



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:18 PM UTC

PDB ID : 5LDD / pdb_00005ldd
Title : Crystal structure of the heterodimeric GEF Mon1-Ccz1 in complex with Ypt7
Authors : Kiontke, S.; Kuemmel, D.
Deposited on : 2016-06-24
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 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

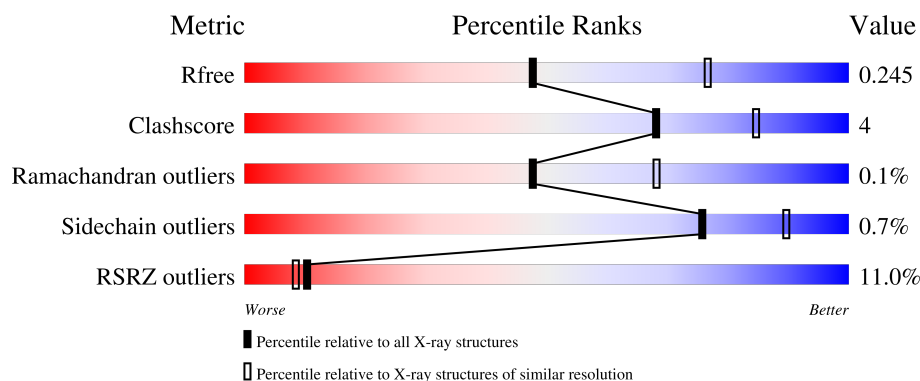
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 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	166	2% 83% 11% 7%
1	D	166	3% 73% 12% 14%
2	B	250	2% 63% 34%
2	E	250	3% 61% 5% 34%
3	C	207	5% 70% 11% 19%

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Mol	Chain	Length	Quality of chain
3	F	207	35% 65% 12% 24%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7670 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 Mon1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1212	779	209	222	2			
1	D	143	Total	C	N	O	S	0	0	0
			1114	719	193	200	2			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	190	GLY	-	expression tag	UNP G0SGS3
A	191	PRO	-	expression tag	UNP G0SGS3
A	192	LEU	-	expression tag	UNP G0SGS3
A	193	GLY	-	expression tag	UNP G0SGS3
A	194	SER	-	expression tag	UNP G0SGS3
D	190	GLY	-	expression tag	UNP G0SGS3
D	191	PRO	-	expression tag	UNP G0SGS3
D	192	LEU	-	expression tag	UNP G0SGS3
D	193	GLY	-	expression tag	UNP G0SGS3
D	194	SER	-	expression tag	UNP G0SGS3

- Molecule 2 is a protein called Ccz1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1323	851	222	249	1			
2	E	165	Total	C	N	O	S	0	0	0
			1315	845	221	248	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP G0SD94
E	0	SER	-	expression tag	UNP G0SD94

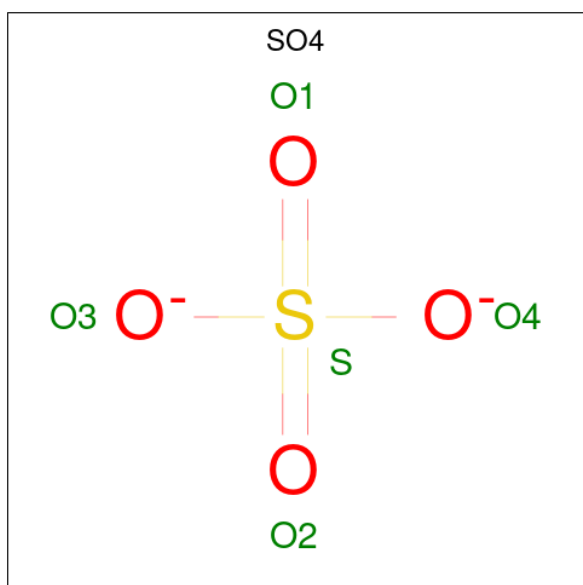
- Molecule 3 is a protein called Rab small monomeric GTPase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	168	Total	C	N	O	S	0	0	0
			1324	846	227	244	7			
3	F	158	Total	C	N	O	S	0	0	0
			1245	798	212	228	7			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLY	-	expression tag	UNP G0SGE1
C	0	SER	-	expression tag	UNP G0SGE1
C	125	ILE	ASN	engineered mutation	UNP G0SGE1
F	-1	GLY	-	expression tag	UNP G0SGE1
F	0	SER	-	expression tag	UNP G0SGE1
F	125	ILE	ASN	engineered mutation	UNP G0SGE1

