



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:19 PM GMT

PDB ID : 5CLQ
Title : Ran Y39A in complex with GPPNHP and RanBD1
Authors : Vetter, I.R.; Brucker, S.
Deposited on : 2015-07-16
Resolution : 3.20 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

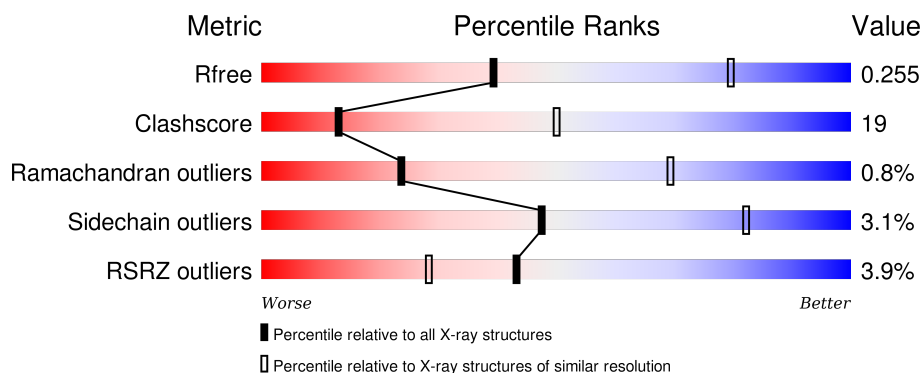
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 $\leq 5\%$. 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>4%</div> <div>64%</div> <div>29%</div> <div>• •</div> </div>
1	C	216	<div> <div>6%</div> <div>57%</div> <div>31%</div> <div>• • 7%</div> </div>
2	B	167	<div> <div>•</div> <div>54%</div> <div>24%</div> <div>• 20%</div> </div>
2	D	167	<div> <div>3%</div> <div>47%</div> <div>28%</div> <div>• • 22%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	A	304	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5524 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	207	Total	C	N	O	S	0	0	0
			1648	1064	285	293	6			
1	C	200	Total	C	N	O	S	0	0	0
			1591	1030	272	283	6			

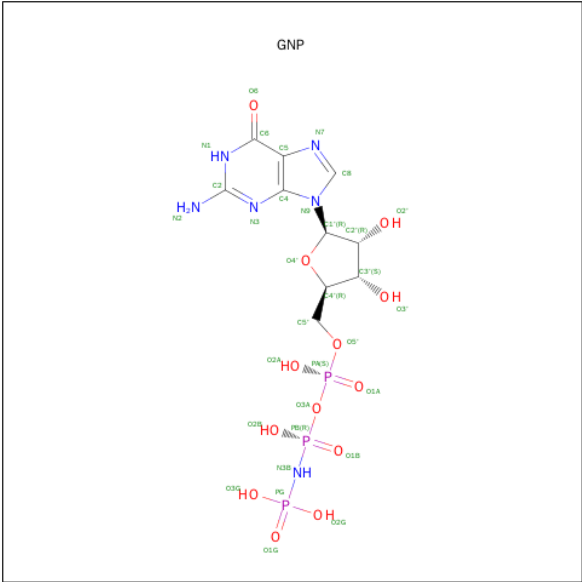
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ALA	TYR	engineered mutation	UNP P62826
C	39	ALA	TYR	engineered mutation	UNP P62826

- Molecule 2 is a protein called E3 SUMO-protein ligase RanBP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	134	Total	C	N	O	S	0	0	0
			1100	703	191	201	5			
2	D	131	Total	C	N	O	S	0	0	0
			1077	688	188	196	5			

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

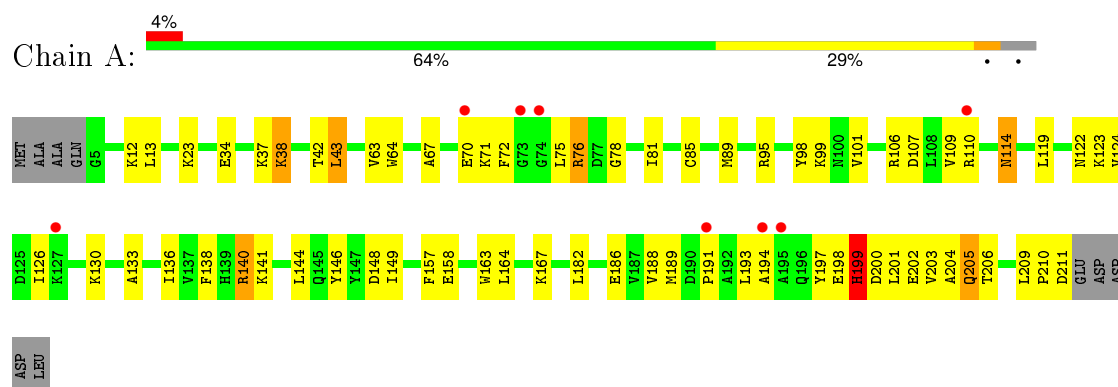
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	4	Total	O	0	0
			4	4		
6	B	2	Total	O	0	0
			2	2		
6	C	4	Total	O	0	0
			4	4		
6	D	2	Total	O	0	0
			2	2		

