wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:59 AM GMT

PDB ID	:	3KGD
Title	:	Crystal structure of E. coli RNA 3' cyclase
Authors	:	Shuman, S.; Tanaka, N.; Smith, P.
Deposited on	:	2009-10-28
Resolution	:	1.68 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

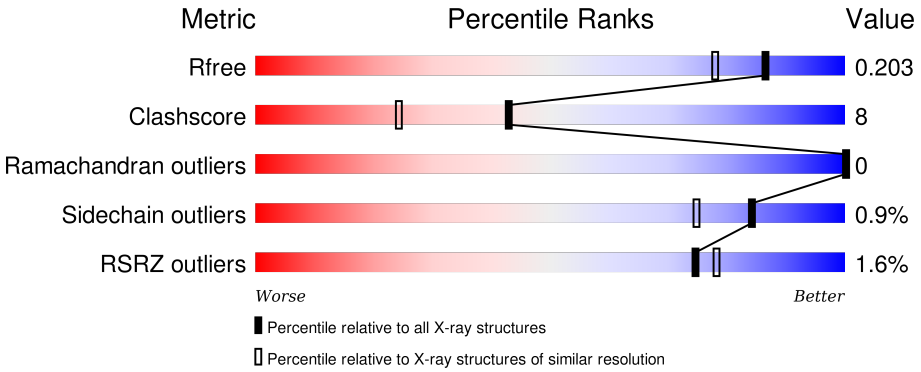
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.68 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	4802 (1.70-1.66)
Clashscore	102246	5317 (1.70-1.66)
Ramachandran outliers	100387	5225 (1.70-1.66)
Sidechain outliers	100360	5224 (1.70-1.66)
RSRZ outliers	91569	4813 (1.70-1.66)

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	358	79% 14% 6%
1	B	358	2% 85% 11% •
1	C	358	2% 80% 15% 6%
1	D	358	2% 80% 14% • 5%

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
3	GOL	A	340	-	-	-	X
3	GOL	A	341	-	-	-	X
3	GOL	B	340	-	-	-	X
3	GOL	C	341	-	-	X	-
3	GOL	C	342	-	-	-	X
3	GOL	D	341	-	-	X	-
3	GOL	D	342	-	-	-	X
5	SO4	C	345	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12204 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 RNA 3'-terminal phosphate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	21	0
			2615	1659	465	483	8			
1	B	342	Total	C	N	O	S	0	21	0
			2658	1681	480	489	8			
1	C	338	Total	C	N	O	S	0	16	0
			2605	1649	463	484	9			
1	D	340	Total	C	N	O	S	0	16	0
			2620	1653	472	486	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	EXPRESSION TAG	UNP P46849
A	-17	HIS	-	EXPRESSION TAG	UNP P46849
A	-16	HIS	-	EXPRESSION TAG	UNP P46849
A	-15	HIS	-	EXPRESSION TAG	UNP P46849
A	-14	HIS	-	EXPRESSION TAG	UNP P46849
A	-13	HIS	-	EXPRESSION TAG	UNP P46849
A	-12	HIS	-	EXPRESSION TAG	UNP P46849
A	-11	HIS	-	EXPRESSION TAG	UNP P46849
A	-10	HIS	-	EXPRESSION TAG	UNP P46849
A	-9	HIS	-	EXPRESSION TAG	UNP P46849
A	-8	HIS	-	EXPRESSION TAG	UNP P46849
A	-7	SER	-	EXPRESSION TAG	UNP P46849
A	-6	SER	-	EXPRESSION TAG	UNP P46849
A	-5	GLY	-	EXPRESSION TAG	UNP P46849
A	-4	HIS	-	EXPRESSION TAG	UNP P46849
A	-3	ILE	-	EXPRESSION TAG	UNP P46849
A	-2	GLU	-	EXPRESSION TAG	UNP P46849
A	-1	GLY	-	EXPRESSION TAG	UNP P46849
A	0	ARG	-	EXPRESSION TAG	UNP P46849
A	1	HIS	-	EXPRESSION TAG	UNP P46849
B	-19	GLY	-	EXPRESSION TAG	UNP P46849