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

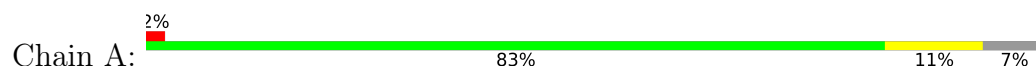
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	31	Total 31	O 31	0	0
5	B	37	Total 37	O 37	0	0
5	C	25	Total 25	O 25	0	0
5	D	13	Total 13	O 13	0	0
5	E	9	Total 9	O 9	0	0
5	F	7	Total 7	O 7	0	0

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.

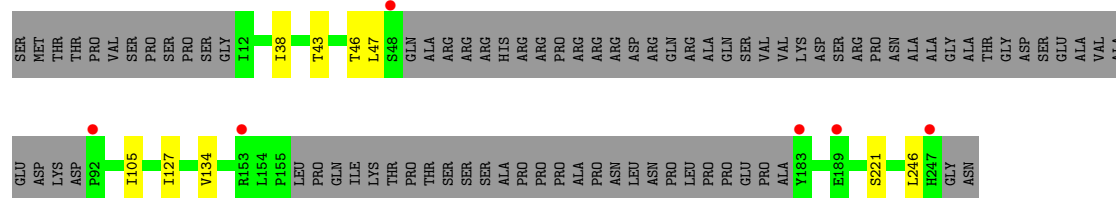
• Molecule 1: Mon1



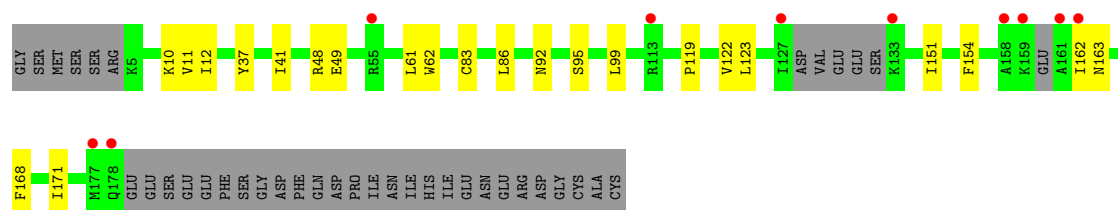
• Molecule 1: Mon1



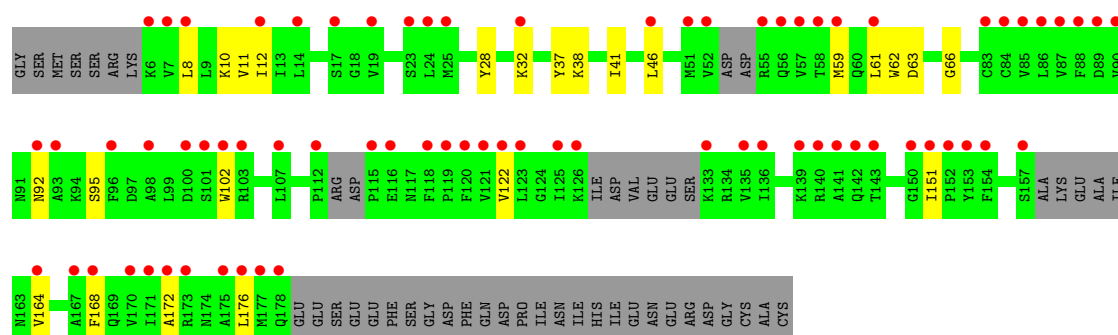
• Molecule 2: Ccz1



- Molecule 3: Rab small monomeric GTPase-like protein



- Molecule 3: Rab small monomeric GTPase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.08Å 103.81Å 206.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.38 – 2.50 46.38 – 2.50	Depositor EDS
% Data completeness (in resolution range)	86.7 (46.38-2.50) 86.8 (46.38-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.72 (at 2.48Å)	Xtriage
Refinement program	PHENIX dev_2439	Depositor
R, R_{free}	0.200 , 0.241 (Not available) , 0.245	Depositor DCC
R_{free} test set	1839 reflections (3.46%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7670	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6328e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.22	0/1236	0.40	0/1676
1	D	0.18	0/1136	0.35	0/1538
2	B	0.23	0/1352	0.42	0/1838
2	E	0.20	0/1344	0.37	0/1827
3	C	0.20	0/1345	0.37	0/1809
3	F	0.15	0/1264	0.32	0/1697
All	All	0.20	0/7677	0.37	0/10385

There are no bond length outliers.

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	1212	0	1252	9	0
