



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:26 AM UTC

PDB ID : 4BJ6 / pdb_00004bj6
Title : Crystal structure Rif2 in complex with the C-terminal domain of Rap1 (Rap1-RCT)
Authors : Shi, T.; Bunker, R.D.; Gut, H.; Scrima, A.; Thoma, N.H.
Deposited on : 2013-04-16
Resolution : 3.26 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

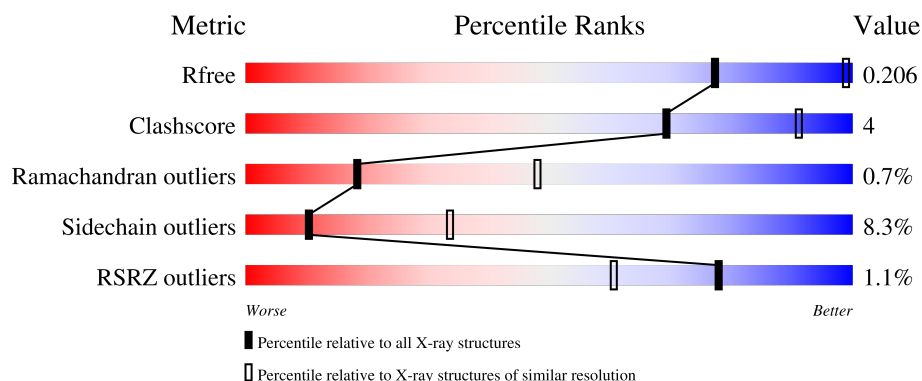
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	365	64% 15% 20%
1	B	365	62% 15% 21%
2	C	202	64% 10% 25%
2	E	202	64% 10% 25%
3	D	13	69% 31%

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Mol	Chain	Length	Quality of chain
3	F	13	 62% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7370 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 RAP1-INTERACTING FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2362	1529	378	442	13			
1	B	290	Total	C	N	O	S	0	0	0
			2332	1510	371	438	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	expression tag	UNP Q06208
A	32	GLY	-	expression tag	UNP Q06208
A	33	GLY	-	expression tag	UNP Q06208
A	34	ARG	-	expression tag	UNP Q06208
B	31	GLY	-	expression tag	UNP Q06208
B	32	GLY	-	expression tag	UNP Q06208
B	33	GLY	-	expression tag	UNP Q06208
B	34	ARG	-	expression tag	UNP Q06208

- Molecule 2 is a protein called DNA-BINDING PROTEIN RAP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	151	Total	C	N	O	S	0	0	0
			1227	779	204	237	7			
2	E	151	Total	C	N	O	S	0	0	0
			1227	779	204	237	7			

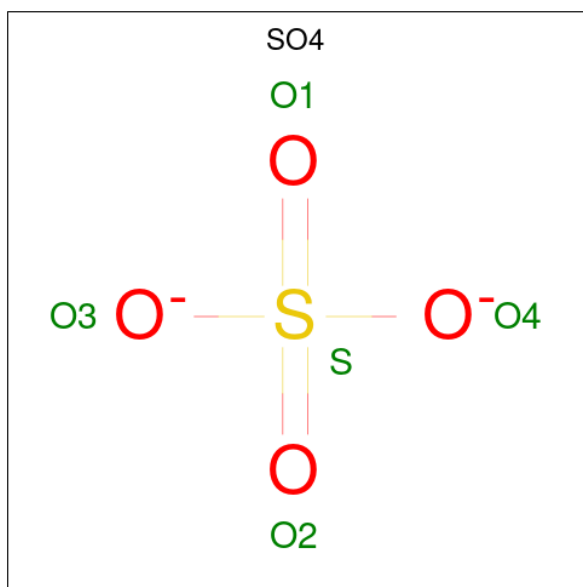
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	626	GLY	-	expression tag	UNP P11938
E	626	GLY	-	expression tag	UNP P11938

