



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:26 PM UTC

PDB ID : 1I2M / pdb_00001i2m
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

<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

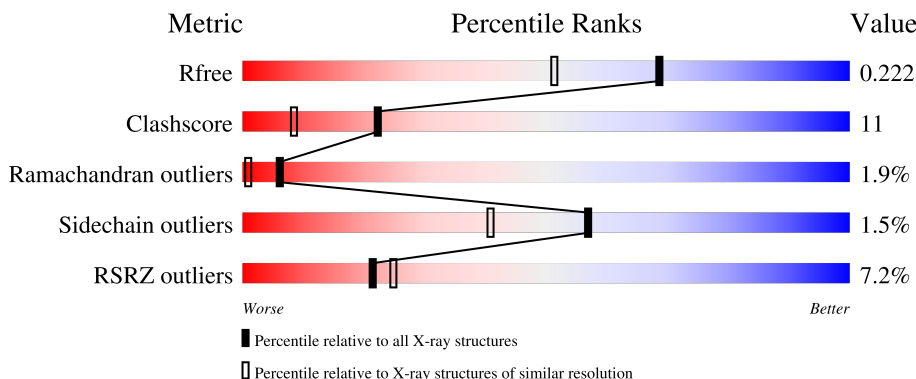
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	216	9% 59% 12% 6% 24%
1	C	216	14% 42% 27% • • 24%
2	B	402	3% 84% 12% •
2	D	402	5% 83% 13% •

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			

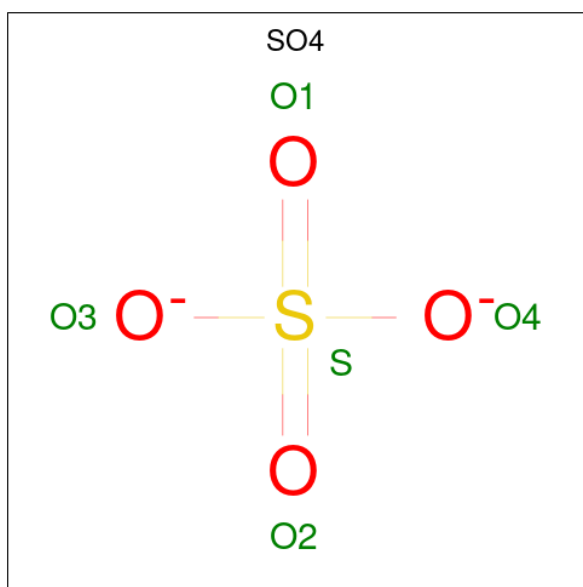
There are 2 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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		

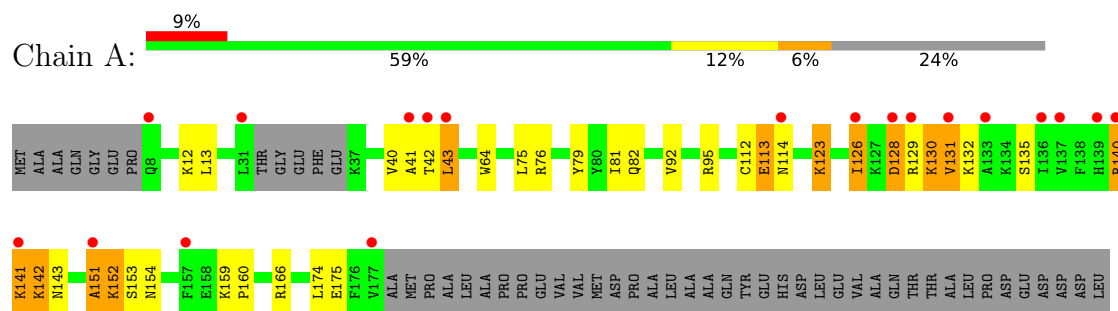
- Molecule 4 is water.