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	HIS	-	EXPRESSION TAG	UNP P46849
B	-17	HIS	-	EXPRESSION TAG	UNP P46849
B	-16	HIS	-	EXPRESSION TAG	UNP P46849
B	-15	HIS	-	EXPRESSION TAG	UNP P46849
B	-14	HIS	-	EXPRESSION TAG	UNP P46849
B	-13	HIS	-	EXPRESSION TAG	UNP P46849
B	-12	HIS	-	EXPRESSION TAG	UNP P46849
B	-11	HIS	-	EXPRESSION TAG	UNP P46849
B	-10	HIS	-	EXPRESSION TAG	UNP P46849
B	-9	HIS	-	EXPRESSION TAG	UNP P46849
B	-7	SER	-	EXPRESSION TAG	UNP P46849
B	-6	SER	-	EXPRESSION TAG	UNP P46849
B	-5	GLY	-	EXPRESSION TAG	UNP P46849
B	-4	HIS	-	EXPRESSION TAG	UNP P46849
B	-3	ILE	-	EXPRESSION TAG	UNP P46849
B	-2	GLU	-	EXPRESSION TAG	UNP P46849
B	-1	GLY	-	EXPRESSION TAG	UNP P46849
B	0	ARG	-	EXPRESSION TAG	UNP P46849
B	1	HIS	-	EXPRESSION TAG	UNP P46849
C	-18	GLY	-	EXPRESSION TAG	UNP P46849
C	-17	HIS	-	EXPRESSION TAG	UNP P46849
C	-16	HIS	-	EXPRESSION TAG	UNP P46849
C	-15	HIS	-	EXPRESSION TAG	UNP P46849
C	-14	HIS	-	EXPRESSION TAG	UNP P46849
C	-13	HIS	-	EXPRESSION TAG	UNP P46849
C	-12	HIS	-	EXPRESSION TAG	UNP P46849
C	-11	HIS	-	EXPRESSION TAG	UNP P46849
C	-10	HIS	-	EXPRESSION TAG	UNP P46849
C	-9	HIS	-	EXPRESSION TAG	UNP P46849
C	-8	HIS	-	EXPRESSION TAG	UNP P46849
C	-7	SER	-	EXPRESSION TAG	UNP P46849
C	-6	SER	-	EXPRESSION TAG	UNP P46849
C	-5	GLY	-	EXPRESSION TAG	UNP P46849
C	-4	HIS	-	EXPRESSION TAG	UNP P46849
C	-3	ILE	-	EXPRESSION TAG	UNP P46849
C	-2	GLU	-	EXPRESSION TAG	UNP P46849
C	-1	GLY	-	EXPRESSION TAG	UNP P46849
C	0	ARG	-	EXPRESSION TAG	UNP P46849
C	1	HIS	-	EXPRESSION TAG	UNP P46849
D	-18	GLY	-	EXPRESSION TAG	UNP P46849
D	-17	HIS	-	EXPRESSION TAG	UNP P46849
D	-16	HIS	-	EXPRESSION TAG	UNP P46849