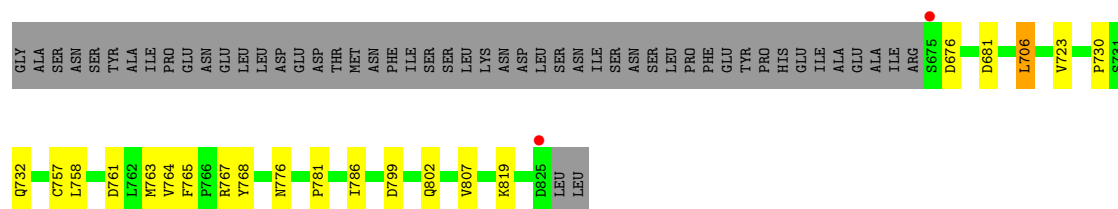
- Molecule 3 is a protein called RAP1-INTERACTING FACTOR 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	0	0	0
			84	56	14	14			
3	F	13	Total	C	N	O	0	0	0
			88	59	15	14			

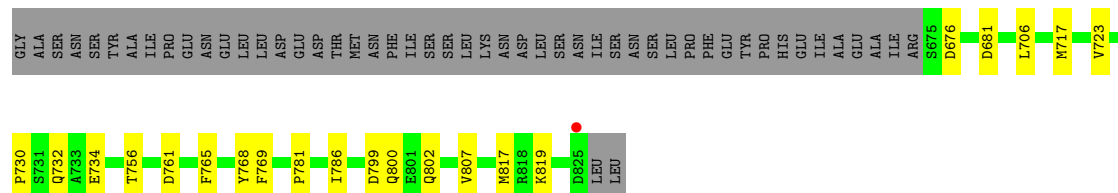
- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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



● Molecule 2: DNA-BINDING PROTEIN RAP1



● Molecule 3: RAP1-INTERACTING FACTOR 2



● Molecule 3: RAP1-INTERACTING FACTOR 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.25Å 112.68Å 140.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.26 48.79 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.79-3.26) 99.6 (48.79-3.26)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.172 , 0.195 0.184 , 0.206	Depositor DCC
R_{free} test set	1361 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	100.3	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 82.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7370	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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	0.90	1/2408 (0.0%)	1.38	18/3257 (0.6%)
1	B	0.91	2/2377 (0.1%)	1.38	17/3216 (0.5%)
2	C	0.81	0/1258	1.34	6/1700 (0.4%)
2	E	0.83	0/1258	1.36	6/1700 (0.4%)
3	D	1.04	0/84	1.49	0/116
3	F	1.01	0/88	1.46	0/120
All	All	0.88	3/7473 (0.0%)	1.37	47/10109 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	334	PHE	CA-C	6.31	1.60	1.52
1	B	136	VAL	CA-C	5.86	1.58	1.52
1	B	334	PHE	CA-C	5.19	1.58	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	ASN	N-CA-C	-7.21	105.10	114.04
1	A	300	ASP	CA-CB-CG	7.18	119.78	112.60
1	B	300	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	137	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	377	ASN	CA-CB-CG	6.61	119.20	112.60
1	B	377	ASN	CA-CB-CG	6.57	119.17	112.60
1	A	139	ASN	CA-CB-CG	6.39	118.99	112.60
2	E	676	ASP	CA-CB-CG	6.38	118.98	112.60
2	E	681	ASP	CA-CB-CG	6.31	118.91	112.60
2	C	681	ASP	CA-CB-CG	6.27	118.87	112.60
1	A	284	CYS	CA-C-N	6.13	128.41	120.44
1	A	284	CYS	C-N-CA	6.13	128.41	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	676	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	189	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	284	CYS	CA-C-N	6.01	128.25	120.44
1	B	284	CYS	C-N-CA	6.01	128.25	120.44
1	A	254	ASN	N-CA-C	-5.93	105.79	114.39
1	A	189	ASP	CA-CB-CG	5.89	118.50	112.60
1	A	74	PHE	CA-C-N	5.80	128.37	120.54
1	A	74	PHE	C-N-CA	5.80	128.37	120.54
1	B	89	ILE	CA-C-N	5.75	128.78	120.38
1	B	89	ILE	C-N-CA	5.75	128.78	120.38
2	C	819	LYS	CA-C-N	5.52	127.67	120.28
2	C	819	LYS	C-N-CA	5.52	127.67	120.28
1	B	139	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	89	ILE	CA-C-N	5.42	128.29	120.38
1	A	89	ILE	C-N-CA	5.42	128.29	120.38
1	B	135	LEU	CA-C-N	-5.33	117.49	122.66
1	B	135	LEU	C-N-CA	-5.33	117.49	122.66
1	A	255	ASN	CA-CB-CG	5.32	117.92	112.60
2	E	723	VAL	CA-C-N	5.27	129.27	120.62
2	E	723	VAL	C-N-CA	5.27	129.27	120.62
1	A	300	ASP	CA-C-N	5.20	127.25	120.28
1	A	300	ASP	C-N-CA	5.20	127.25	120.28
2	C	723	VAL	CA-C-N	5.16	129.08	120.62
2	C	723	VAL	C-N-CA	5.16	129.08	120.62
1	B	300	ASP	CA-C-N	5.15	127.19	120.28
1	B	300	ASP	C-N-CA	5.15	127.19	120.28
2	E	819	LYS	CA-C-N	5.13	127.67	120.28
2	E	819	LYS	C-N-CA	5.13	127.67	120.28
1	B	74	PHE	CA-C-N	5.11	127.44	120.54
1	B	74	PHE	C-N-CA	5.11	127.44	120.54
1	A	243	ASN	CA-CB-CG	5.11	117.71	112.60
1	A	312	LEU	CA-C-N	5.05	126.93	120.56
1	A	312	LEU	C-N-CA	5.05	126.93	120.56
1	B	367	THR	CA-C-N	5.05	128.44	120.47
1	B	367	THR	C-N-CA	5.05	128.44	120.47

