Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:57 PM 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

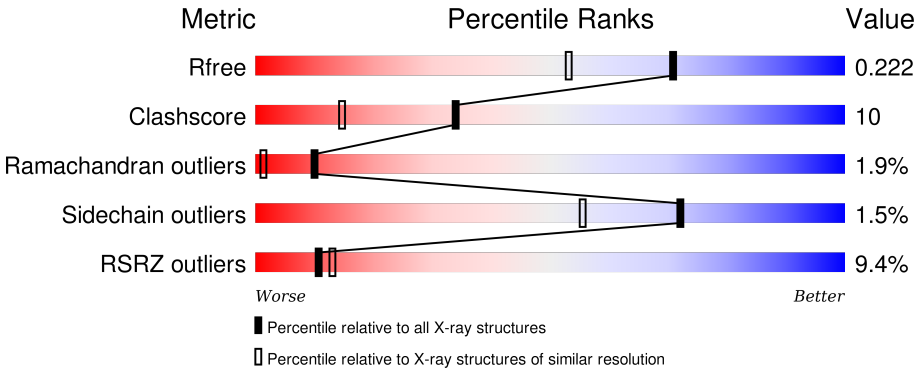
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (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. 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 <=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	13% 61% 13% • 24%
1	C	216	19% 44% 26% 5% • 24%
2	B	402	3% 88% 9% •
2	D	402	6% 85% 12% •

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			

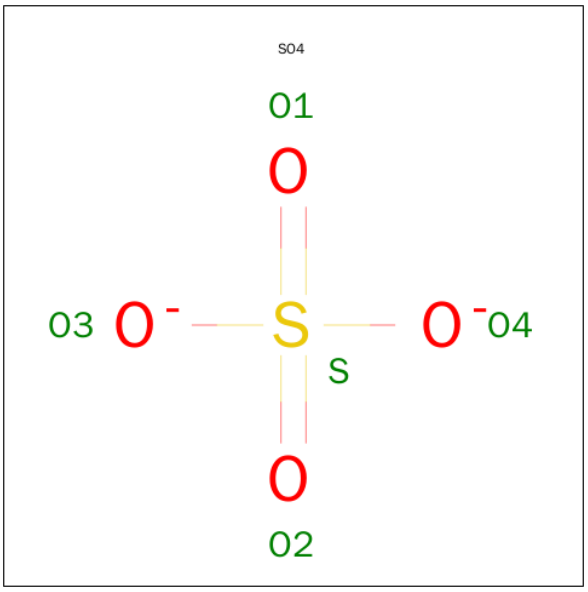
There are 2 discrepancies between the modelled and reference sequences:

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_4S).



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

- Molecule 4 is water.

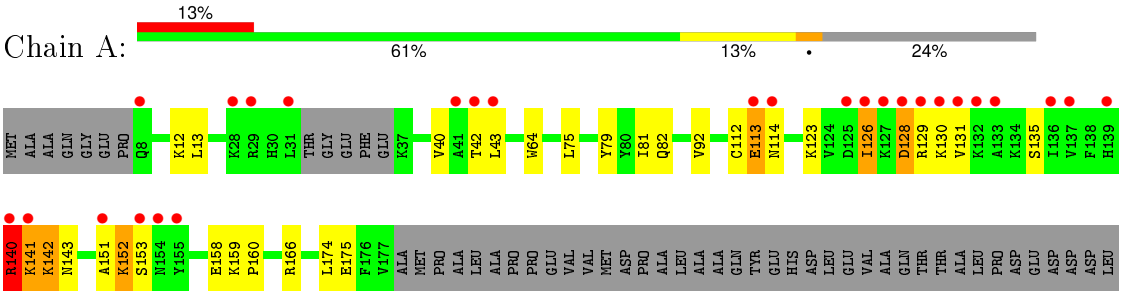
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	62	Total O 62 62	0	0
4	B	180	Total O 180 180	0	0
4	C	57	Total O 57 57	0	0
4	D	176	Total O 176 176	0	0

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 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.

