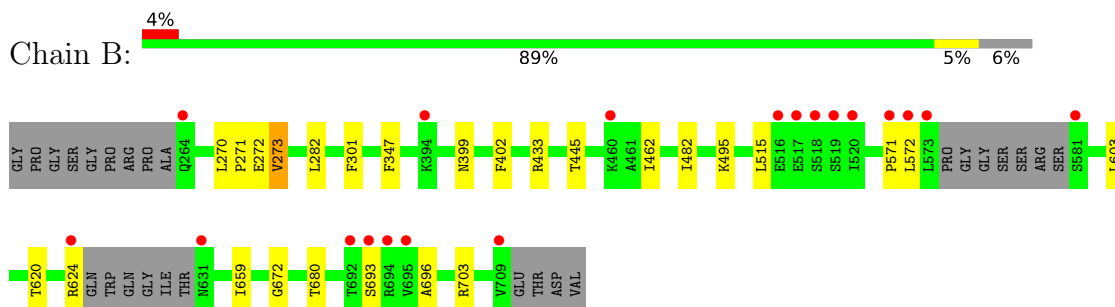
3 Residue-property plots [i](#)

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

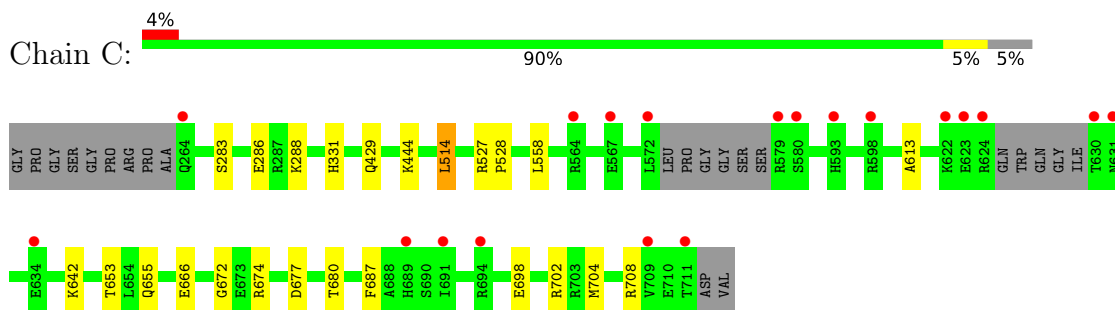
- Molecule 1: Rho guanine nucleotide exchange factor 16



- Molecule 1: Rho guanine nucleotide exchange factor 16

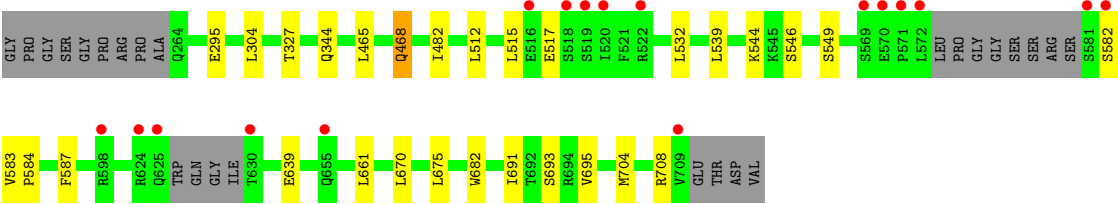


- Molecule 1: Rho guanine nucleotide exchange factor 16



- Molecule 1: Rho guanine nucleotide exchange factor 16





4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	144.44Å 144.44Å 290.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.42 – 2.39 48.42 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.42-2.39) 99.8 (48.42-2.39)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.176 , 0.204 0.185 , 0.209	Depositor DCC
R_{free} test set	6640 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	43.5	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14658	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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	0.53	0/3535	0.80	3/4781 (0.1%)
1	B	0.50	0/3567	0.78	0/4819
1	C	0.46	0/3567	0.69	0/4825
1	D	0.55	0/3577	0.82	4/4833 (0.1%)
All	All	0.51	0/14246	0.77	7/19258 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	520	ILE	N-CA-C	-8.88	104.48	113.10
1	D	582	SER	N-CA-C	-6.63	105.19	113.28
1	D	468	GLN	CB-CA-C	5.72	121.65	110.67
1	D	587	PHE	CA-CB-CG	5.49	119.29	113.80
1	A	582	SER	N-CA-C	-5.36	106.58	113.01
1	A	486	ASN	N-CA-C	-5.20	105.73	111.71
1	D	584	PRO	N-CA-C	5.02	120.51	113.53