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	2362	0	2353	18	0
1	B	2332	0	2310	21	0
2	C	1227	0	1171	7	0
2	E	1227	0	1171	6	0
3	D	84	0	77	2	0
3	F	88	0	88	3	0
4	A	15	0	0	0	0
4	B	20	0	0	0	0
4	C	5	0	0	0	0
4	E	10	0	0	0	0
All	All	7370	0	7170	51	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 (51) 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:B:256:VAL:HA	1:B:259:SER:HB3	1.70	0.73
1:A:256:VAL:HA	1:A:259:SER:HB3	1.70	0.72
1:B:145:MET:HA	1:B:145:MET:HE2	1.73	0.70
1:A:145:MET:HA	1:A:145:MET:HE2	1.73	0.69
1:B:354:THR:HG23	1:B:357:GLU:HB2	1.81	0.62
1:A:312:LEU:O	1:A:316:GLN:HB2	2.01	0.61
1:B:312:LEU:O	1:B:316:GLN:HB2	2.02	0.59
1:A:354:THR:HG23	1:A:357:GLU:H	1.68	0.57
1:B:259:SER:O	1:B:263:SER:HB2	2.05	0.57
1:A:199:ASN:HB3	1:A:202:GLU:HG2	1.87	0.57
1:B:199:ASN:HB3	1:B:202:GLU:HG2	1.87	0.56
1:B:330:PHE:CE1	1:B:334:PHE:HB2	2.40	0.55
1:A:207:ILE:HD12	1:A:248:LYS:HE2	1.90	0.54
2:C:761:ASP:HA	3:D:45:VAL:HB	1.88	0.54
2:E:717:MET:HE1	2:E:769:PHE:HB3	1.89	0.53
1:A:240:GLU:HB2	1:A:247:PHE:HE2	1.74	0.53
1:B:379:LYS:HB3	1:B:382:GLN:HG2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:LYS:HB3	1:A:382:GLN:HG2	1.91	0.52
1:B:207:ILE:HD12	1:B:248:LYS:HE2	1.91	0.52
1:B:240:GLU:HB2	1:B:247:PHE:HE2	1.75	0.52
1:B:119:ILE:HG12	1:B:380:LYS:HA	1.93	0.50
1:A:330:PHE:CE1	1:A:334:PHE:HB2	2.46	0.50
1:A:119:ILE:HG12	1:A:380:LYS:HA	1.93	0.50
1:B:379:LYS:O	1:B:382:GLN:HB2	2.13	0.49
1:A:379:LYS:O	1:A:382:GLN:HB2	2.13	0.48
1:B:139:ASN:HB3	1:B:206:HIS:CD2	2.49	0.48
2:E:799:ASP:HB3	2:E:802:GLN:HE21	1.79	0.48
2:E:761:ASP:HA	3:F:45:VAL:HB	1.95	0.47
2:C:764:VAL:HG23	2:C:767:ARG:HD2	1.96	0.46
2:C:799:ASP:HB3	2:C:802:GLN:HE21	1.79	0.46
1:A:66:VAL:HA	1:A:354:THR:OG1	2.14	0.46
1:A:207:ILE:HG23	1:A:248:LYS:HD3	1.98	0.46
1:B:384:LEU:HD12	2:C:706:LEU:HD12	1.98	0.45
1:B:299:PHE:O	1:B:306:LEU:HD22	2.16	0.45
1:A:299:PHE:O	1:A:306:LEU:HD22	2.17	0.45
1:B:143:ILE:HG22	1:B:145:MET:HE3	2.00	0.44
1:B:207:ILE:HG23	1:B:248:LYS:HD3	1.98	0.44
1:A:143:ILE:HG22	1:A:145:MET:HE3	1.99	0.43
2:E:734:GLU:HG3	3:F:39:LEU:HD13	2.01	0.43
2:C:730:PRO:HA	3:D:44:LEU:HB2	2.00	0.42
1:A:346:THR:O	1:A:350:VAL:HB	2.19	0.42
1:B:75:LYS:HD2	1:B:350:VAL:HA	2.02	0.42
2:E:768:TYR:HA	2:E:786:ILE:HD11	2.02	0.42
1:B:312:LEU:HD22	1:B:359:LEU:HD13	2.02	0.41
2:C:768:TYR:HA	2:C:786:ILE:HD11	2.01	0.41
1:B:139:ASN:HB3	1:B:206:HIS:HD2	1.85	0.41
1:B:346:THR:O	1:B:350:VAL:HB	2.20	0.41
2:C:758:LEU:HD13	2:C:764:VAL:HG13	2.03	0.41
2:E:730:PRO:HA	3:F:44:LEU:HB2	2.03	0.41
1:A:354:THR:HG22	1:A:357:GLU:HB2	2.02	0.40
1:A:312:LEU:HD22	1:A:359:LEU:HD13	2.04	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	289/365 (79%)	276 (96%)	12 (4%)	1 (0%)	36	66
1	B	286/365 (78%)	272 (95%)	13 (4%)	1 (0%)	36	66
2	C	149/202 (74%)	144 (97%)	3 (2%)	2 (1%)	9	34
2	E	149/202 (74%)	145 (97%)	2 (1%)	2 (1%)	9	34
3	D	11/13 (85%)	11 (100%)	0	0	100	100
3	F	11/13 (85%)	11 (100%)	0	0	100	100
All	All	895/1160 (77%)	859 (96%)	30 (3%)	6 (1%)	18	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	732	GLN
2	C	781	PRO
2	E	781	PRO
2	C	732	GLN
1	A	387	LYS
1	B	387	LYS

