



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:48 AM GMT

PDB ID : 1I2M
Title : RAN-RCC1-SO4 COMPLEX
Authors : Renault, L.; Kuhlmann, J.; Henkel, A.; Wittinghofer, A.
Deposited on : 2001-02-11
Resolution : 1.76 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

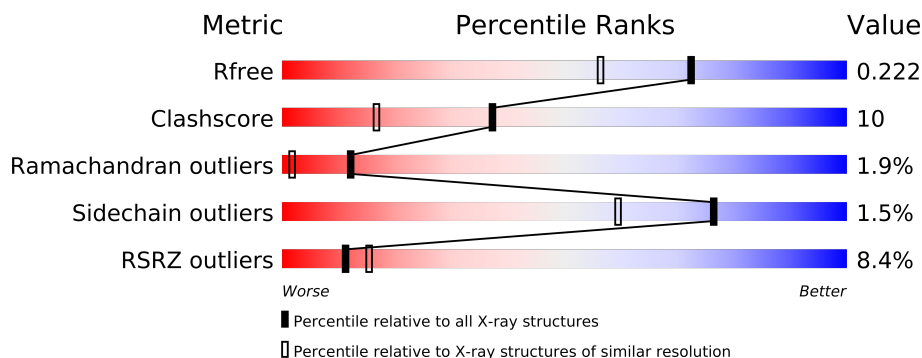
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.76 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}	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	216	
1	C	216	
2	B	402	
2	D	402	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8984 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GTP-BINDING NUCLEAR PROTEIN RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	0	0
			1346	875	239	228	4			
1	C	164	Total	C	N	O	S	0	0	0
			1337	869	237	227	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	129	ARG	SER	SEE REMARK 999	UNP P62826
C	129	ARG	SER	SEE REMARK 999	UNP P62826

- Molecule 2 is a protein called REGULATOR OF CHROMOSOME CONDENSATION 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	388	Total	C	N	O	S	0	0	0
			2899	1809	509	562	19			
2	D	390	Total	C	N	O	S	0	0	0
			2917	1820	512	566	19			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

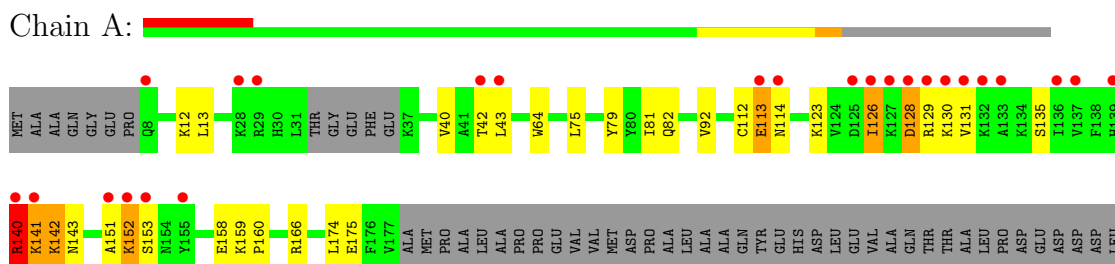
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	180	Total	O	0	0
			180	180		
4	C	57	Total	O	0	0
			57	57		
4	D	176	Total	O	0	0
			176	176		

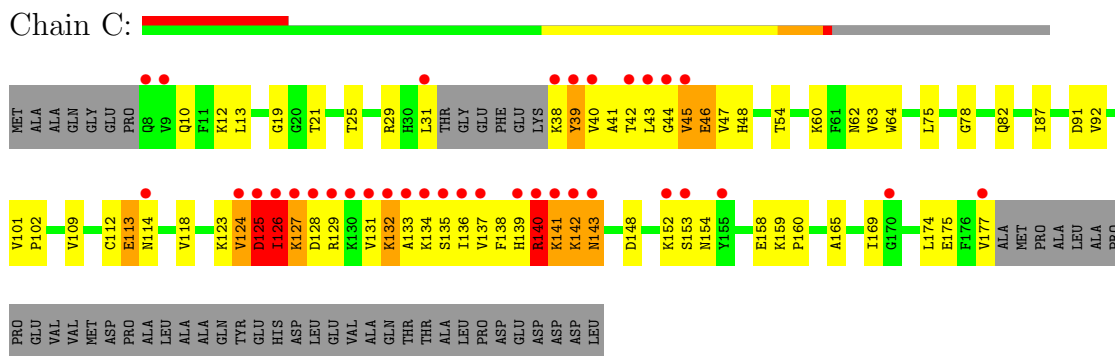
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