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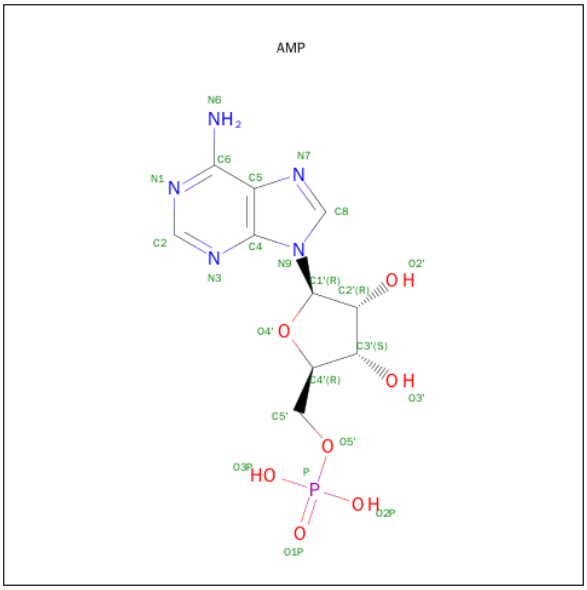
Chain	Residue	Modelled	Actual	Comment	Reference
D	-15	HIS	-	EXPRESSION TAG	UNP P46849
D	-14	HIS	-	EXPRESSION TAG	UNP P46849
D	-13	HIS	-	EXPRESSION TAG	UNP P46849
D	-12	HIS	-	EXPRESSION TAG	UNP P46849
D	-11	HIS	-	EXPRESSION TAG	UNP P46849
D	-10	HIS	-	EXPRESSION TAG	UNP P46849
D	-9	HIS	-	EXPRESSION TAG	UNP P46849
D	-8	HIS	-	EXPRESSION TAG	UNP P46849
D	-7	SER	-	EXPRESSION TAG	UNP P46849
D	-6	SER	-	EXPRESSION TAG	UNP P46849
D	-5	GLY	-	EXPRESSION TAG	UNP P46849
D	-4	HIS	-	EXPRESSION TAG	UNP P46849
D	-3	ILE	-	EXPRESSION TAG	UNP P46849
D	-2	GLU	-	EXPRESSION TAG	UNP P46849
D	-1	GLY	-	EXPRESSION TAG	UNP P46849
D	0	ARG	-	EXPRESSION TAG	UNP P46849
D	1	HIS	-	EXPRESSION TAG	UNP P46849

- Molecule 2 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
2	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

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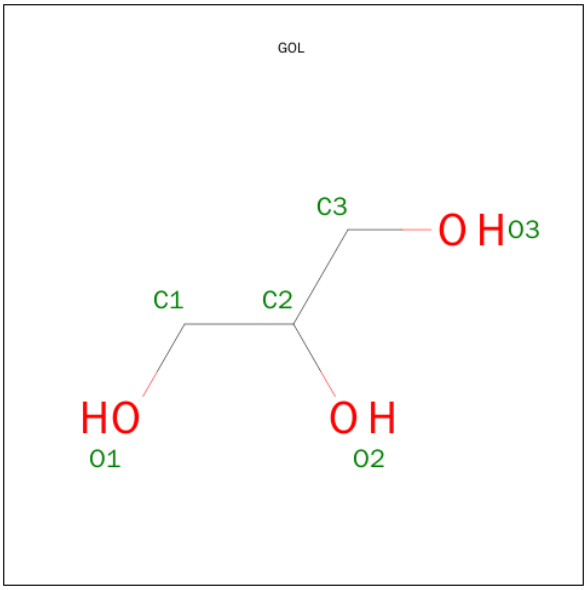
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

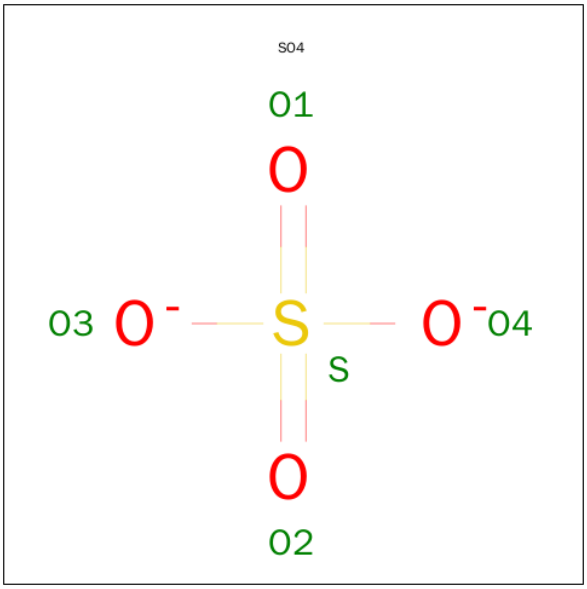


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			6	3	3			
3	A	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	B	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	C	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			
3	D	1	Total	C	O		0	0
			6	3	3			

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Na 1 1	0	0
4	A	1	Total Na 1 1	0	0
4	D	1	Total Na 1 1	0	0
4	C	2	Total Na 2 2	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 6 is water.