1	D	1114	0	1159	14	0
2	B	1323	0	1314	4	0
2	E	1315	0	1303	6	0
3	C	1324	0	1336	12	0
3	F	1245	0	1251	15	0
4	C	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	5	0	0	0	0
5	A	31	0	0	1	0
5	B	37	0	0	0	0
5	C	25	0	0	1	0
5	D	13	0	0	0	0
5	E	9	0	0	0	0
5	F	7	0	0	0	0
All	All	7670	0	7615	55	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 4.

All (55) 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)
2:E:199:ASP:OD1	2:E:202:ARG:NH2	2.21	0.74
1:D:234:PRO:HB3	1:D:249:MET:HG3	1.75	0.69
1:A:219:LYS:NZ	5:A:701:HOH:O	2.26	0.68
1:D:220:GLY:HA2	1:D:291:ARG:HH22	1.56	0.67
2:E:191:LYS:HD3	2:E:195:LEU:HD22	1.80	0.64
1:D:234:PRO:HD2	3:F:8:LEU:HD21	1.82	0.62
2:E:127:ILE:HB	2:E:134:VAL:HB	1.82	0.61
3:F:11:VAL:HB	3:F:61:LEU:HD23	1.83	0.60
2:B:127:ILE:HB	2:B:134:VAL:HB	1.85	0.59
2:B:38:ILE:HG12	2:B:105:ILE:HD12	1.85	0.59
3:C:11:VAL:HB	3:C:61:LEU:HD23	1.86	0.57
3:C:86:LEU:HB3	3:C:99:LEU:HD22	1.85	0.57
1:D:224:HIS:HB2	1:D:289:ILE:HB	1.87	0.56
3:C:10:LYS:HE3	3:C:62:TRP:CE2	2.40	0.56
1:D:222:LEU:HA	1:D:291:ARG:HG3	1.88	0.55
3:F:37:TYR:HB3	3:F:41:ILE:HG12	1.91	0.53
1:A:234:PRO:HB3	1:A:249:MET:HG3	1.89	0.53
3:C:163:ASN:ND2	5:C:402:HOH:O	2.42	0.53
1:D:279:LEU:HB3	1:D:286:PHE:HB2	1.92	0.51
1:D:242:LEU:HD11	3:F:8:LEU:HD13	1.93	0.50
3:F:12:ILE:HD13	3:F:62:TRP:HB2	1.94	0.48
1:D:218:TRP:O	1:D:224:HIS:NE2	2.39	0.48
3:C:37:TYR:HB3	3:C:41:ILE:HG12	1.95	0.48
3:F:46:LEU:HB2	3:F:61:LEU:HB2	1.95	0.48
1:D:228:LEU:HG	1:D:285:TYR:HB2	1.96	0.47
3:C:48:ARG:NH1	3:C:49:GLU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:122:VAL:HG23	3:C:151:ILE:HG21	1.97	0.47