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		

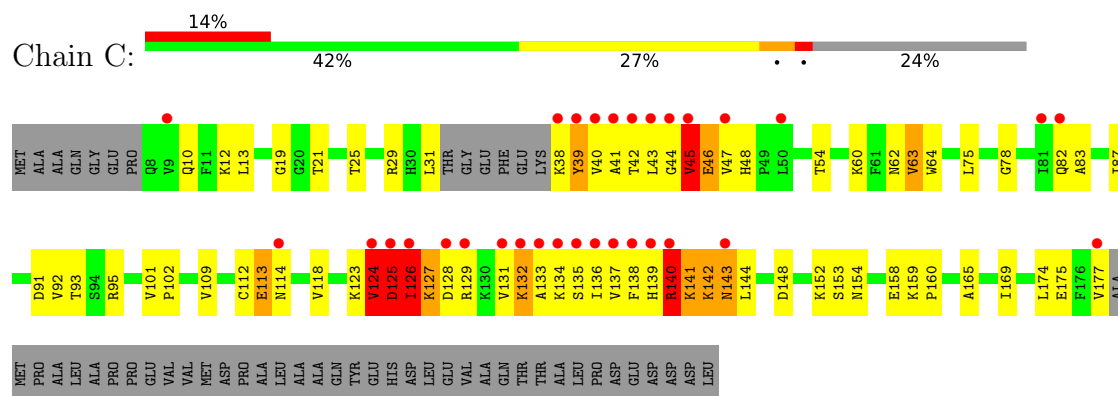
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

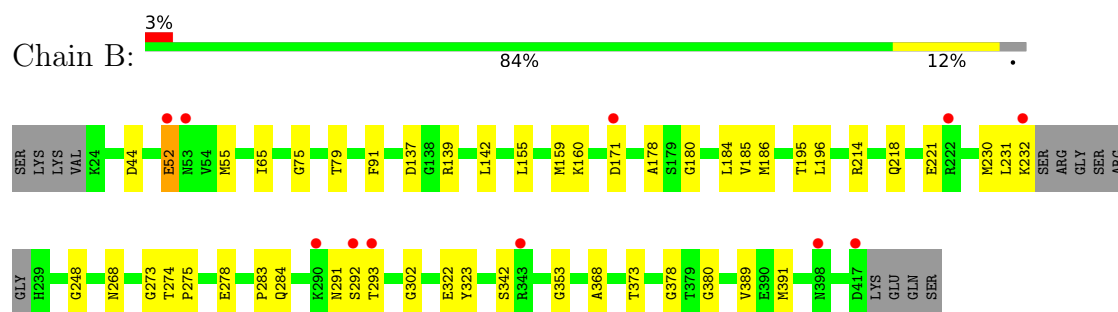
• Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN



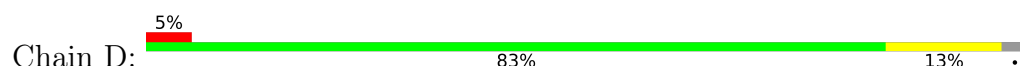
• Molecule 1: GTP-BINDING NUCLEAR PROTEIN RAN

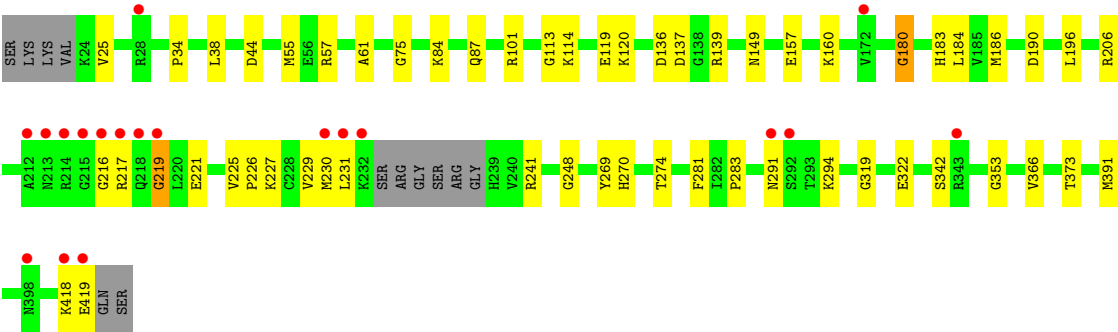


• Molecule 2: REGULATOR OF CHROMOSOME CONDENSATION 1



• 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 19.79 – 1.76	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.79-1.76) 99.7 (19.79-1.76)	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 (6.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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 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.