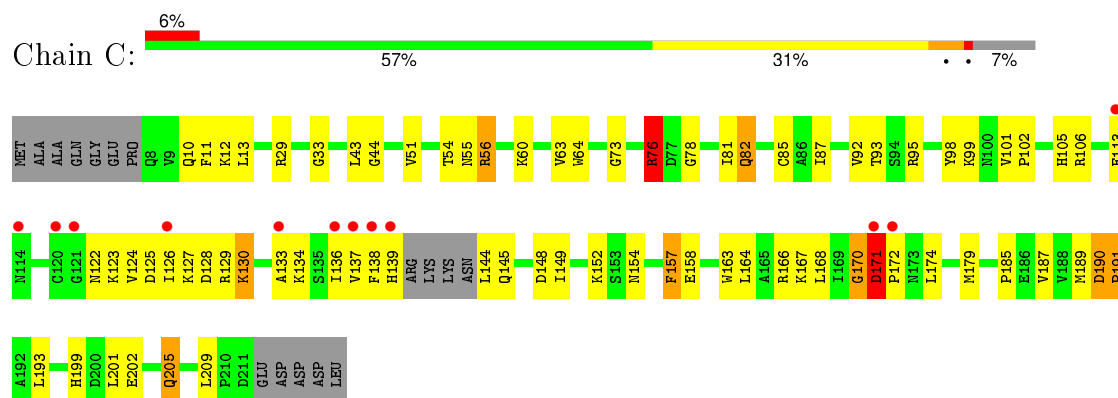
3 Residue-property plots [i](#)

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.

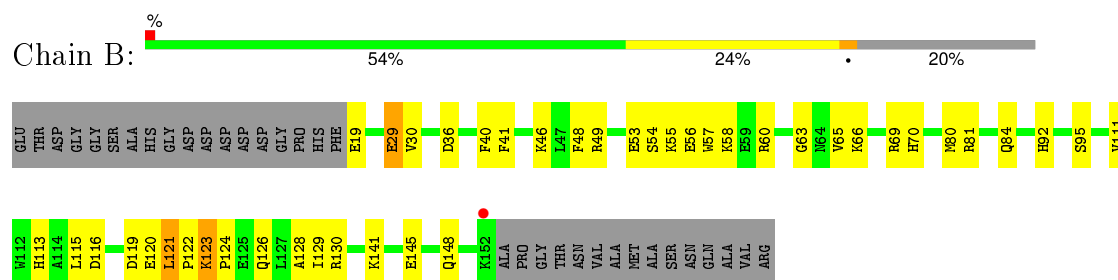
- Molecule 1: GTP-binding nuclear protein Ran



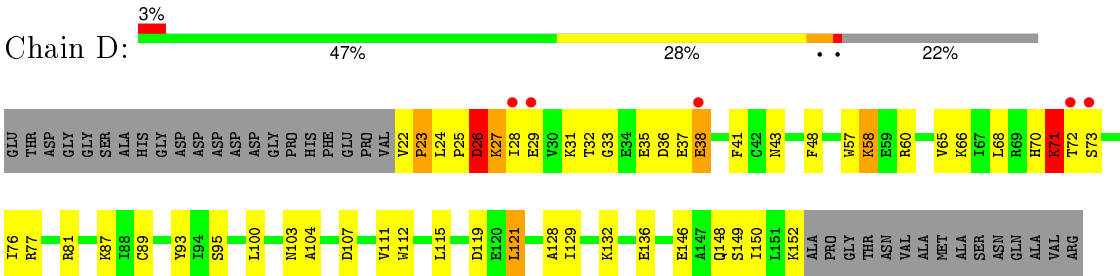
- Molecule 1: GTP-binding nuclear protein Ran



