



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:10 am BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

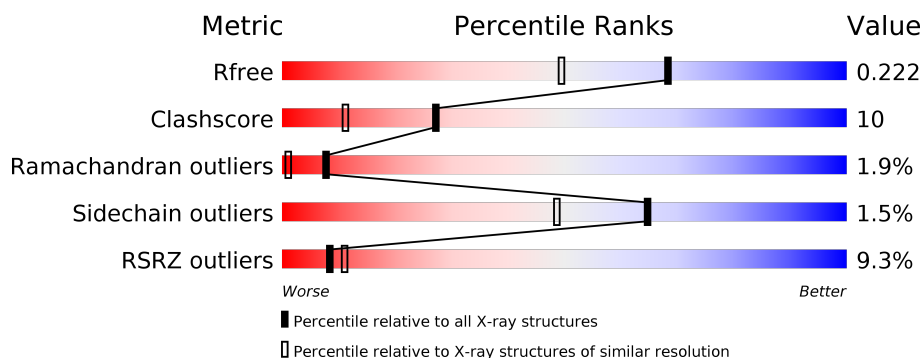
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (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  $\geq 3$ , 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	216	<div> <div>12%</div> <div> <div></div> <div>61%</div> <div>13%</div> <div>•</div> <div>24%</div> </div> </div>
1	C	216	<div> <div>19%</div> <div> <div></div> <div>44%</div> <div>26%</div> <div>5%</div> <div>•</div> <div>24%</div> </div> </div>
2	B	402	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>9%</div> <div>•</div> </div> </div>
2	D	402	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>•</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8984 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 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: O<sub>4</sub>S).



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		

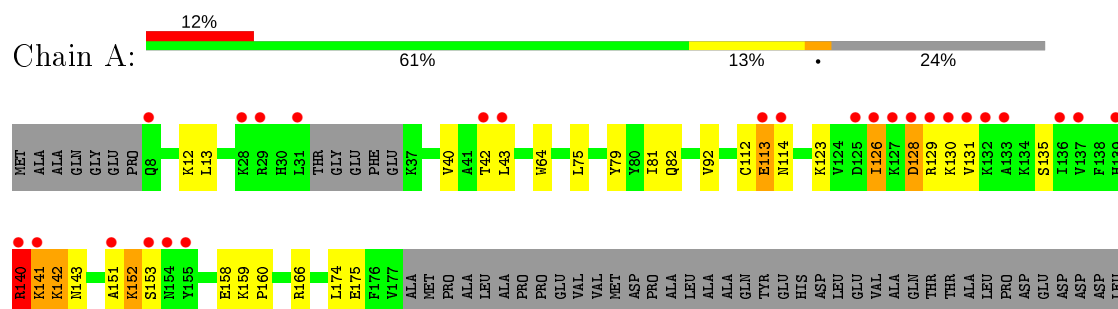
- Molecule 4 is water.

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		

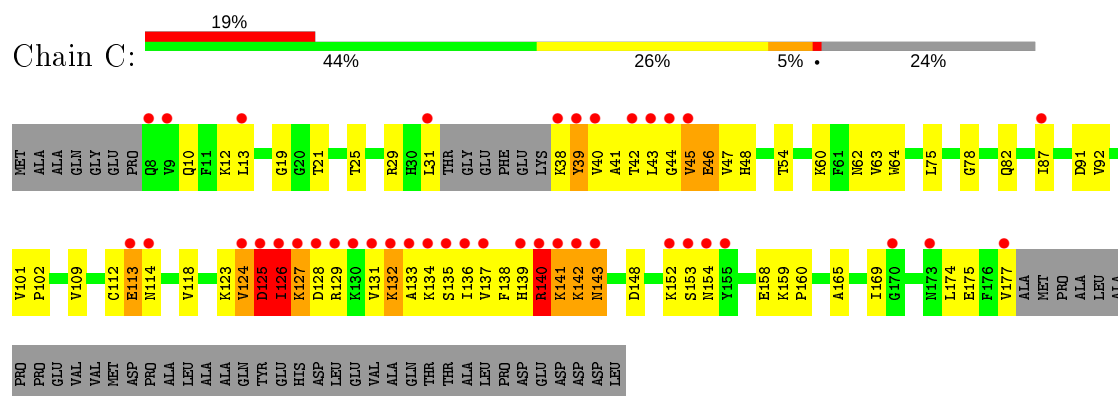
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