1:D:346:ALA:O	1:D:350:THR:HG23	2.15	0.47
1:A:206:PRO:HB2	1:A:209:LEU:HD13	1.97	0.46
1:A:228:LEU:HG	1:A:285:TYR:HB2	1.98	0.46
3:F:38:LYS:NZ	3:F:63:ASP:OD2	2.39	0.45
1:A:288:ALA:HB2	1:A:303:LEU:HD21	1.99	0.45
3:F:92:ASN:OD1	3:F:95:SER:N	2.44	0.45
1:A:279:LEU:HB3	1:A:286:PHE:HB2	2.00	0.44
3:F:122:VAL:HG23	3:F:151:ILE:HG21	2.00	0.44
3:F:66:GLY:HA2	3:F:102:TRP:HH2	1.81	0.44
2:B:221:SER:O	2:E:95:LYS:HE2	2.17	0.44
1:D:259:TYR:CE2	2:E:107:LEU:HD21	2.54	0.43
2:B:43:THR:N	2:B:46:THR:OG1	2.42	0.43
3:C:168:PHE:HA	3:C:171:ILE:HG22	1.98	0.43
3:F:59:MET:HE1	3:F:168:PHE:CD1	2.53	0.43
3:C:123:LEU:HD23	3:C:154:PHE:HB2	2.00	0.43
2:E:43:THR:HG23	2:E:46:THR:H	1.84	0.43
1:A:214:ARG:NH1	1:A:241:ASP:OD1	2.51	0.43
1:A:259:TYR:HB3	1:A:264:ASN:O	2.18	0.42
1:D:212:ASP:OD1	3:F:32:LYS:HD2	2.20	0.42
3:C:12:ILE:HD13	3:C:62:TRP:HB2	2.01	0.42
1:A:252:VAL:HG11	1:A:287:VAL:HG21	2.02	0.42
3:F:172:ALA:O	3:F:176:LEU:HG	2.20	0.42
3:C:83:CYS:HB3	3:C:119:PRO:HB2	2.02	0.41
3:F:10:LYS:HE3	3:F:62:TRP:CE2	2.55	0.41
3:C:92:ASN:OD1	3:C:95:SER:N	2.45	0.41
1:D:246:ASN:OD1	1:D:247:SER:N	2.53	0.41
1:D:316:LEU:HB3	1:D:317:PRO:HD3	2.03	0.40
3:F:28:TYR:HB2	3:F:164:VAL:HG11	2.03	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	153/166 (92%)	153 (100%)	0	0	100	100
1	D	141/166 (85%)	141 (100%)	0	0	100	100
2	B	160/250 (64%)	157 (98%)	3 (2%)	0	100	100
2	E	159/250 (64%)	156 (98%)	3 (2%)	0	100	100
3	C	162/207 (78%)	157 (97%)	4 (2%)	1 (1%)	21	38
3	F	148/207 (72%)	145 (98%)	3 (2%)	0	100	100
All	All	923/1246 (74%)	909 (98%)	13 (1%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	162	ILE