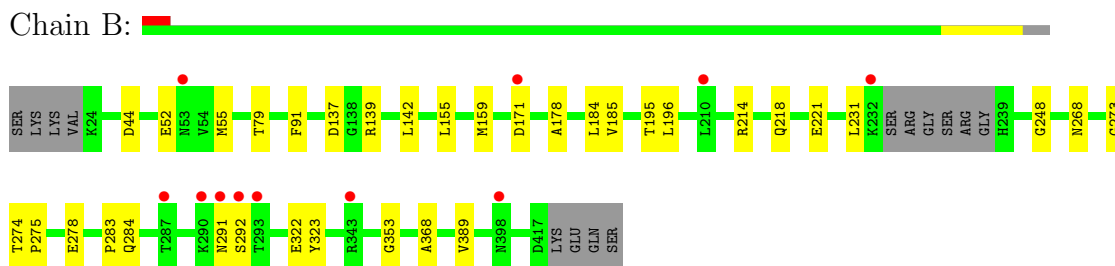
• Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN



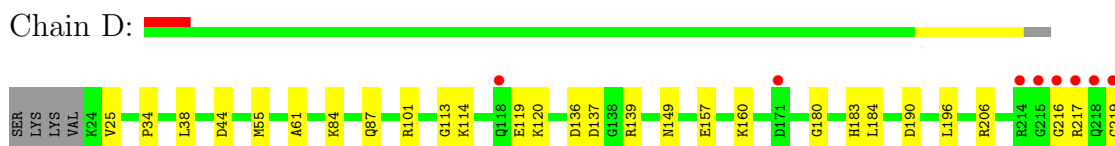
• Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN

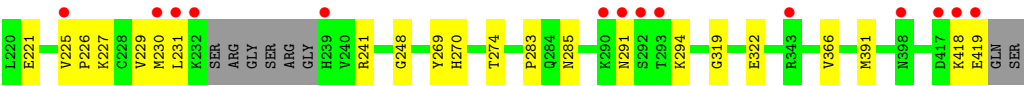


• Molecule 2: REGULATOR OF CHROMOSOME CONDENSATION 1



• Molecule 2: REGULATOR OF CHROMOSOME CONDENSATION 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	50.33Å 71.45Å 77.73Å 100.92° 92.05° 104.47°	Depositor
Resolution (Å)	19.79 – 1.76 19.80 – 1.63	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.79-1.76) 97.0 (19.80-1.63)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 1.63Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.192 , 0.223 0.192 , 0.222	Depositor DCC
R_{free} test set	8466 reflections (9.11%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 44.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 123475 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8984	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.30	0/1378	0.62	0/1859
1	C	0.32	0/1369	0.66	0/1848
2	B	0.31	0/2953	0.62	2/3989 (0.1%)
2	D	0.30	0/2971	0.61	1/4012 (0.0%)
All	All	0.31	0/8671	0.62	3/11708 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	248	GLY	N-CA-C	-5.12	100.30	113.10
2	B	353	GLY	N-CA-C	-5.03	100.52	113.10
2	B	248	GLY	N-CA-C	-5.02	100.56	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1346	0	1378	31	0
1	C	1337	0	1365	90	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2899	0	2842	22	0
2	D	2917	0	2861	39	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	62	0	0	0	0
4	B	180	0	0	1	0
4	C	57	0	0	0	0
4	D	176	0	0	0	0
All	All	8984	0	8446	172	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:ARG:HG2	1:A:141:LYS:H	1.16	1.08
1:A:141:LYS:HE2	1:A:143:ASN:HD21	1.35	0.89
1:A:140:ARG:HG2	1:A:141:LYS:N	1.93	0.83
2:D:231:LEU:HD13	2:D:283:PRO:HB2	1.63	0.81
1:C:60:LYS:HD3	1:C:62:ASN:HD21	1.46	0.80
1:C:10:GLN:HE21	1:C:60:LYS:HD2	1.47	0.79
1:C:39:TYR:H	1:C:46:GLU:HA	1.45	0.79
1:C:42:THR:HG21	1:C:78:GLY:O	1.83	0.79
1:C:141:LYS:O	1:C:142:LYS:HG3	1.84	0.77
1:C:126:ILE:HG23	1:C:126:ILE:O	1.83	0.76
1:C:38:LYS:N	1:C:47:VAL:HB	2.03	0.73
1:C:29:ARG:HH11	1:C:154:ASN:HD21	1.36	0.73
1:A:140:ARG:CG	1:A:141:LYS:H	1.97	0.72
1:C:141:LYS:HE2	1:C:143:ASN:HD21	1.55	0.71
1:C:126:ILE:HD12	1:C:128:ASP:HB2	1.74	0.70
1:A:141:LYS:HE2	1:A:143:ASN:ND2	2.07	0.70
1:C:124:VAL:CG1	1:C:125:ASP:N	2.54	0.69
1:C:43:LEU:N	1:C:43:LEU:HD12	2.08	0.67
1:C:126:ILE:HD12	1:C:128:ASP:CB	2.26	0.66
1:A:112:CYS:O	1:A:113:GLU:HB2	1.94	0.66
2:D:221:GLU:H	2:D:221:GLU:CD	1.99	0.66
1:A:126:ILE:HG13	1:A:126:ILE:O	1.95	0.66