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	3468	0	3442	11	0
1	B	3501	0	3501	16	0
1	C	3501	0	3470	14	0
1	D	3510	0	3506	14	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	20	0	0	0	0
3	A	152	0	0	2	0
3	B	132	0	0	1	0
3	C	139	0	0	1	0
3	D	190	0	0	1	0
All	All	14658	0	13919	54	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 2.

All (54) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:661:LEU:HD11	1:D:704:MET:HE1	1.82	0.60
1:B:515:LEU:HB2	1:B:603:LEU:HB3	1.82	0.60
1:C:653:THR:O	1:C:674:ARG:NH2	2.36	0.57
1:C:331:HIS:CE1	1:D:327:THR:HA	2.41	0.56
1:C:674:ARG:HD2	1:C:677:ASP:OD1	2.06	0.55
1:B:433:ARG:NH1	3:B:902:HOH:O	2.33	0.54
1:D:465:LEU:HA	1:D:468:GLN:HG2	1.91	0.53
1:A:671:HIS:HD2	3:A:983:HOH:O	1.91	0.53
1:C:698:GLU:O	1:C:702:ARG:HG3	2.09	0.53
1:B:571:PRO:O	1:B:572:LEU:HB2	2.11	0.51
1:A:515:LEU:HB2	1:A:603:LEU:HB3	1.92	0.51
1:D:639:GLU:HB2	1:D:691:ILE:HD11	1.94	0.50
1:B:445:THR:HG22	1:B:445:THR:O	2.14	0.47
1:A:396:SER:O	1:A:403:ARG:HD3	2.15	0.47
1:C:283:SER:HB2	1:C:286:GLU:H	1.79	0.47
1:C:642:LYS:HG3	1:C:687:PHE:CD2	2.50	0.47
1:D:675:LEU:HA	1:D:704:MET:HE2	1.97	0.47
1:C:558:LEU:O	3:C:901:HOH:O	2.20	0.47
1:C:514:LEU:HD12	1:C:514:LEU:HA	1.77	0.46
1:C:429:GLN:HB3	1:C:655:GLN:NE2	2.30	0.46
1:B:270:LEU:HB2	1:B:273:VAL:HG13	1.97	0.46
1:D:512:LEU:HD12	1:D:532:LEU:HD22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:ASN:HB3	1:B:402:PHE:HB3	1.98	0.45
1:D:304:LEU:HD21	1:D:344:GLN:HG3	2.00	0.44
1:A:386:VAL:O	1:A:390:ARG:HG2	2.17	0.44
1:C:613:ALA:HB2	1:C:666:GLU:HG2	1.99	0.44
1:D:544:LYS:NZ	3:D:905:HOH:O	2.50	0.44
1:A:376:HIS:N	1:A:377:PRO:HD2	2.33	0.44
1:B:672:GLY:O	1:B:680:THR:HA	2.18	0.44
1:B:659:ILE:HG13	1:B:703:ARG:HH22	1.82	0.44