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	271/346 (78%)	246 (91%)	25 (9%)	8	29
1	B	266/346 (77%)	238 (90%)	28 (10%)	6	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	140/188 (74%)	134 (96%)	6 (4%)	26	52
2	E	140/188 (74%)	134 (96%)	6 (4%)	26	52
3	D	7/13 (54%)	5 (71%)	2 (29%)	0	1
3	F	8/13 (62%)	6 (75%)	2 (25%)	0	2
All	All	832/1094 (76%)	763 (92%)	69 (8%)	10	34

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	VAL
1	A	77	MET
1	A	92	VAL
1	A	94	SER
1	A	96	SER
1	A	114	ASP
1	A	127	ARG
1	A	147	ASP
1	A	193	MET
1	A	200	ASN
1	A	213	GLU
1	A	214	GLN
1	A	215	LEU
1	A	219	SER
1	A	220	THR
1	A	224	ILE
1	A	256	VAL
1	A	258	ILE
1	A	275	THR
1	A	276	VAL
1	A	350	VAL
1	A	359	LEU
1	A	365	ARG
1	A	369	LYS
1	A	380	LYS
1	B	69	VAL
1	B	77	MET
1	B	92	VAL
1	B	96	SER
1	B	103	LEU
1	B	114	ASP
1	B	127	ARG