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	0.33	0/1378	0.92	8/1859 (0.4%)
1	C	0.38	0/1369	0.95	6/1848 (0.3%)
2	B	0.35	0/2953	0.89	13/3989 (0.3%)
2	D	0.34	0/2971	0.87	7/4012 (0.2%)
All	All	0.35	0/8671	0.90	34/11708 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	353	GLY	N-CA-C	-8.81	100.65	112.81
2	B	248	GLY	N-CA-C	-8.77	100.56	112.57
2	B	180	GLY	N-CA-C	-8.27	101.24	112.57
2	D	180	GLY	N-CA-C	-7.78	102.07	112.81
2	D	248	GLY	N-CA-C	-7.77	100.30	112.58
1	C	83	ALA	N-CA-C	7.75	121.75	110.28
2	D	342	SER	N-CA-C	7.11	120.06	111.82
1	A	131	VAL	N-CA-C	-6.98	105.82	113.43
2	B	353	GLY	N-CA-C	-6.96	100.52	112.64
1	A	95	ARG	N-CA-C	6.71	120.92	112.87
2	D	75	GLY	N-CA-C	-6.69	103.41	112.57
2	B	342	SER	N-CA-C	6.62	119.50	111.82
2	D	219	GLY	N-CA-C	6.45	120.46	112.14
2	B	75	GLY	N-CA-C	-6.40	102.81	112.41
2	B	160	LYS	N-CA-C	6.27	118.62	108.34
2	B	52	GLU	N-CA-C	6.20	120.39	112.34
1	A	41	ALA	N-CA-C	-6.16	105.72	113.72
2	B	293	THR	N-CA-C	-6.16	105.56	114.12
1	C	144	LEU	N-CA-C	6.08	119.28	110.28
2	B	380	GLY	N-CA-C	-6.08	107.46	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	95	ARG	N-CA-C	5.86	119.91	112.87
1	C	63	VAL	N-CA-C	5.83	117.40	108.71
1	A	151	ALA	N-CA-C	-5.62	101.06	109.15
2	B	373	THR	N-CA-C	5.53	118.03	111.33
1	C	45	VAL	N-CA-C	-5.46	100.49	109.12
2	D	373	THR	N-CA-C	5.45	117.93	111.33
1	A	132	LYS	N-CA-C	-5.40	106.88	112.93
1	A	76	ARG	CB-CA-C	-5.39	110.38	116.63
1	A	130	LYS	N-CA-C	-5.21	102.61	110.06
2	B	302	GLY	N-CA-C	-5.12	105.18	112.55
2	B	65	ILE	CA-C-N	5.11	124.83	119.82
2	B	65	ILE	C-N-CA	5.11	124.83	119.82
1	C	124	VAL	N-CA-C	5.09	119.92	109.34
1	A	43	LEU	N-CA-C	5.01	117.57	110.10

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	32	0
1	C	1337	0	1365	92	0
2	B	2899	0	2842	25	0
2	D	2917	0	2861	41	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	179	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 11.