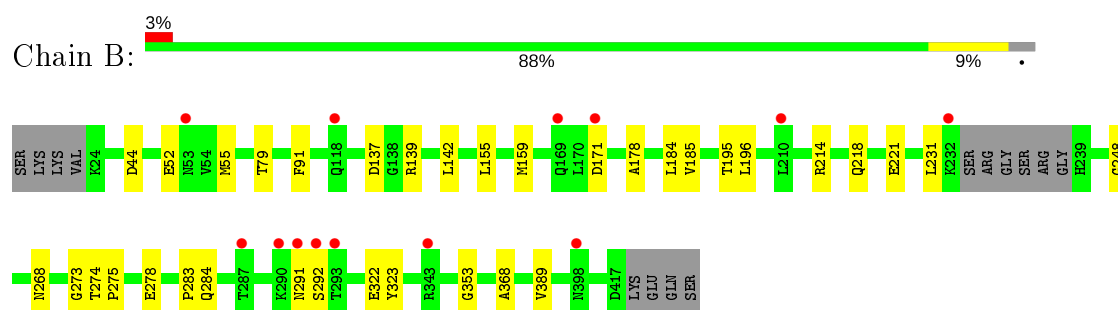
#### • Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN



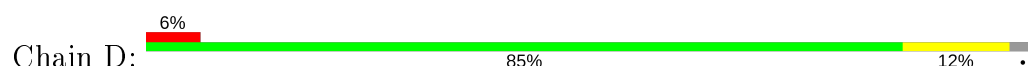
#### • Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN

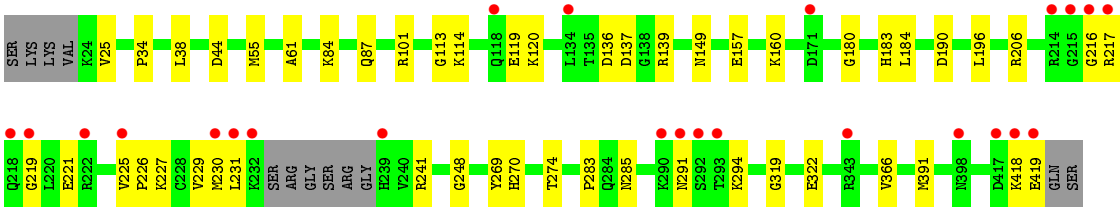


#### • Molecule 2: REGULATOR OF CHROMOSOME CONDENSATION 1



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (6.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.30	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 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	1346	0	1378	31	0
1	C	1337	0	1365	90	0
2	B	2899	0	2842	22	0
2	D	2917	0	2861	39	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (172) 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: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:A:112:CYS:O	1:A:113:GLU:HB2	1.94	0.66
1:C:126:ILE:HD12	1:C:128:ASP:CB	2.26	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	Interatomic distance (Å)	Clash overlap (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:129:ARG:HA	1:C:129:ARG:CZ	2.32	0.59
1:C:43:LEU:C	1:C:45:VAL:H	2.06	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
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
2:D:291:ASN:CB	2:D:294:LYS:HB2	2.36	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LYS:HB3	2:D:136:ASP:OD2	2.07	0.54
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
2:B:221:GLU:OE2	1:C:75:LEU:HG	2.10	0.51
1:C:60:LYS:HD3	1:C:62:ASN:ND2	2.21	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
2:B:52:GLU:O	2:B:52:GLU:HG2	2.09	0.50
1:C:31:LEU:HD21	1:C:48:HIS:HB3	1.93	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:13:LEU:HD23	1:C:13:LEU:C	2.32	0.50
1:C:42:THR:O	1:C:75:LEU:HD13	2.12	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:184:LEU:HD23	2:B:196:LEU:HD21	1.94	0.49
2:B:273:GLY:C	2:B:275:PRO:HD3	2.33	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
2:B:275:PRO:HA	2:B:284:GLN:HE22	1.78	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
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:112:CYS:O	1:C:113:GLU:HB2	2.15	0.47
1:C:126:ILE:CD1	1:C:128:ASP:HB2	2.43	0.46
1:C:42:THR:HB	1:C:43:LEU:HD12	1.98	0.46
1:C:165:ALA:O	1:C:169:ILE:HG12	2.16	0.46
2:D:157:GLU:OE1	2:D:160:LYS:HD3	2.15	0.46
2:D:196:LEU:HD23	2:D:196:LEU:N	2.30	0.46
1:C:87:ILE:HG12	1:C:118:VAL:CG1	2.46	0.46
2:B:274:THR:N	2:B:275:PRO:HD3	2.31	0.46
1:C:10:GLN:HE21	1:C:60:LYS:CD	2.23	0.46
1:A:151:ALA:O	1:A:152:LYS:HB3	2.15	0.46
1:C:12:LYS:HB3	1:C:64:TRP:HZ3	1.81	0.45
2:B:159:MET:CG	1:C:41:ALA:HA	2.45	0.45
2:D:229:VAL:CG1	2:D:283:PRO:HG2	2.46	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:O	2:D:84:LYS:HG3	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:B:142:LEU:HG	2:B:155:LEU:HD11	1.99	0.44
2:D:206:ARG:NE	2:D:227:LYS:HB2	2.32	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: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
1:C:29:ARG:NH1	1:C:154:ASN:ND2	2.64	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
2:B:368:ALA:O	2:B:389:VAL:HG12	2.20	0.42
2:B:79:THR:HB	2:B:91:PHE:CE2	2.54	0.42
1:C:139:HIS:CE1	1:C:148:ASP:OD1	2.68	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:92:VAL:O	1:C:134:LYS:HE2	2.20	0.41
1:C:169:ILE:CD1	1:C:174:LEU:HD22	2.50	0.41
2:D:119:GLU:CD	2:D:139:ARG:HH22	2.23	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:21:THR:HA	1:C:124:VAL:HG21	2.01	0.41
1:C:140:ARG:O	1:C:141:LYS:C	2.59	0.41
2:B:268:ASN:HA	2:B:278:GLU:HG2	2.03	0.40
1:A:40:VAL:HG13	1:A:42:THR:O	2.22	0.40
2:B:322:GLU:HG3	2:B:323:TYR:CD2	2.57	0.40
1:C:39:TYR:CA	1:C:46:GLU:HA	2.52	0.40
1:C:13:LEU:HB3	1:C:63:VAL:HG22	2.04	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 [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	A	161/216 (74%)	146 (91%)	8 (5%)	7 (4%)	<b>2</b> <b>0</b>
1	C	160/216 (74%)	144 (90%)	4 (2%)	12 (8%)	<b>1</b> <b>0</b>
2	B	384/402 (96%)	373 (97%)	9 (2%)	2 (0%)	<b>29</b> <b>12</b>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	386/402 (96%)	373 (97%)	13 (3%)	0	100	100
All	All	1091/1236 (88%)	1036 (95%)	34 (3%)	21 (2%)	8	1

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%)	37	14
1	C	145/185 (78%)	139 (96%)	6 (4%)	30	10
2	B	313/325 (96%)	312 (100%)	1 (0%)	92	89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	315/325 (97%)	313 (99%)	2 (1%)	86	79
All	All	919/1020 (90%)	905 (98%)	14 (2%)	65	49