- Molecule 2: E3 SUMO-protein ligase RanBP2



- Molecule 2: E3 SUMO-protein ligase RanBP2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.53Å 170.92Å 135.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.98-3.20) 99.9 (19.98-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 3.22Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.224 , 0.254 0.222 , 0.255	Depositor DCC
R_{free} test set	996 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	85.4	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.6	EDS
Estimated twinning fraction	0.016 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 19912 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5524	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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, 0.375 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: MG, GNP, 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	0.49	0/1689	0.92	7/2291 (0.3%)
1	C	0.45	0/1630	0.96	10/2212 (0.5%)
2	B	0.46	0/1124	0.85	1/1510 (0.1%)
2	D	0.60	1/1100 (0.1%)	1.11	6/1476 (0.4%)
All	All	0.50	1/5543 (0.0%)	0.96	24/7489 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	D	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	26	ASP	CB-CG	6.14	1.64	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	GLY	N-CA-C	9.32	136.39	113.10
2	B	121	LEU	CB-CG-CD2	-7.47	98.31	111.00
1	C	56	ARG	NE-CZ-NH1	-7.00	116.80	120.30
2	D	26	ASP	N-CA-CB	6.91	123.04	110.60
1	A	75	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	199	HIS	CB-CA-C	6.37	123.13	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	38	GLU	CB-CA-C	-6.34	97.71	110.40
1	C	171	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	171	ASP	CB-CG-OD1	-6.28	112.65	118.30
2	D	38	GLU	CA-CB-CG	6.15	126.93	113.40
1	A	107	ASP	CB-CG-OD1	-5.96	112.94	118.30
1	C	82	GLN	CA-CB-CG	5.95	126.50	113.40
1	A	76	ARG	CG-CD-NE	-5.90	99.42	111.80
1	C	134	LYS	CA-CB-CG	-5.87	100.49	113.40
1	A	43	LEU	CB-CG-CD1	-5.57	101.54	111.00
2	D	28	ILE	N-CA-C	-5.53	96.06	111.00
1	A	71	LYS	N-CA-C	5.50	125.84	111.00
1	C	130	LYS	CD-CE-NZ	-5.48	99.09	111.70
2	D	23	PRO	C-N-CA	-5.32	108.41	121.70
2	D	71	LYS	CB-CA-C	-5.30	99.81	110.40
1	C	56	ARG	CG-CD-NE	5.28	122.89	111.80
1	A	114	ASN	N-CA-CB	-5.27	101.11	110.60
1	C	106	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	C	76	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	171	ASP	Peptide
2	D	26	ASP	Peptide
2	D	27	LYS	Mainchain

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	1648	0	1660	65	0
1	C	1591	0	1598	81	0
2	B	1100	0	1110	38	0
2	D	1077	0	1088	59	0
3	A	32	0	13	0	0
3	C	32	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	10	0	0	1	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
6	A	4	0	0	0	0
6	B	2	0	0	1	0
6	C	4	0	0	0	0
6	D	2	0	0	0	0
All	All	5524	0	5482	209	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 19.