All (179) 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
2:B:230:MET:HE1	2:D:281:PHE:HB2	1.68	0.75
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
2:D:221:GLU:H	2:D:221:GLU:CD	1.99	0.70
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
2:D:44:ASP:HA	2:D:55:MET:HE3	1.75	0.67
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: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:A:112:CYS:O	1:A:113:GLU:HB2	1.94	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
1:C:43:LEU:C	1:C:45:VAL:H	2.06	0.64
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:O	1:C:126:ILE:CG2	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
2:B:221:GLU:CD	1:C:75:LEU:HG	2.25	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CZ	1:C:129:ARG:HA	2.32	0.59
2:D:291:ASN:ND2	2:D:294:LYS:HD2	2.17	0.59
1:C:43:LEU:C	1:C:45:VAL:N	2.59	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
1:A:92:VAL:HG21	1:A:135:SER:HB2	1.86	0.56
1:A:140:ARG:CG	1:A:141:LYS:N	2.60	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:131:VAL:C	1:C:133:ALA:H	2.14	0.55
1:C:137:VAL:HG12	1:C:137:VAL:O	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:13:LEU:C	1:C:13:LEU:HD23	2.32	0.54
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:91:ASP:CG	1:C:124:VAL:HB	2.33	0.54
1:C:124:VAL:HG13	1:C:125:ASP:H	1.72	0.54
2:B:273:GLY:C	2:B:275:PRO:HD3	2.33	0.54
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
1:C:137:VAL:HG11	2:D:55:MET:HE2	1.90	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
1:C:126:ILE:C	1:C:128:ASP:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:270:HIS:HD2	2:D:274:THR:O	1.93	0.52
1:A:13:LEU:C	1:A:13:LEU:HD23	2.35	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
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:HG2	2:B:52:GLU:O	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: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:137:VAL:CG1	2:D:55:MET:HE2	2.42	0.50
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
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
2:B:186:MET:HE2	2:B:196:LEU:HD22	1.96	0.47
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
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:119:GLU:CD	2:D:139:ARG:HH22	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:C:131:VAL:C	1:C:133:ALA:N	2.75	0.45
2:B:185:VAL:HG12	2:B:195:THR:HG22	1.99	0.45
1:C:140:ARG:O	1:C:141:LYS:C	2.59	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
1:C:93:THR:HA	1:C:134:LYS:HZ3	1.83	0.44
2:D:186:MET:HE2	2:D:196:LEU:HD22	1.98	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
2:B:378:GLY:HA3	2:B:391:MET:HE3	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:A:75:LEU:HB2	1:A:79:TYR:CE1	2.55	0.42
1:A:123:LYS:CE	1:A:131:VAL:HG21	2.48	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
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:C:139:HIS:CE1	1:C:148:ASP:OD1	2.68	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:92:VAL:O	1:C:134:LYS:HE2	2.20	0.41
1:C:152:LYS:O	1:C:153:SER:HB2	2.19	0.41
1:C:169:ILE:CD1	1:C:174:LEU:HD22	2.50	0.41
2:D:38:LEU:HA	2:D:61:ALA:O	2.20	0.41
2:D:34:PRO:HD3	2:D:84:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:SER:O	1:A:154:ASN:C	2.64	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:140:ARG:CG	1:C:141:LYS:N	2.83	0.41
1:C:177:VAL:O	1:C:177:VAL:HG23	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
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:13:LEU:HB3	1:C:63:VAL:HG22	2.04	0.40
1:C:39:TYR:CA	1:C:46:GLU:HA	2.52	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%)	20
1	C	160/216 (74%)	144 (90%)	4 (2%)	12 (8%)	10
2	B	384/402 (96%)	373 (97%)	9 (2%)	2 (0%)	2411
2	D	386/402 (96%)	373 (97%)	13 (3%)	0	100100
All	All	1091/1236 (88%)	1036 (95%)	34 (3%)	21 (2%)	61

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%)	142 (97%)	4 (3%)	39	19
1	C	145/185 (78%)	139 (96%)	6 (4%)	27	8
2	B	313/325 (96%)	311 (99%)	2 (1%)	78	71
2	D	315/325 (97%)	313 (99%)	2 (1%)	78	71
All	All	919/1020 (90%)	905 (98%)	14 (2%)	57	41