1:A:482:ILE:HD12	1:A:482:ILE:HA	1.86	0.43
1:B:495:LYS:HB2	1:B:495:LYS:HE2	1.78	0.43
1:B:693:SER:HB3	1:B:696:ALA:HB3	1.99	0.43
1:D:482:ILE:HD12	1:D:482:ILE:HA	1.85	0.43
1:D:670:LEU:O	1:D:682:TRP:HA	2.19	0.43
1:C:704:MET:O	1:C:708:ARG:HG2	2.19	0.43
1:D:532:LEU:HG	1:D:539:LEU:HD11	2.00	0.43
1:B:620:THR:O	1:B:624:ARG:HG3	2.19	0.42
1:D:693:SER:OG	1:D:695:VAL:HG12	2.19	0.42
1:A:458:ALA:O	1:A:462:ILE:HG22	2.20	0.42
1:A:370:HIS:HD2	3:A:907:HOH:O	2.03	0.42
1:B:482:ILE:HD12	1:B:482:ILE:HA	1.86	0.42
1:C:288:LYS:HB3	1:C:444:LYS:HD2	2.00	0.42
1:D:704:MET:O	1:D:708:ARG:HG2	2.19	0.41
1:A:614:ARG:HG2	1:A:682:TRP:CE2	2.55	0.41
1:A:362:ASP:HB2	1:A:451:ARG:HD2	2.02	0.41
1:B:282:LEU:HD12	1:B:282:LEU:HA	1.93	0.41
1:A:439:ASP:OD1	1:A:706:ARG:HD2	2.21	0.41
1:B:462:ILE:HD12	1:B:462:ILE:HA	1.84	0.41
1:D:546:SER:HB3	1:D:549:SER:HB3	2.03	0.41
1:B:301:PHE:HB2	1:B:347:PHE:CE1	2.57	0.40
1:B:270:LEU:HA	1:B:271:PRO:HD3	1.97	0.40
1:C:527:ARG:HA	1:C:528:PRO:HD3	1.98	0.40
1:C:672:GLY:O	1:C:680:THR:HA	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/459 (93%)	417 (98%)	9 (2%)	0	100	100
1	B	427/459 (93%)	419 (98%)	8 (2%)	0	100	100
1	C	431/459 (94%)	423 (98%)	8 (2%)	0	100	100
1	D	428/459 (93%)	422 (99%)	6 (1%)	0	100	100
All	All	1712/1836 (93%)	1681 (98%)	31 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	383/411 (93%)	379 (99%)	4 (1%)	68	84
1	B	389/411 (95%)	387 (100%)	2 (0%)	81	91
1	C	386/411 (94%)	385 (100%)	1 (0%)	86	93
1	D	390/411 (95%)	386 (99%)	4 (1%)	68	84
All	All	1548/1644 (94%)	1537 (99%)	11 (1%)	76	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	GLN
1	A	482	ILE
1	A	519	SER
1	A	520	ILE
1	B	272	GLU
1	B	273	VAL
1	C	514	LEU
1	D	295	GLU