All (209) 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:C:56:ARG:HH12	2:D:24:LEU:HG	1.35	0.91
1:C:163:TRP:O	1:C:167:LYS:NZ	2.09	0.83
2:D:60:ARG:NH2	2:D:119:ASP:OD2	2.14	0.80
2:D:32:THR:N	2:D:35:GLU:OE2	2.15	0.79
1:C:123:LYS:HB3	1:C:126:ILE:HD12	1.63	0.78
1:A:106:ARG:O	1:A:110:ARG:HG2	1.84	0.76
2:B:65:VAL:HG21	2:B:129:ILE:HD11	1.68	0.76
2:D:65:VAL:HG21	2:D:129:ILE:HD11	1.70	0.74
1:C:55:ASN:O	2:D:27:LYS:HG3	1.88	0.73
1:C:205:GLN:HB3	2:D:111:VAL:HG21	1.70	0.72
2:B:49:ARG:HD3	2:B:60:ARG:HD3	1.71	0.72
1:C:13:LEU:HD23	1:C:63:VAL:HG22	1.72	0.71
1:A:114:ASN:N	1:A:114:ASN:OD1	2.17	0.71
2:D:37:GLU:HA	2:D:71:LYS:NZ	2.08	0.69
2:D:70:HIS:HD2	2:D:71:LYS:H	1.42	0.68
2:B:121:LEU:HD21	2:D:121:LEU:HD22	1.78	0.66
1:C:179:MET:O	2:D:81:ARG:NH1	2.27	0.65
1:C:98:TYR:CE2	1:C:136:ILE:HG13	2.31	0.65
1:C:201:LEU:O	1:C:205:GLN:HG2	1.97	0.64
1:C:85:CYS:HB2	1:C:164:LEU:HD22	1.78	0.64
2:B:60:ARG:NH2	2:B:119:ASP:OD1	2.30	0.64
1:A:200:ASP:OD2	2:B:126:GLN:NE2	2.31	0.64
2:D:70:HIS:HD2	2:D:71:LYS:N	1.96	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:VAL:HG11	1:C:148:ASP:HB3	1.81	0.63
2:D:95:SER:O	2:D:148:GLN:NE2	2.26	0.62
1:A:200:ASP:O	1:A:203:VAL:HG22	1.99	0.61
1:A:201:LEU:O	1:A:205:GLN:HG3	2.01	0.61
1:A:106:ARG:CZ	1:A:110:ARG:HG3	2.31	0.61
1:C:209:LEU:HD13	2:D:103:ASN:ND2	2.15	0.61
1:C:102:PRO:HG3	1:C:138:PHE:HE1	1.67	0.60
1:A:191:PRO:HA	1:A:194:ALA:HB2	1.83	0.60
1:A:189:MET:HE3	2:B:124:PRO:HB3	1.84	0.60
1:C:13:LEU:HD11	1:C:87:ILE:HG13	1.83	0.60
1:C:122:ASN:HA	1:C:149:ILE:HG13	1.82	0.60
1:C:139:HIS:HD2	1:C:144:LEU:O	1.85	0.59
1:A:205:GLN:HG2	2:B:111:VAL:HG21	1.85	0.58
1:A:194:ALA:HA	1:A:197:TYR:CD2	2.39	0.58
1:C:209:LEU:HD13	2:D:103:ASN:HD22	1.69	0.58
1:A:136:ILE:HG21	1:A:146:TYR:CG	2.39	0.58
1:C:154:ASN:O	1:C:157:PHE:HB3	2.03	0.58
1:C:29:ARG:HG2	1:C:157:PHE:CE1	2.39	0.58
1:A:95:ARG:HH12	1:A:130:LYS:HE2	1.68	0.57
1:A:78:GLY:O	1:A:81:ILE:HG12	2.04	0.57
1:A:209:LEU:HB3	2:B:130:ARG:HH21	1.69	0.57
1:A:202:GLU:HG3	1:A:206:THR:HG23	1.87	0.57
1:A:200:ASP:HA	1:A:203:VAL:HG13	1.87	0.57
1:C:73:GLY:O	1:C:76:ARG:HG2	2.04	0.57
1:A:85:CYS:HB2	1:A:164:LEU:HD22	1.87	0.57
1:C:163:TRP:CZ3	1:C:167:LYS:HE3	2.40	0.57
1:C:95:ARG:HE	1:C:130:LYS:HD2	1.69	0.57
1:C:92:VAL:HG11	1:C:129:ARG:HG2	1.86	0.56
2:D:70:HIS:CD2	2:D:71:LYS:N	2.73	0.56
2:B:53:GLU:O	2:B:55:LYS:HD3	2.05	0.56
1:A:38:LYS:H	1:A:38:LYS:HD3	1.69	0.56
2:B:54:SER:OG	2:B:56:GLU:HG2	2.05	0.56
1:A:13:LEU:HD22	1:A:63:VAL:HG22	1.88	0.56
2:B:40:PHE:HZ	2:B:69:ARG:HE	1.52	0.56
1:A:188:VAL:HG13	1:C:190:ASP:HB2	1.88	0.56
2:D:37:GLU:OE1	2:D:68:LEU:HB3	2.06	0.56
1:C:56:ARG:HH21	2:D:26:ASP:HB2	1.70	0.55
2:D:70:HIS:CD2	2:D:71:LYS:H	2.22	0.55
1:A:110:ARG:N	1:A:110:ARG:HD2	2.22	0.55
1:C:44:GLY:HA2	1:C:73:GLY:HA2	1.89	0.54
1:C:56:ARG:HH22	2:D:24:LEU:CD2	2.20	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:36:ASP:O	2:B:70:HIS:HD2	1.90	0.54
1:C:95:ARG:HG2	1:C:130:LYS:HB3	1.89	0.54
1:C:78:GLY:O	1:C:81:ILE:HG12	2.08	0.54
1:A:140:ARG:NH2	5:A:303:SO4:O3	2.38	0.54
2:D:37:GLU:HA	2:D:71:LYS:HZ3	1.72	0.53
1:C:56:ARG:HH22	2:D:24:LEU:HD21	1.72	0.53
1:C:93:THR:HG22	1:C:126:ILE:HG21	1.90	0.53