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

Mol	Chain	Res	Type
1	A	43	LEU
1	A	128	ASP
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 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 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	0.20	0	6,6,6	0.06	0
3	SO4	C	2250	-	4,4,4	0.25	0	6,6,6	0.06	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	165/216 (76%)	0.83	26 (15%)	2 3	18, 32, 80, 99	0
1	C	164/216 (75%)	1.27	40 (24%)	0 0	19, 36, 90, 99	0
2	B	388/402 (96%)	0.08	13 (3%)	45 51	16, 26, 57, 92	0
2	D	390/402 (97%)	0.27	24 (6%)	20 26	15, 27, 66, 99	0
All	All	1107/1236 (89%)	0.44	103 (9%)	8 11	15, 29, 73, 99	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	VAL	14.3
1	A	129	ARG	11.3
1	C	125	ASP	10.6
2	D	215	GLY	10.2
1	C	129	ARG	9.9
1	C	128	ASP	9.3
1	A	128	ASP	8.9
1	C	126	ILE	8.4
2	D	218	GLN	8.1
1	C	130	LYS	8.0
1	C	133	ALA	7.7
1	C	132	LYS	7.2
1	A	126	ILE	6.9
1	A	43	LEU	6.6
2	D	232	LYS	6.2
1	C	42	THR	6.2
2	D	217	ARG	6.2
1	C	31	LEU	6.2
1	A	153	SER	6.0
1	A	132	LYS	5.9
2	D	292	SER	5.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	141	LYS	5.6
1	A	136	ILE	5.3
1	C	39	TYR	5.3
1	C	141	LYS	5.2
1	C	127	LYS	5.2
1	C	40	VAL	5.1
2	D	171	ASP	5.1
1	A	127	LYS	5.0
2	B	292	SER	5.0
2	D	291	ASN	4.8
2	D	419	GLU	4.6
1	C	140	ARG	4.6
1	A	133	ALA	4.5
2	D	293	THR	4.4
1	A	151	ALA	4.3
2	B	232	LYS	4.3
1	C	124	VAL	4.3
1	A	114	ASN	4.3
1	C	153	SER	4.2
2	B	291	ASN	4.1
2	D	230	MET	4.1
1	C	143	ASN	4.1
2	B	398	ASN	4.0
2	D	216	GLY	3.9
1	C	136	ILE	3.8
1	A	131	VAL	3.8
2	D	219	GLY	3.7
1	C	114	ASN	3.7
2	D	239	HIS	3.7
2	D	231	LEU	3.6
2	D	343	ARG	3.6
2	D	118	GLN	3.6
2	B	290	LYS	3.4
2	B	171	ASP	3.4
1	C	135	SER	3.4
1	A	130	LYS	3.4
1	C	170	GLY	3.4
2	D	290	LYS	3.4
1	C	139	HIS	3.4
1	C	43	LEU	3.3
1	A	29	ARG	3.3
1	A	139	HIS	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	38	LYS	3.2
2	B	210	LEU	3.2
1	C	152	LYS	3.2
1	A	137	VAL	3.1
1	C	177	VAL	3.1
2	B	287	THR	3.0
1	C	44	GLY	2.9
2	B	53	ASN	2.8
1	A	28	LYS	2.8
2	D	398	ASN	2.8
1	C	142	LYS	2.7
2	B	293	THR	2.7
1	A	125	ASP	2.7
2	D	214	ARG	2.6
1	C	134	LYS	2.6
1	A	42	THR	2.6
1	A	8	GLN	2.6
2	D	417	ASP	2.6
1	A	155	TYR	2.5
1	A	113	GLU	2.5
1	C	137	VAL	2.5
1	C	45	VAL	2.4
1	C	173	ASN	2.4
2	B	343	ARG	2.4
2	D	225	VAL	2.3
1	C	155	TYR	2.3
1	C	8	GLN	2.3
1	C	9	VAL	2.3
1	A	140	ARG	2.3
2	D	222	ARG	2.2
1	A	31	LEU	2.2
2	B	118	GLN	2.1
1	C	13	LEU	2.1
1	C	87	ILE	2.1
2	B	169	GLN	2.1
1	C	154	ASN	2.1
1	A	154	ASN	2.1
2	D	418	LYS	2.1
2	D	134	LEU	2.0
1	C	113	GLU	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 carbohydrates 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, 95<sup>th</sup> 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
3	SO4	A	1250	5/5	0.99	0.12	36,36,37,38	0
3	SO4	C	2250	5/5	0.99	0.08	35,36,38,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.