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	133/141 (94%)	132 (99%)	1 (1%)	73	88
1	D	121/141 (86%)	120 (99%)	1 (1%)	73	88
2	B	143/213 (67%)	141 (99%)	2 (1%)	59	81
2	E	142/213 (67%)	140 (99%)	2 (1%)	59	81
3	C	143/178 (80%)	143 (100%)	0	100	100
3	F	135/178 (76%)	135 (100%)	0	100	100
All	All	817/1064 (77%)	811 (99%)	6 (1%)	76	89

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	284	LEU
2	B	47	LEU
2	B	246	LEU
1	D	242	LEU

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Mol	Chain	Res	Type
2	E	47	LEU
2	E	246	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	99	HIS
2	B	243	ASN
2	E	99	HIS
3	F	56	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](#)

3 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	$\# Z > 2$
4	SO4	F	301	-	4,4,4	0.25	0	6,6,6	0.18	0
4	SO4	C	301	-	4,4,4	0.23	0	6,6,6	0.22	0
4	SO4	C	302	-	4,4,4	0.23	0	6,6,6	0.16	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	155/166 (93%)	-0.04	4 (2%) 57 52	23, 47, 110, 137	0
1	D	143/166 (86%)	0.24	5 (3%) 47 42	35, 63, 110, 145	0
2	B	166/250 (66%)	-0.26	6 (3%) 46 41	22, 44, 83, 115	0
2	E	165/250 (66%)	0.16	7 (4%) 40 36	27, 64, 108, 147	0
3	C	168/207 (81%)	0.28	10 (5%) 27 24	23, 68, 111, 144	0
3	F	158/207 (76%)	1.99	73 (46%) 0 0	52, 122, 161, 192	0
All	All	955/1246 (76%)	0.39	105 (10%) 10 8	22, 64, 137, 192	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	115	PRO	6.7
3	F	83	CYS	5.8
3	C	161	ALA	5.7
3	F	52	VAL	5.5
3	C	127	ILE	5.0
3	C	158	ALA	4.6
3	F	164	VAL	4.3
2	B	92	PRO	4.2
3	F	102	TRP	4.1
3	F	93	ALA	4.0
3	F	123	LEU	3.9
2	E	183	TYR	3.8
3	F	133	LYS	3.7
3	F	55	ARG	3.7
3	F	135	VAL	3.7
3	F	175	ALA	3.7
3	F	152	PRO	3.7
3	F	98	ALA	3.6
3	F	125	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
3	F	177	MET	3.6
3	F	136	ILE	3.5
3	F	87	VAL	3.4
2	B	48	SER	3.4
3	F	122	VAL	3.4
2	B	247	HIS	3.3
3	C	159	LYS	3.3
3	F	168	PHE	3.2
3	F	85	VAL	3.2
3	F	58	THR	3.1
3	F	126	LYS	3.1
3	F	120	PHE	3.1
3	F	90	VAL	3.1
3	C	177	MET	3.0
3	F	24	LEU	3.0
3	F	89	ASP	3.0
1	A	353	SER	3.0
3	F	178	GLN	3.0
3	F	88	PHE	3.0
3	F	17	SER	3.0
3	F	172	ALA	2.9
2	E	155	PRO	2.9
3	F	6	LYS	2.9
3	F	151	ILE	2.9
3	F	112	PRO	2.9
3	F	59	MET	2.9
3	F	153	TYR	2.9
3	F	12	ILE	2.8
1	D	214	ARG	2.8
3	F	19	VAL	2.8
1	D	216	ALA	2.8
3	F	86	LEU	2.8
3	C	133	LYS	2.8
3	F	157	SER	2.8
2	B	183	TYR	2.7
1	A	311	LEU	2.7
3	F	150	GLY	2.7
3	C	162	ILE	2.7
3	F	176	LEU	2.7
3	F	154	PHE	2.6
3	F	121	VAL	2.6
3	F	143	THR	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	100	ASP	2.6
3	F	140	ARG	2.6
3	F	56	GLN	2.5
3	C	55	ARG	2.5
3	F	141	ALA	2.5
3	F	23	SER	2.4
3	F	118	PHE	2.4
3	F	7	VAL	2.4
3	C	178	GLN	2.4
3	F	103	ARG	2.4
2	E	189	GLU	2.4
2	E	247	HIS	2.4
3	F	14	LEU	2.3
3	F	84	CYS	2.3
3	F	96	PHE	2.3
1	A	208	THR	2.3
3	F	61	LEU	2.3
3	F	101	SER	2.3
3	F	139	LYS	2.3
3	F	116	GLU	2.3
3	F	92	ASN	2.3
1	A	326	ARG	2.2
2	E	233	ARG	2.2
3	F	170	VAL	2.2
3	F	8	LEU	2.2
3	C	113	ARG	2.2
3	F	119	PRO	2.2
3	F	171	ILE	2.2
2	B	153	ARG	2.2
3	F	173	ARG	2.2
3	F	57	VAL	2.1
3	F	46	LEU	2.1
1	D	213	GLU	2.1
2	E	246	LEU	2.1
3	F	167	ALA	2.1
1	D	353	SER	2.1
3	F	25	MET	2.1
3	F	51	MET	2.1
3	F	32	LYS	2.0
2	E	48	SER	2.0
3	F	142	GLN	2.0
2	B	189	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	107	LEU	2.0
1	D	218	TRP	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
4	SO4	F	301	5/5	0.82	0.10	79,96,101,109	0
4	SO4	C	302	5/5	0.87	0.16	123,123,124,124	0
4	SO4	C	301	5/5	0.94	0.09	59,63,71,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.