1:A:204:ALA:HB1	2:B:57:TRP:CZ2	2.44	0.53
1:A:34:GLU:OE1	2:B:58:LYS:HE3	2.08	0.52
1:A:123:LYS:HB3	1:A:126:ILE:HD12	1.91	0.52
1:C:54:THR:HG21	1:C:174:LEU:HD21	1.91	0.52
1:A:72:PHE:O	1:A:76:ARG:NH2	2.41	0.52
1:A:76:ARG:HD3	1:A:76:ARG:N	2.25	0.52
1:C:95:ARG:HH21	1:C:130:LYS:HD3	1.75	0.52
1:A:189:MET:CE	2:B:124:PRO:HB3	2.40	0.51
1:C:51:VAL:HG13	2:D:87:LYS:NZ	2.25	0.51
1:A:202:GLU:O	1:A:206:THR:N	2.43	0.51
2:B:95:SER:O	2:B:148:GLN:NE2	2.32	0.51
2:D:107:ASP:N	2:D:107:ASP:OD1	2.28	0.51
1:A:199:HIS:O	1:A:202:GLU:N	2.43	0.51
1:C:95:ARG:HE	1:C:130:LYS:CD	2.24	0.51
1:A:109:VAL:HG23	1:A:110:ARG:HD2	1.92	0.51
1:A:122:ASN:HA	1:A:149:ILE:HG13	1.93	0.51
2:B:122:PRO:O	2:B:123:LYS:HE3	2.11	0.51
2:B:121:LEU:CD2	2:D:121:LEU:HD22	2.40	0.51
1:C:167:LYS:O	1:C:170:GLY:HA2	2.10	0.50
1:C:163:TRP:CH2	1:C:167:LYS:HE3	2.46	0.50
1:C:56:ARG:HA	2:D:27:LYS:HA	1.94	0.50
2:D:72:THR:OG1	2:D:73:SER:N	2.43	0.50
2:B:46:LYS:HG2	2:B:48:PHE:CE1	2.46	0.50
1:C:12:LYS:HE3	1:C:64:TRP:CE2	2.46	0.50
1:A:198:GLU:O	1:A:201:LEU:N	2.45	0.50
1:C:56:ARG:NH1	2:D:24:LEU:HG	2.16	0.50
1:A:95:ARG:HH12	1:A:130:LYS:HB3	1.77	0.50
1:C:105:HIS:CE1	1:C:144:LEU:HD21	2.47	0.50
1:A:201:LEU:O	1:A:204:ALA:HB3	2.12	0.49
1:C:166:ARG:NE	1:C:172:PRO:O	2.44	0.49
2:D:68:LEU:O	2:D:76:ILE:HA	2.13	0.49
1:C:127:LYS:HG2	1:C:128:ASP:N	2.26	0.49
2:B:48:PHE:HB2	2:B:128:ALA:HB3	1.95	0.49
1:C:127:LYS:CG	1:C:128:ASP:N	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:29:GLU:CD	2:B:30:VAL:H	2.16	0.49
1:C:93:THR:HG21	1:C:126:ILE:HD13	1.94	0.49
2:D:37:GLU:HA	2:D:71:LYS:HZ1	1.76	0.49
1:A:70:GLU:C	1:A:70:GLU:CD	2.71	0.49
2:D:146:GLU:O	2:D:149:SER:HB2	2.12	0.49
1:A:158:GLU:N	1:A:158:GLU:OE2	2.41	0.48
1:A:205:GLN:HG2	2:B:111:VAL:CG2	2.43	0.48
1:A:198:GLU:O	1:A:201:LEU:HB3	2.13	0.48
1:A:157:PHE:CE2	2:B:84:GLN:HB2	2.48	0.48
2:D:37:GLU:CD	2:D:38:GLU:H	2.17	0.48
1:C:209:LEU:HD12	2:D:57:TRP:CD1	2.49	0.48
1:A:119:LEU:HB2	1:A:138:PHE:CE2	2.49	0.48
2:D:103:ASN:OD1	2:D:104:ALA:N	2.47	0.48
1:C:139:HIS:ND1	1:C:139:HIS:O	2.47	0.48
1:A:12:LYS:HE3	1:A:64:TRP:CE2	2.49	0.47
1:C:98:TYR:HA	1:C:101:VAL:HG23	1.96	0.47
1:A:95:ARG:NH1	1:A:130:LYS:HB3	2.29	0.47
1:A:189:MET:O	1:A:191:PRO:HD3	2.14	0.47
2:D:43:ASN:ND2	2:D:136:GLU:OE2	2.33	0.47
2:D:37:GLU:CD	2:D:38:GLU:N	2.69	0.46
1:A:72:PHE:O	1:A:76:ARG:NH1	2.47	0.46
1:C:171:ASP:HB3	1:C:172:PRO:HD3	1.97	0.46
2:D:150:ILE:HD12	2:D:150:ILE:H	1.81	0.46
1:C:93:THR:CG2	1:C:126:ILE:HG21	2.45	0.46
1:C:125:ASP:OD2	1:C:152:LYS:HD3	2.16	0.46
2:D:115:LEU:HD12	2:D:115:LEU:HA	1.31	0.45
2:D:70:HIS:HB3	2:D:73:SER:OG	2.16	0.45
1:C:92:VAL:HG23	1:C:122:ASN:O	2.17	0.45
1:A:124:VAL:HG11	1:A:148:ASP:HB3	1.99	0.45
2:B:60:ARG:NH1	6:B:301:HOH:O	2.50	0.45
2:D:41:PHE:O	2:D:66:LYS:HA	2.17	0.45
2:D:100:LEU:HD23	2:D:112:TRP:HB3	1.99	0.44
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.81	0.44
1:A:163:TRP:O	1:A:167:LYS:HG2	2.18	0.44
2:D:29:GLU:H	2:D:29:GLU:HG2	1.65	0.44
1:A:133:ALA:O	1:A:136:ILE:HB	2.18	0.44
2:B:115:LEU:HD12	2:B:115:LEU:HA	1.77	0.44
1:C:145:GLN:HG3	1:C:163:TRP:NE1	2.33	0.44
1:C:199:HIS:O	1:C:202:GLU:HB2	2.16	0.44
2:D:36:ASP:O	2:D:71:LYS:CE	2.66	0.44