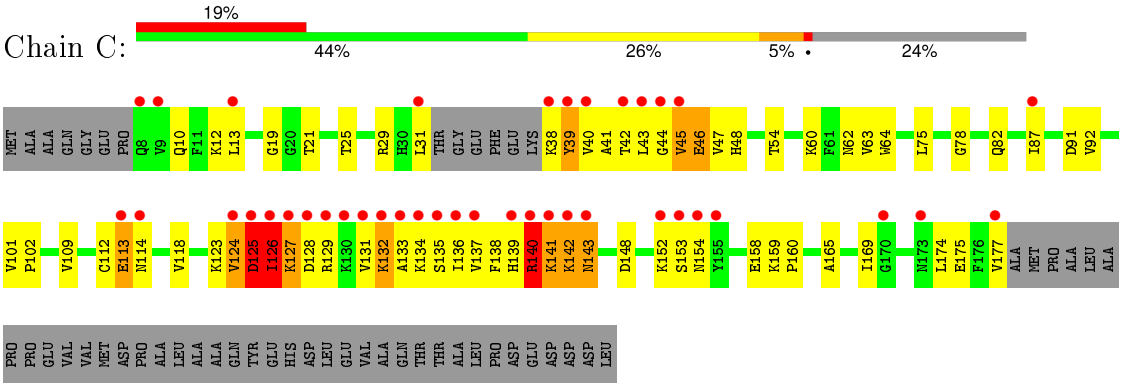
- Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN

Chain A:



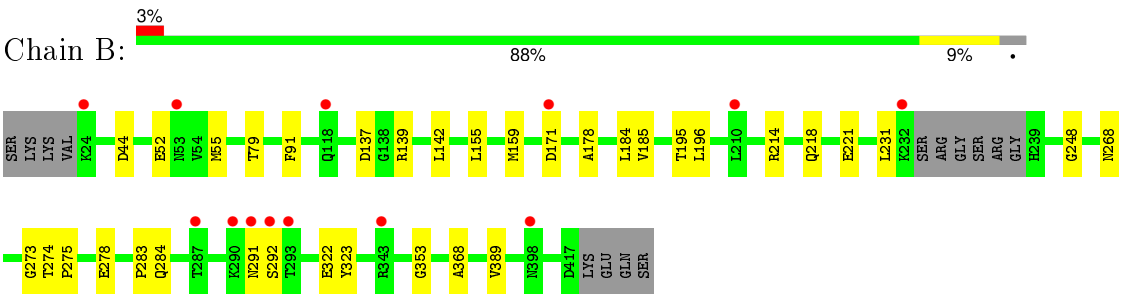
- Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN

Chain C:



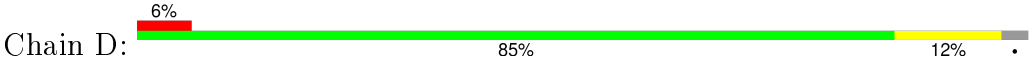
- Molecule 2: REGULATOR OF CHROMOSOME CONDENSATION 1

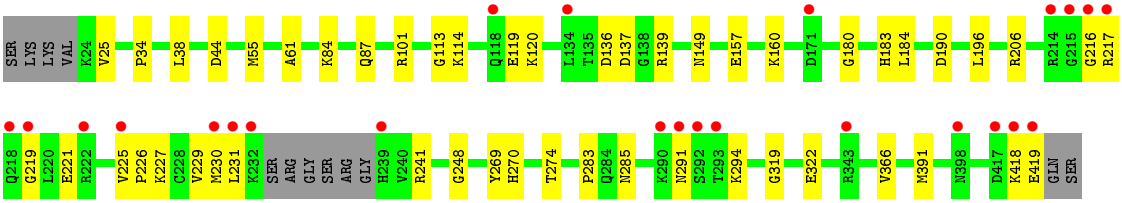
Chain B:



- Molecule 2: REGULATOR OF CHROMOSOME CONDENSATION 1

Chain D:




SER LYS LYS VAL K24 V25 P34 L38 D44 M55 A61 K84 Q87 R101 G113 K114 Q118 E119 K120 L134 T135 D136 D137 G138 R139 N149 E157 K160 D171 G180 H183 L184 D190 L196 R206 R214 G215 G216 R217
Q218 G219 L220 E221 R222 V225 P226 K227 C228 V229 M230 L231 K232 SER ARG GLY SER ARG GLY H239 V240 R241 G248 Y269 H270 T274 P283 Q284 N285 K290 N291 S292 T293 K294 G319 E322 R343 V366 M391 N398 D417 K418 E419 GLN SER

4 Data and refinement statistics (i)

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) 91.3 (19.80-1.63)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	8465 reflections (8.35%)	DCC
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.30	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(^{o})	Ideal(^{o})
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

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

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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: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

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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: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

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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
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

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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: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

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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: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
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 (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%)	3 0
1	C	160/216 (74%)	144 (90%)	4 (2%)	12 (8%)	1 0
2	B	384/402 (96%)	373 (97%)	9 (2%)	2 (0%)	34 14

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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%)	10 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 (i)

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%)	44 18
1	C	145/185 (78%)	139 (96%)	6 (4%)	37 13
2	B	313/325 (96%)	312 (100%)	1 (0%)	94 92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	315/325 (97%)	313 (99%)	2 (1%)	90 83
All	All	919/1020 (90%)	905 (98%)	14 (2%)	72 55

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	0.08	0	6,6,6	0.07	0
3	SO4	C	2250	-	4,4,4	0.15	0	6,6,6	0.08	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.