1:C:137:VAL:HG11	2:D:55:MET:CE	2.27	0.65
1:C:39:TYR:HD2	1:C:44:GLY:O	1.80	0.64
1:C:125:ASP:O	1:C:126:ILE:HB	1.98	0.64
1:C:124:VAL:O	1:C:126:ILE:N	2.31	0.64
1:C:139:HIS:HE1	1:C:148:ASP:OD1	1.81	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:LYS:HD2	1:C:129:ARG:HB3	1.81	0.63
2:B:137:ASP:OD2	2:B:139:ARG:HD3	1.98	0.63
2:B:159:MET:HG3	1:C:41:ALA:HA	1.81	0.62
1:C:126:ILE:CG2	1:C:126:ILE:O	2.48	0.62
1:C:133:ALA:HA	1:C:136:ILE:HG12	1.82	0.62
1:C:124:VAL:HG12	1:C:125:ASP:N	2.15	0.61
1:C:131:VAL:O	1:C:133:ALA:N	2.33	0.61
1:C:39:TYR:N	1:C:46:GLU:HA	2.15	0.61
1:A:159:LYS:HB2	1:A:160:PRO:HD3	1.83	0.60
2:D:291:ASN:HB3	2:D:294:LYS:HB2	1.82	0.60
1:A:123:LYS:HE3	1:A:131:VAL:HG21	1.84	0.60
1:C:133:ALA:HA	1:C:136:ILE:CG1	2.32	0.60
1:A:42:THR:OG1	1:A:75:LEU:HD11	2.02	0.60
1:C:43:LEU:C	1:C:45:VAL:H	2.06	0.59
1:C:129:ARG:HA	1:C:129:ARG:CZ	2.32	0.59
2:D:291:ASN:ND2	2:D:294:LYS:HD2	2.17	0.59
2:D:44:ASP:HA	2:D:55:MET:HE1	1.84	0.58
1:A:151:ALA:O	1:A:152:LYS:CB	2.52	0.58
1:C:40:VAL:HG12	1:C:82:GLN:NE2	2.19	0.58
2:D:44:ASP:HA	2:D:55:MET:CE	2.33	0.58
1:C:129:ARG:HA	1:C:129:ARG:NH1	2.19	0.58
1:C:42:THR:OG1	1:C:82:GLN:NE2	2.34	0.57
1:A:152:LYS:O	1:A:153:SER:HB3	2.05	0.57
1:A:141:LYS:O	1:A:142:LYS:HB2	2.04	0.57
2:B:221:GLU:CD	1:C:75:LEU:HG	2.25	0.57
1:A:140:ARG:CG	1:A:141:LYS:N	2.60	0.56
1:A:92:VAL:HG21	1:A:135:SER:HB2	1.86	0.56
1:C:43:LEU:C	1:C:45:VAL:N	2.59	0.56
1:A:140:ARG:O	1:A:141:LYS:HB3	2.06	0.56
2:D:291:ASN:CB	2:D:294:LYS:HB2	2.36	0.56
1:C:159:LYS:HB2	1:C:160:PRO:HD3	1.87	0.56
1:C:169:ILE:HD11	1:C:174:LEU:HD22	1.87	0.56
1:C:141:LYS:HE2	1:C:143:ASN:ND2	2.22	0.55
1:C:140:ARG:HD3	1:C:141:LYS:H	1.71	0.55
1:C:124:VAL:CG1	1:C:125:ASP:H	2.20	0.55
1:C:137:VAL:O	1:C:137:VAL:HG12	2.07	0.55
1:C:126:ILE:O	1:C:128:ASP:N	2.35	0.55
2:D:184:LEU:HD23	2:D:196:LEU:HD21	1.89	0.55
1:C:29:ARG:NH1	1:C:154:ASN:HD21	2.02	0.54
1:A:75:LEU:HB2	1:A:79:TYR:CZ	2.43	0.54
1:C:124:VAL:HG13	1:C:125:ASP:H	1.72	0.54
2:D:120:LYS:HB3	2:D:136:ASP:OD2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:219:GLY:HA3	2:D:221:GLU:OE1	2.07	0.54
1:C:46:GLU:HG2	1:C:48:HIS:CE1	2.43	0.54
1:A:141:LYS:O	1:A:142:LYS:CB	2.56	0.53
1:C:25:THR:O	1:C:29:ARG:HG2	2.08	0.53
2:D:206:ARG:CZ	2:D:227:LYS:HB2	2.39	0.52
1:C:141:LYS:HG2	1:C:142:LYS:H	1.74	0.52
2:D:270:HIS:HD2	2:D:274:THR:O	1.93	0.52
2:D:217:ARG:O	2:D:217:ARG:HD3	2.10	0.52
1:C:40:VAL:HG12	1:C:82:GLN:HE22	1.74	0.52