2:B:41:PHE:O	2:B:66:LYS:HA	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:GLU:N	1:C:158:GLU:OE2	2.43	0.44
1:A:99:LYS:HA	1:A:99:LYS:HD3	1.84	0.44
1:C:56:ARG:NH2	2:D:26:ASP:HB2	2.33	0.43
2:D:23:PRO:O	2:D:25:PRO:HD3	2.18	0.43
1:C:145:GLN:HG3	1:C:163:TRP:CE2	2.53	0.43
1:C:105:HIS:CE1	1:C:144:LEU:HD11	2.53	0.43
1:C:99:LYS:HB3	1:C:99:LYS:HE3	1.63	0.43
1:A:98:TYR:HA	1:A:101:VAL:HG23	1.99	0.43
1:C:51:VAL:HG13	2:D:87:LYS:HZ1	1.83	0.43
1:C:171:ASP:CB	1:C:172:PRO:HD3	2.48	0.43
1:C:185:PRO:O	1:C:187:VAL:HG22	2.19	0.43
2:D:71:LYS:HD3	2:D:71:LYS:N	2.33	0.43
1:A:70:GLU:O	1:A:76:ARG:NH2	2.50	0.43
1:C:43:LEU:HA	1:C:43:LEU:HD23	1.78	0.43
2:D:33:GLY:N	2:D:35:GLU:OE2	2.40	0.43
1:C:127:LYS:HG2	1:C:128:ASP:H	1.83	0.43
2:B:81:ARG:HG2	2:B:81:ARG:HH11	1.84	0.43
1:A:23:LYS:HG2	1:A:89:MET:HE3	2.01	0.43
2:D:58:LYS:HE2	2:D:58:LYS:HB2	1.65	0.43
1:C:133:ALA:HA	1:C:136:ILE:HD13	2.01	0.43
1:C:29:ARG:NH2	1:C:33:GLY:O	2.44	0.43
1:A:42:THR:O	1:A:67:ALA:HB2	2.19	0.43
1:C:145:GLN:HG3	1:C:163:TRP:CD1	2.53	0.43
1:A:81:ILE:HG13	1:A:81:ILE:O	2.19	0.43
1:C:10:GLN:HB3	1:C:60:LYS:HB3	2.00	0.43
1:A:141:LYS:HB2	1:A:144:LEU:HD12	2.01	0.43
2:D:132:LYS:HA	2:D:132:LYS:HD2	1.54	0.43
2:B:65:VAL:HG22	2:B:80:MET:SD	2.59	0.43
2:D:81:ARG:HG2	2:D:81:ARG:HH11	1.84	0.43
1:C:139:HIS:CD2	1:C:144:LEU:O	2.68	0.43
2:D:48:PHE:HB2	2:D:128:ALA:HB3	2.01	0.42
1:C:56:ARG:CZ	2:D:25:PRO:O	2.67	0.42
2:B:141:LYS:O	2:B:145:GLU:HG3	2.19	0.42
2:B:121:LEU:HD21	2:D:121:LEU:CD2	2.49	0.42
1:C:98:TYR:CZ	1:C:138:PHE:HE2	2.37	0.42
1:A:193:LEU:HD11	1:A:197:TYR:CE1	2.55	0.42
1:A:72:PHE:O	1:A:76:ARG:CZ	2.67	0.42
1:C:11:PHE:CG	1:C:168:LEU:HD13	2.54	0.42
2:D:77:ARG:HB3	2:D:93:TYR:CD1	2.55	0.42
2:B:92:HIS:HB3	2:B:116:ASP:HA	2.01	0.42
1:A:209:LEU:HD12	2:B:57:TRP:CD1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:26:ASP:OD2	2:D:27:LYS:N	2.37	0.41
1:C:56:ARG:HD3	1:C:56:ARG:HH11	1.65	0.41
1:C:145:GLN:HB2	1:C:163:TRP:CZ2	2.55	0.41
1:A:189:MET:SD	2:B:113:HIS:NE2	2.92	0.41
2:D:87:LYS:HB3	2:D:87:LYS:HE3	1.89	0.41
2:B:121:LEU:HB3	2:B:123:LYS:HD3	2.02	0.41
1:C:56:ARG:HH12	2:D:24:LEU:CG	2.19	0.41
2:B:63:GLY:HA3	2:B:81:ARG:O	2.19	0.41
1:A:37:LYS:HE3	1:A:37:LYS:HB3	1.97	0.41
2:B:121:LEU:HB3	2:B:123:LYS:CD	2.50	0.41
1:C:189:MET:O	1:C:191:PRO:HD3	2.21	0.41
1:C:98:TYR:OH	1:C:138:PHE:HE2	2.03	0.41
1:A:43:LEU:HD23	1:A:43:LEU:O	2.20	0.41
1:C:102:PRO:HG3	1:C:138:PHE:CE1	2.50	0.41
1:A:186:GLU:HB2	1:C:193:LEU:HD21	2.01	0.41
2:D:60:ARG:HH11	2:D:60:ARG:HG3	1.86	0.40
2:B:29:GLU:OE1	2:B:29:GLU:HA	2.20	0.40
1:C:98:TYR:OH	1:C:136:ILE:HA	2.21	0.40
1:C:129:ARG:HH22	1:C:148:ASP:CG	2.24	0.40
2:D:60:ARG:HD3	2:D:89:CYS:O	2.21	0.40
1:A:157:PHE:HE2	2:B:84:GLN:HB2	1.85	0.40
1:A:210:PRO:O	1:A:211:ASP:HB3	2.21	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	205/216 (95%)	188 (92%)	15 (7%)	2 (1%)	19	65
1	C	196/216 (91%)	179 (91%)	14 (7%)	3 (2%)	13	55
2	B	132/167 (79%)	127 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	129/167 (77%)	122 (95%)	7 (5%)	0	100	100
All	All	662/766 (86%)	616 (93%)	41 (6%)	5 (1%)	24	69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	C	113	GLU
1	A	140	ARG
1	C	171	ASP
1	C	205	GLN