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^{th} 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%)	0.85	27 (16%) 2 4	18, 32, 80, 99	0
1	C	164/216 (75%)	1.28	40 (24%) 1 1	19, 36, 90, 99	0
2	B	388/402 (96%)	0.09	13 (3%) 49 55	16, 26, 57, 92	0
2	D	390/402 (97%)	0.29	24 (6%) 24 29	15, 27, 66, 99	0
All	All	1107/1236 (89%)	0.45	104 (9%) 11 13	15, 29, 73, 99	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	VAL	14.5
2	D	215	GLY	11.4
1	A	129	ARG	11.0
1	C	125	ASP	10.8
1	C	128	ASP	9.8
1	C	129	ARG	9.7
1	A	128	ASP	8.8
2	D	218	GLN	8.3
1	C	126	ILE	8.2
1	C	133	ALA	7.7
1	C	130	LYS	7.7
1	C	132	LYS	6.9
1	A	126	ILE	6.8
1	A	43	LEU	6.7
2	D	232	LYS	6.3
2	D	217	ARG	6.3
1	C	42	THR	6.2
2	D	292	SER	6.1
1	A	153	SER	6.0
1	A	132	LYS	5.9
1	A	141	LYS	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	31	LEU	5.8
1	A	136	ILE	5.5
2	B	292	SER	5.2
1	C	39	TYR	5.2
1	A	127	LYS	5.1
2	D	171	ASP	4.9
1	C	127	LYS	4.9
1	C	40	VAL	4.9
1	C	141	LYS	4.9
2	D	419	GLU	4.8
1	A	151	ALA	4.7
1	C	140	ARG	4.6
2	D	291	ASN	4.5
2	B	232	LYS	4.3
1	C	124	VAL	4.2
1	A	114	ASN	4.1
2	D	293	THR	4.1
2	B	291	ASN	4.1
1	A	133	ALA	4.1
1	C	153	SER	4.1
2	D	219	GLY	3.9
2	D	230	MET	3.9
1	C	143	ASN	3.9
2	D	231	LEU	3.8
2	B	398	ASN	3.8
1	C	136	ILE	3.8
2	D	343	ARG	3.7
1	C	114	ASN	3.7
2	D	239	HIS	3.7
1	A	131	VAL	3.6
2	D	216	GLY	3.6
1	A	130	LYS	3.6
1	C	139	HIS	3.5
2	B	171	ASP	3.5
1	C	170	GLY	3.5
1	C	135	SER	3.4
2	B	290	LYS	3.4
1	C	43	LEU	3.4
2	D	290	LYS	3.4
2	D	118	GLN	3.3
1	A	29	ARG	3.3
1	A	137	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	210	LEU	3.3
1	C	177	VAL	3.2
1	C	38	LYS	3.1
1	A	28	LYS	3.0
1	C	44	GLY	3.0
2	B	293	THR	2.9
1	C	152	LYS	2.9
1	A	139	HIS	2.9
1	A	125	ASP	2.8
2	B	53	ASN	2.8
1	C	142	LYS	2.8
2	B	287	THR	2.7
1	C	134	LYS	2.7
1	A	42	THR	2.7
2	D	398	ASN	2.7
2	D	214	ARG	2.7
1	A	8	GLN	2.6
2	D	225	VAL	2.5
1	C	173	ASN	2.5
2	D	417	ASP	2.4
1	C	45	VAL	2.4
2	B	343	ARG	2.4
1	C	9	VAL	2.4
1	A	113	GLU	2.4
1	A	155	TYR	2.4
1	C	137	VAL	2.4
1	C	8	GLN	2.3
1	C	13	LEU	2.2
2	D	222	ARG	2.2
1	A	31	LEU	2.2
1	A	140	ARG	2.2
1	A	154	ASN	2.2
1	C	87	ILE	2.1
2	B	118	GLN	2.1
1	C	155	TYR	2.1
1	C	113	GLU	2.1
2	D	418	LYS	2.1
2	B	24	LYS	2.0
1	C	154	ASN	2.0
1	A	41	ALA	2.0
2	D	134	LEU	2.0

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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	A	1250	5/5	0.98	0.12	0.86	36,36,37,38	0
3	SO4	C	2250	5/5	0.99	0.08	-0.07	35,36,38,39	0

6.5 Other polymers

There are no such residues in this entry.