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Mol	Chain	Res	Type
1	D	515	LEU
1	D	517	GLU
1	D	583	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	ASN
1	A	429	GLN
1	A	457	GLN
1	A	588	GLN
1	B	316	GLN
1	B	376	HIS
1	B	384	ASN
1	B	429	GLN
1	B	448	HIS
1	B	671	HIS
1	C	357	GLN
1	C	446	GLN
1	C	448	HIS
1	C	671	HIS
1	D	264	GLN
1	D	326	GLN
1	D	376	HIS
1	D	429	GLN
1	D	446	GLN
1	D	560	HIS
1	D	655	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](#)

13 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	$\# Z > 2$
2	SO4	A	803	-	4,4,4	0.51	0	6,6,6	0.08	0
2	SO4	D	803	-	4,4,4	0.26	0	6,6,6	0.35	0
2	SO4	D	802	-	4,4,4	0.52	0	6,6,6	0.10	0
2	SO4	A	802	-	4,4,4	0.31	0	6,6,6	0.24	0
2	SO4	C	802	-	4,4,4	0.29	0	6,6,6	0.52	0
2	SO4	B	801	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	D	801	-	4,4,4	0.51	0	6,6,6	0.09	0
2	SO4	C	803	-	4,4,4	0.51	0	6,6,6	0.08	0
2	SO4	B	802	-	4,4,4	0.34	0	6,6,6	0.44	0
2	SO4	C	801	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	B	803	-	4,4,4	0.49	0	6,6,6	0.08	0
2	SO4	D	804	-	4,4,4	0.23	0	6,6,6	0.31	0
2	SO4	A	801	-	4,4,4	0.30	0	6,6,6	0.28	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	432/459 (94%)	0.09	23 (5%) 32 28	32, 50, 83, 107	0
1	B	433/459 (94%)	0.15	19 (4%) 39 34	33, 52, 88, 122	0
1	C	437/459 (95%)	0.12	19 (4%) 40 36	33, 55, 90, 126	0
1	D	434/459 (94%)	-0.07	17 (3%) 43 39	30, 47, 78, 121	0
All	All	1736/1836 (94%)	0.08	78 (4%) 38 34	30, 50, 87, 126	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	572	LEU	11.1
1	B	573	LEU	9.2
1	A	572	LEU	8.6
1	D	572	LEU	6.2
1	C	579	ARG	6.1
1	A	709	VAL	5.6
1	B	709	VAL	5.4
1	A	520	ILE	5.3
1	A	581	SER	5.2
1	C	711	THR	5.2
1	B	572	LEU	5.0
1	D	571	PRO	5.0
1	C	630	THR	4.7
1	A	582	SER	4.7
1	D	581	SER	4.7
1	D	630	THR	4.6
1	C	624	ARG	4.6
1	B	519	SER	4.5
1	B	695	VAL	4.4
1	D	582	SER	4.2
1	B	571	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	570	GLU	4.1
1	D	709	VAL	4.1
1	A	519	SER	4.1
1	D	625	GLN	4.0
1	B	624	ARG	3.9
1	A	631	ASN	3.8
1	D	518	SER	3.5
1	B	516	GLU	3.5
1	B	581	SER	3.5
1	B	520	ILE	3.3
1	D	569	SER	3.3
1	A	264	GLN	3.2
1	C	631	ASN	3.1
1	A	571	PRO	3.1
1	A	583	VAL	3.1
1	B	692	THR	3.0
1	A	517	GLU	3.0
1	C	634	GLU	3.0
1	C	593	HIS	2.9
1	A	569	SER	2.8
1	C	709	VAL	2.8
1	C	580	SER	2.8
1	A	705	GLU	2.8
1	C	689	HIS	2.8
1	B	631	ASN	2.7
1	A	522	ARG	2.7
1	A	518	SER	2.7
1	C	691	ILE	2.7
1	A	516	GLU	2.7
1	D	624	ARG	2.7
1	A	476	MET	2.6
1	A	376	HIS	2.5
1	D	522	ARG	2.4
1	D	570	GLU	2.4
1	B	264	GLN	2.4
1	B	694	ARG	2.4
1	B	460	LYS	2.4
1	C	264	GLN	2.4
1	B	518	SER	2.4
1	C	564	ARG	2.4
1	A	580	SER	2.3
1	B	693	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	520	ILE	2.3
1	A	695	VAL	2.2
1	B	394	LYS	2.2
1	C	567	GLU	2.2
1	D	519	SER	2.2
1	C	623	GLU	2.1
1	A	447	GLY	2.1
1	C	694	ARG	2.1
1	D	598	ARG	2.1
1	A	623	GLU	2.1
1	D	516	GLU	2.1
1	D	655	GLN	2.1
1	B	517	GLU	2.0
1	C	598	ARG	2.0
1	C	622	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	803	5/5	0.83	0.10	64,69,97,103	0
2	SO4	B	803	5/5	0.86	0.12	67,82,91,96	0
2	SO4	A	803	5/5	0.86	0.12	71,72,80,92	0
2	SO4	B	802	5/5	0.87	0.10	58,58,95,100	0
2	SO4	C	803	5/5	0.90	0.10	76,80,92,95	0
2	SO4	A	802	5/5	0.90	0.12	62,70,85,93	0
2	SO4	B	801	5/5	0.91	0.15	55,64,80,91	0
2	SO4	A	801	5/5	0.92	0.12	54,63,75,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	801	5/5	0.93	0.11	64,69,79,80	0
2	SO4	C	802	5/5	0.93	0.12	50,51,71,79	0
2	SO4	D	802	5/5	0.94	0.10	51,71,75,83	0
2	SO4	D	804	5/5	0.94	0.09	56,61,73,79	0
2	SO4	C	801	5/5	0.99	0.05	46,46,47,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.