1:C:131:VAL:C	1:C:133:ALA:H	2.14	0.51
1:C:60:LYS:HD3	1:C:62:ASN:ND2	2.21	0.51
2:B:221:GLU:OE2	1:C:75:LEU:HG	2.10	0.51
2:D:190:ASP:O	2:D:241:ARG:HD3	2.10	0.51
2:B:178:ALA:HB3	2:B:185:VAL:CG2	2.41	0.51
1:C:31:LEU:HD21	1:C:48:HIS:HB3	1.93	0.50
2:B:52:GLU:O	2:B:52:GLU:HG2	2.09	0.50
1:C:39:TYR:HA	1:C:45:VAL:O	2.11	0.50
2:D:366:VAL:HG13	2:D:391:MET:HB2	1.93	0.50
2:D:25:VAL:HG22	2:D:136:ASP:O	2.11	0.50
1:A:12:LYS:HE3	1:A:64:TRP:CE2	2.47	0.50
1:C:19:GLY:HA3	2:D:149:ASN:O	2.12	0.50
1:C:42:THR:O	1:C:75:LEU:HD13	2.12	0.50
1:C:13:LEU:HD23	1:C:13:LEU:C	2.32	0.50
1:C:42:THR:CB	1:C:82:GLN:HE21	2.25	0.50
1:C:91:ASP:CG	1:C:124:VAL:HB	2.33	0.49
1:A:166:ARG:NH2	1:A:175:GLU:OE2	2.45	0.49
2:B:273:GLY:C	2:B:275:PRO:HD3	2.33	0.49
2:B:184:LEU:HD23	2:B:196:LEU:HD21	1.94	0.49
1:C:127:LYS:HG2	1:C:152:LYS:HD2	1.94	0.49
1:C:132:LYS:O	1:C:136:ILE:HG12	2.13	0.48
2:D:101:ARG:CZ	2:D:113:GLY:HA3	2.43	0.48
1:C:140:ARG:O	1:C:141:LYS:O	2.31	0.48
2:D:196:LEU:HD13	2:D:226:PRO:HG3	1.95	0.48
2:B:275:PRO:HA	2:B:284:GLN:HE22	1.78	0.48
1:C:29:ARG:HH11	1:C:154:ASN:ND2	2.06	0.47
2:B:214:ARG:HD2	1:C:39:TYR:CZ	2.49	0.47
2:D:231:LEU:CD1	2:D:283:PRO:HB2	2.40	0.47
1:C:126:ILE:C	1:C:128:ASP:H	2.18	0.47
1:C:137:VAL:HG11	2:D:55:MET:HE2	1.95	0.47
1:A:13:LEU:HD23	1:A:13:LEU:C	2.35	0.47
2:D:230:MET:O	2:D:231:LEU:HB3	2.15	0.47
2:D:137:ASP:OD2	2:D:139:ARG:HD3	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:112:CYS:O	1:C:113:GLU:HB2	2.15	0.47
1:C:42:THR:HB	1:C:43:LEU:HD12	1.98	0.46
1:C:126:ILE:CD1	1:C:128:ASP:HB2	2.43	0.46
1:C:165:ALA:O	1:C:169:ILE:HG12	2.16	0.46
2:D:196:LEU:HD23	2:D:196:LEU:N	2.30	0.46
2:D:157:GLU:OE1	2:D:160:LYS:HD3	2.15	0.46
1:C:87:ILE:HG12	1:C:118:VAL:CG1	2.46	0.46
1:C:10:GLN:HE21	1:C:60:LYS:CD	2.23	0.46
2:B:274:THR:N	2:B:275:PRO:HD3	2.31	0.46
1:A:151:ALA:O	1:A:152:LYS:HB3	2.15	0.46
2:D:229:VAL:CG1	2:D:283:PRO:HG2	2.46	0.45
2:B:159:MET:CG	1:C:41:ALA:HA	2.45	0.45
1:C:12:LYS:HB3	1:C:64:TRP:HZ3	1.81	0.45
2:B:44:ASP:HA	2:B:55:MET:CE	2.46	0.45
1:C:39:TYR:HA	1:C:46:GLU:HA	1.98	0.45
2:B:185:VAL:HG12	2:B:195:THR:HG22	1.99	0.45
1:A:140:ARG:O	1:A:141:LYS:CB	2.65	0.44
2:D:84:LYS:HG3	2:D:84:LYS:O	2.18	0.44
1:C:101:VAL:HB	1:C:102:PRO:HD3	2.00	0.44
2:D:216:GLY:O	2:D:217:ARG:CB	2.65	0.44
2:D:87:GLN:OE1	2:D:114:LYS:HE3	2.17	0.44
2:D:206:ARG:NE	2:D:227:LYS:HB2	2.32	0.44
2:B:142:LEU:HG	2:B:155:LEU:HD11	1.99	0.44
1:C:42:THR:CG2	1:C:78:GLY:O	2.62	0.43