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	177/184 (96%)	175 (99%)	2 (1%)	80	94
1	C	171/184 (93%)	165 (96%)	6 (4%)	43	80
2	B	120/143 (84%)	116 (97%)	4 (3%)	45	81
2	D	117/143 (82%)	111 (95%)	6 (5%)	29	70
All	All	585/654 (89%)	567 (97%)	18 (3%)	47	82

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	199	HIS
2	B	19	GLU
2	B	29	GLU
2	B	120	GLU
2	B	123	LYS
1	C	76	ARG
1	C	82	GLN
1	C	137	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	157	PHE
1	C	190	ASP
1	C	191	PRO
2	D	22	VAL
2	D	31	LYS
2	D	58	LYS
2	D	71	LYS
2	D	121	LEU
2	D	152	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	82	GLN
1	C	105	HIS
1	C	139	HIS
2	D	70	HIS

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 ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	GNP	A	301	4	29,34,34	1.92	6 (20%)	29,54,54	2.64	7 (24%)
5	SO4	A	303	-	4,4,4	0.19	0	6,6,6	0.12	0
5	SO4	A	304	-	4,4,4	0.21	0	6,6,6	0.08	0
5	SO4	B	201	-	4,4,4	0.20	0	6,6,6	0.09	0
5	SO4	C	301	-	4,4,4	0.17	0	6,6,6	0.18	0
3	GNP	C	302	4	29,34,34	1.84	5 (17%)	29,54,54	2.59	7 (24%)
5	SO4	D	201	-	4,4,4	0.17	0	6,6,6	0.09	0
5	SO4	D	202	-	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	GNP	A	301	4	-	0/13/38/38	0/3/3/3
5	SO4	A	303	-	-	0/0/0/0	0/0/0/0
5	SO4	A	304	-	-	0/0/0/0	0/0/0/0
5	SO4	B	201	-	-	0/0/0/0	0/0/0/0
5	SO4	C	301	-	-	0/0/0/0	0/0/0/0
3	GNP	C	302	4	-	0/13/38/38	0/3/3/3
5	SO4	D	201	-	-	0/0/0/0	0/0/0/0
5	SO4	D	202	-	-	0/0/0/0	0/0/0/0