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

Mol	Chain	Res	Type
1	A	43	LEU

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Mol	Chain	Res	Type
1	A	123	LYS
1	A	128	ASP
1	A	129	ARG
2	B	171	ASP
2	B	232	LYS
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	57	ARG
2	D	322	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	103	ASN
1	A	139	HIS
1	A	145	GLN
2	B	118	GLN
2	B	218	GLN
2	B	284	GLN
2	B	303	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 [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	2250	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	A	1250	-	4,4,4	0.32	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	165/216 (76%)	0.65	19 (11%) 9 11	18, 32, 80, 99	0
1	C	164/216 (75%)	0.94	31 (18%) 3 3	19, 36, 90, 99	0
2	B	388/402 (96%)	0.08	11 (2%) 55 61	16, 26, 57, 92	0
2	D	390/402 (97%)	0.21	19 (4%) 35 40	15, 27, 66, 99	0
All	All	1107/1236 (89%)	0.34	80 (7%) 21 25	15, 29, 73, 99	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	VAL	5.8
1	A	42	THR	5.7
1	C	40	VAL	5.6
1	A	43	LEU	5.6
1	C	124	VAL	5.6
2	D	215	GLY	4.8
1	A	151	ALA	4.7
1	C	42	THR	4.7
1	C	43	LEU	4.5
1	C	126	ILE	4.5
1	C	39	TYR	4.4
1	C	177	VAL	4.2
1	C	133	ALA	4.0
1	C	143	ASN	3.9
2	D	219	GLY	3.9
1	C	44	GLY	3.8
2	D	231	LEU	3.8
1	C	136	ILE	3.7
1	A	177	VAL	3.7
1	A	41	ALA	3.7
2	D	343	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	137	VAL	3.5
1	C	125	ASP	3.4
1	C	47	VAL	3.4
1	C	134	LYS	3.3
1	A	131	VAL	3.3
1	C	135	SER	3.2
2	D	292	SER	3.2
1	C	129	ARG	3.2
2	D	419	GLU	3.1
1	A	141	LYS	3.1
1	C	138	PHE	3.0
2	B	171	ASP	3.0
2	D	398	ASN	3.0
2	D	291	ASN	2.9
1	C	137	VAL	2.9
2	D	218	GLN	2.8
2	D	232	LYS	2.8
1	C	41	ALA	2.8
2	D	212	ALA	2.8
1	C	139	HIS	2.8
1	C	45	VAL	2.7
2	D	418	LYS	2.7
2	B	292	SER	2.7
2	D	230	MET	2.7
1	C	140	ARG	2.6
2	B	417	ASP	2.6
2	D	214	ARG	2.6
1	A	129	ARG	2.6
1	A	128	ASP	2.5
2	B	398	ASN	2.5
1	A	114	ASN	2.5
1	C	114	ASN	2.5
1	A	136	ILE	2.5
1	C	50	LEU	2.4
2	D	216	GLY	2.4
2	D	217	ARG	2.4
1	C	81	ILE	2.4
1	C	128	ASP	2.4
2	B	232	LYS	2.4
1	A	139	HIS	2.4
1	A	8	GLN	2.3
1	C	82	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	213	ASN	2.3
1	C	38	LYS	2.3
2	B	290	LYS	2.3
2	B	343	ARG	2.3
1	A	126	ILE	2.3
2	D	172	VAL	2.3
1	A	133	ALA	2.2
1	C	9	VAL	2.2
1	A	157	PHE	2.2
2	D	28	ARG	2.2
2	B	53	ASN	2.2
2	B	293	THR	2.2
2	B	52	GLU	2.1
1	C	132	LYS	2.1
1	A	31	LEU	2.1
1	A	140	ARG	2.0
2	B	222	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	1250	5/5	0.97	0.08	36,36,37,38	0
3	SO4	C	2250	5/5	0.97	0.08	35,36,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.