2:D:180:GLY:HA3	2:D:183:HIS:CE1	2.53	0.43
1:A:166:ARG:HG2	1:A:174:LEU:HB3	2.00	0.43
1:C:109:VAL:O	1:C:113:GLU:HA	2.17	0.43
1:C:135:SER:HA	1:C:138:PHE:CD1	2.54	0.43
2:B:231:LEU:HD21	2:B:283:PRO:HB2	2.01	0.43
1:A:81:ILE:O	1:A:82:GLN:HB2	2.19	0.42
1:C:152:LYS:O	1:C:153:SER:HB2	2.19	0.42
1:C:29:ARG:NH1	1:C:154:ASN:ND2	2.64	0.42
1:A:123:LYS:CE	1:A:131:VAL:HG21	2.48	0.42
1:A:75:LEU:HB2	1:A:79:TYR:CE1	2.55	0.42
2:D:418:LYS:O	2:D:419:GLU:HB3	2.20	0.42
1:C:137:VAL:CG1	2:D:55:MET:HE2	2.50	0.42
1:C:139:HIS:CE1	1:C:148:ASP:OD1	2.68	0.42
2:B:79:THR:HB	2:B:91:PHE:CE2	2.54	0.42
2:B:368:ALA:O	2:B:389:VAL:HG12	2.20	0.42
1:A:130:LYS:HA	1:A:130:LYS:HD2	1.74	0.41
2:B:214:ARG:HD2	1:C:39:TYR:CE2	2.55	0.41
1:C:169:ILE:CD1	1:C:174:LEU:HD22	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:119:GLU:CD	2:D:139:ARG:HH22	2.23	0.41
1:C:92:VAL:O	1:C:134:LYS:HE2	2.20	0.41
2:D:38:LEU:HA	2:D:61:ALA:O	2.20	0.41
1:C:140:ARG:CG	1:C:141:LYS:N	2.83	0.41
2:D:34:PRO:HD3	2:D:84:LYS:HE3	2.03	0.41
1:A:113:GLU:HB3	1:A:114:ASN:H	1.59	0.41
2:B:218:GLN:HB2	4:B:587:HOH:O	2.21	0.41
1:C:177:VAL:HG23	1:C:177:VAL:O	2.20	0.41
2:D:269:TYR:O	2:D:319:GLY:HA2	2.21	0.41
1:C:140:ARG:O	1:C:141:LYS:C	2.59	0.41
1:C:21:THR:HA	1:C:124:VAL:HG21	2.01	0.41
2:B:268:ASN:HA	2:B:278:GLU:HG2	2.03	0.40
1:C:39:TYR:CA	1:C:46:GLU:HA	2.52	0.40
1:A:40:VAL:HG13	1:A:42:THR:O	2.22	0.40
1:C:13:LEU:HB3	1:C:63:VAL:HG22	2.04	0.40
2:B:322:GLU:HG3	2:B:323:TYR:CD2	2.57	0.40
1:C:54:THR:HB	1:C:175:GLU:O	2.21	0.40
1:A:141:LYS:O	1:A:142:LYS:HG2	2.21	0.40
2:D:225:VAL:O	2:D:227:LYS:HG2	2.22	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	161/216 (74%)	146 (91%)	8 (5%)	7 (4%)	4	0
1	C	160/216 (74%)	144 (90%)	4 (2%)	12 (8%)	2	0
2	B	384/402 (96%)	373 (97%)	9 (2%)	2 (0%)	38	15
2	D	386/402 (96%)	373 (97%)	13 (3%)	0	100	100
All	All	1091/1236 (88%)	1036 (95%)	34 (3%)	21 (2%)	12	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ASP
1	A	152	LYS
2	B	291	ASN
2	B	292	SER
1	C	39	TYR
1	C	125	ASP
1	C	126	ILE
1	C	132	LYS
1	C	141	LYS
1	C	143	ASN
1	A	113	GLU
1	A	142	LYS
1	A	126	ILE
1	A	141	LYS
1	C	113	GLU
1	C	114	ASN
1	C	124	VAL
1	C	127	LYS
1	A	140	ARG
1	C	140	ARG
1	C	142	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	146/185 (79%)	141 (97%)	5 (3%)	49	21
1	C	145/185 (78%)	139 (96%)	6 (4%)	41	15
2	B	313/325 (96%)	312 (100%)	1 (0%)	96	93
2	D	315/325 (97%)	313 (99%)	2 (1%)	92	85
All	All	919/1020 (90%)	905 (98%)	14 (2%)	76	59