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	GNP	PB-O3A	-5.28	1.52	1.59
3	C	302	GNP	PB-O3A	-4.76	1.53	1.59
3	A	301	GNP	PB-O2B	-3.01	1.48	1.56
3	C	302	GNP	PB-O2B	-3.01	1.48	1.56
3	C	302	GNP	PG-O2G	-2.13	1.51	1.56
3	A	301	GNP	C8-N7	-2.03	1.30	1.34
3	A	301	GNP	PB-O1B	2.33	1.48	1.46
3	C	302	GNP	C6-N1	3.70	1.39	1.33
3	A	301	GNP	C6-N1	3.98	1.40	1.33
3	C	302	GNP	PG-O1G	4.99	1.51	1.46
3	A	301	GNP	PG-O1G	5.05	1.51	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	GNP	C5-C6-N1	-9.30	111.36	123.52
3	A	301	GNP	C5-C6-N1	-9.01	111.75	123.52
3	A	301	GNP	PA-O3A-PB	-3.48	120.10	132.71
3	A	301	GNP	O3G-PG-O1G	-3.18	105.21	113.58
3	A	301	GNP	N3-C2-N1	-2.83	123.71	127.56
3	C	302	GNP	O3G-PG-O1G	-2.81	106.18	113.58
3	C	302	GNP	PA-O3A-PB	-2.50	123.63	132.71
3	C	302	GNP	N3-C2-N1	-2.41	124.27	127.56
3	C	302	GNP	O3G-PG-O2G	2.48	114.86	107.67
3	A	301	GNP	O3G-PG-O2G	2.77	115.73	107.67
3	C	302	GNP	O2B-PB-O1B	3.49	116.88	110.02
3	A	301	GNP	O2B-PB-O1B	3.68	117.26	110.02
3	A	301	GNP	C6-N1-C2	7.70	124.90	115.88
3	C	302	GNP	C6-N1-C2	7.74	124.96	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	303	SO4	1	0

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	207/216 (95%)	0.10	8 (3%) 43 28	52, 83, 131, 141	0
1	C	200/216 (92%)	0.23	12 (6%) 25 14	61, 90, 128, 145	0
2	B	134/167 (80%)	0.02	1 (0%) 89 83	66, 85, 112, 126	0
2	D	131/167 (78%)	0.14	5 (3%) 44 29	60, 83, 132, 138	0
All	All	672/766 (87%)	0.13	26 (3%) 43 28	52, 86, 129, 145	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	GLY	4.5
1	C	133	ALA	4.4
2	D	72	THR	4.1
1	A	73	GLY	3.8
1	C	171	ASP	3.8
1	A	194	ALA	3.6
2	D	28	ILE	3.3
1	C	139	HIS	3.1
2	D	38	GLU	3.0
1	C	120	CYS	3.0
1	A	195	ALA	2.9
1	A	70	GLU	2.9
1	C	136	ILE	2.9
2	B	152	LYS	2.8
2	D	73	SER	2.7
1	C	114	ASN	2.7
2	D	29	GLU	2.7
1	C	113	GLU	2.7
1	C	172	PRO	2.5
1	C	126	ILE	2.5
1	C	138	PHE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	191	PRO	2.3
1	C	121	GLY	2.3
1	C	137	VAL	2.1
1	A	110	ARG	2.1
1	A	127	LYS	2.1

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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	SO4	A	304	5/5	0.83	0.46	1.27	121,126,143,152	0
4	MG	C	303	1/1	0.99	0.19	-0.41	74,74,74,74	0
5	SO4	A	303	5/5	0.93	0.17	-0.58	105,107,122,126	0
3	GNP	C	302	32/32	0.95	0.18	-0.74	66,74,85,88	0
3	GNP	A	301	32/32	0.94	0.19	-0.83	72,81,91,96	0
4	MG	A	302	1/1	0.99	0.17	-0.91	80,80,80,80	0
5	SO4	B	201	5/5	0.86	0.33	-	123,130,136,146	0
5	SO4	D	201	5/5	0.84	0.20	-	102,103,121,131	0
5	SO4	D	202	5/5	0.72	0.37	-	108,110,116,128	0
5	SO4	C	301	5/5	0.93	0.15	-	77,103,118,119	0

6.5 Other polymers [i](#)

There are no such residues in this entry.