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Mol	Chain	Res	Type
1	B	135	LEU
1	B	137	ASP
1	B	138	ILE
1	B	147	ASP
1	B	193	MET
1	B	213	GLU
1	B	214	GLN
1	B	215	LEU
1	B	219	SER
1	B	220	THR
1	B	224	ILE
1	B	256	VAL
1	B	258	ILE
1	B	275	THR
1	B	276	VAL
1	B	350	VAL
1	B	354	THR
1	B	359	LEU
1	B	369	LYS
1	B	380	LYS
1	B	384	LEU
2	C	706	LEU
2	C	757	CYS
2	C	763	MET
2	C	765	PHE
2	C	776	ASN
2	C	807	VAL
3	D	42	LEU
3	D	47	ILE
2	E	706	LEU
2	E	756	THR
2	E	765	PHE
2	E	800	GLN
2	E	807	VAL
2	E	817	MET
3	F	42	LEU
3	F	47	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	206	HIS
1	A	244	ASN
1	A	288	GLN
1	A	318	ASN
1	A	323	ASN
1	A	370	ASN
1	A	377	ASN
1	B	80	GLN
1	B	102	ASN
1	B	206	HIS
1	B	244	ASN
1	B	254	ASN
1	B	288	GLN
1	B	318	ASN
1	B	319	ASN
1	B	323	ASN
1	B	370	ASN
1	B	377	ASN
2	C	685	ASN
2	C	709	HIS
2	C	749	ASN
2	C	776	ASN
2	C	802	GLN
2	E	685	ASN
2	E	709	HIS
2	E	749	ASN
2	E	802	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

10 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	B	1392	-	4,4,4	0.32	0	6,6,6	0.17	0
4	SO4	B	1391	-	4,4,4	0.28	0	6,6,6	0.08	0
4	SO4	B	1390	-	4,4,4	0.35	0	6,6,6	0.32	0
4	SO4	A	1390	-	4,4,4	0.31	0	6,6,6	0.12	0
4	SO4	A	1389	-	4,4,4	0.44	0	6,6,6	0.28	0
4	SO4	B	1389	-	4,4,4	0.29	0	6,6,6	0.38	0
4	SO4	A	1391	-	4,4,4	0.26	0	6,6,6	0.18	0
4	SO4	E	1827	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	C	1826	-	4,4,4	0.24	0	6,6,6	0.25	0
4	SO4	E	1826	-	4,4,4	0.37	0	6,6,6	0.37	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

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	293/365 (80%)	-0.40	2 (0%) 84 70	62, 94, 145, 190	0
1	B	290/365 (79%)	-0.26	5 (1%) 69 50	72, 106, 176, 196	0
2	C	151/202 (74%)	-0.31	2 (1%) 75 56	87, 116, 177, 199	0
2	E	151/202 (74%)	-0.40	1 (0%) 84 70	73, 106, 166, 186	0
3	D	13/13 (100%)	0.42	0 100 100	126, 148, 164, 165	0
3	F	13/13 (100%)	0.65	0 100 100	116, 140, 160, 163	0
All	All	911/1160 (78%)	-0.31	10 (1%) 78 60	62, 105, 168, 199	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	825	ASP	4.4
2	E	825	ASP	3.6
1	B	65	ARG	2.9
1	A	218	LEU	2.7
1	A	151	LYS	2.7
1	B	220	THR	2.7
1	B	151	LYS	2.7
1	B	388	LEU	2.6
1	B	373	HIS	2.2
2	C	675	SER	2.2

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

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	A	1390	5/5	0.30	0.11	187,187,187,188	0
4	SO4	A	1391	5/5	0.39	0.12	235,235,235,235	0
4	SO4	B	1391	5/5	0.52	0.09	213,214,214,214	0
4	SO4	E	1827	5/5	0.62	0.08	230,230,230,230	0
4	SO4	C	1826	5/5	0.83	0.09	181,181,182,183	0
4	SO4	E	1826	5/5	0.87	0.14	135,136,138,138	0
4	SO4	B	1392	5/5	0.91	0.12	174,175,176,176	0
4	SO4	B	1390	5/5	0.97	0.07	113,113,118,119	0
4	SO4	B	1389	5/5	0.98	0.06	79,80,82,84	0
4	SO4	A	1389	5/5	0.99	0.03	74,77,78,82	0

6.5 Other polymers [i](#)

There are no such residues in this entry.