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	128	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	129	ARG
1	A	140	ARG
1	A	158	GLU
2	B	171	ASP
1	C	45	VAL
1	C	46	GLU
1	C	125	ASP
1	C	126	ILE
1	C	140	ARG
1	C	158	GLU
2	D	285	ASN
2	D	322	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	139	HIS
1	A	145	GLN
2	B	118	GLN
2	B	218	GLN
2	B	284	GLN
1	C	10	GLN
1	C	48	HIS
1	C	53	HIS
1	C	62	ASN
1	C	139	HIS
1	C	145	GLN
1	C	154	ASN
2	D	218	GLN
2	D	285	ASN
2	D	398	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
3	SO4	A	1250	-	4,4,4	0.11	0	6,6,6	0.06	0
3	SO4	C	2250	-	4,4,4	0.18	0	6,6,6	0.07	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1250	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2250	-	-	0/0/0/0	0/0/0/0

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.

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	165/216 (76%)	0.77	25 (15%) 3 4	18, 32, 80, 99	0
1	C	164/216 (75%)	1.16	35 (21%) 1 2	19, 36, 90, 99	0
2	B	388/402 (96%)	0.01	11 (2%) 50 60	16, 26, 57, 92	0
2	D	390/402 (97%)	0.21	22 (5%) 24 30	15, 27, 66, 99	0
All	All	1107/1236 (89%)	0.36	93 (8%) 11 15	15, 29, 73, 99	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	129	ARG	12.5
1	C	131	VAL	11.9
1	C	125	ASP	11.5
1	C	128	ASP	10.2
1	C	129	ARG	9.6
2	D	215	GLY	8.2
1	C	126	ILE	7.8
1	A	128	ASP	7.4
2	D	218	GLN	7.4
1	C	133	ALA	7.4
1	C	130	LYS	7.3
1	A	126	ILE	7.1
1	C	132	LYS	6.9
2	D	232	LYS	6.8
1	A	43	LEU	6.6
2	D	292	SER	6.3
1	C	42	THR	6.2
1	A	132	LYS	5.4
1	A	153	SER	5.3
1	C	31	LEU	5.1
1	A	136	ILE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	151	ALA	5.0
1	A	141	LYS	4.9
1	C	140	ARG	4.9
2	D	217	ARG	4.9
2	D	419	GLU	4.8
2	D	171	ASP	4.7
1	C	141	LYS	4.6
1	C	127	LYS	4.6
1	C	40	VAL	4.6
1	A	127	LYS	4.6
1	C	39	TYR	4.5
1	C	124	VAL	4.4
2	D	291	ASN	4.4
2	D	293	THR	4.4
2	B	291	ASN	4.4
2	B	292	SER	4.3
2	B	232	LYS	4.3
2	D	239	HIS	4.1
1	A	114	ASN	4.1
1	C	136	ILE	4.0
1	A	130	LYS	3.8
2	D	290	LYS	3.7
2	B	398	ASN	3.6
2	D	230	MET	3.6
1	C	135	SER	3.5
1	C	43	LEU	3.5
2	D	343	ARG	3.4
1	C	153	SER	3.4
1	C	139	HIS	3.4
1	A	131	VAL	3.4
1	C	177	VAL	3.4
2	D	219	GLY	3.3
2	D	118	GLN	3.3
1	C	170	GLY	3.2
2	B	210	LEU	3.2
1	A	139	HIS	3.1
1	C	38	LYS	3.1
2	B	171	ASP	3.1
1	C	142	LYS	3.1
1	C	143	ASN	3.0
2	D	231	LEU	3.0
1	A	137	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	287	THR	2.9
2	D	216	GLY	2.9
2	B	290	LYS	2.9
1	A	125	ASP	2.8
1	A	133	ALA	2.8
1	C	114	ASN	2.8
1	C	44	GLY	2.7
1	A	155	TYR	2.7
1	A	29	ARG	2.7
1	A	42	THR	2.6
2	D	398	ASN	2.6
2	D	225	VAL	2.5
1	A	8	GLN	2.5
1	A	28	LYS	2.5
2	B	53	ASN	2.4
1	C	8	GLN	2.4
1	C	152	LYS	2.4
1	C	134	LYS	2.3
1	A	113	GLU	2.3
2	B	343	ARG	2.2
1	C	9	VAL	2.2
1	A	140	ARG	2.2
2	D	214	ARG	2.2
2	B	293	THR	2.2
1	C	155	TYR	2.1
2	D	417	ASP	2.1
2	D	418	LYS	2.1
1	C	45	VAL	2.1
1	C	137	VAL	2.1
1	A	152	LYS	2.1

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	A	1250	5/5	0.11	0.82	36,36,37,38	0
3	SO4	C	2250	5/5	0.08	-0.09	35,36,38,39	0

6.5 Other polymers

There are no such residues in this entry.