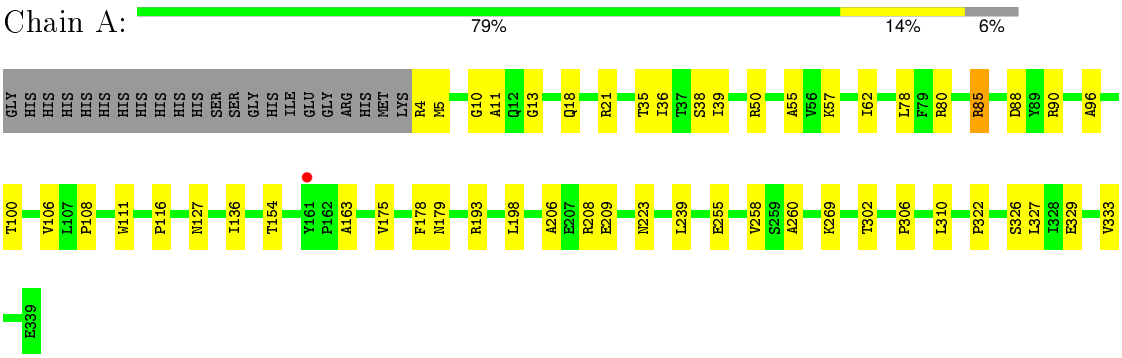
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	375	Total O 376 376	0	1
6	B	411	Total O 413 413	0	2
6	C	363	Total O 364 364	0	1
6	D	359	Total O 360 360	0	1

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.

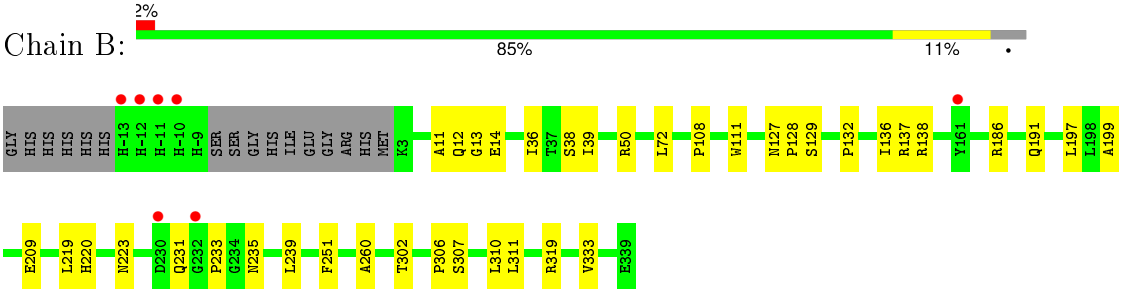
- Molecule 1: RNA 3'-terminal phosphate cyclase

Chain A:



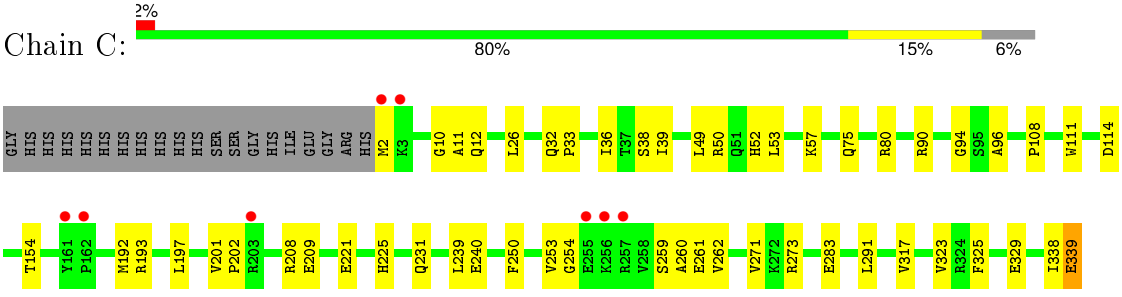
- Molecule 1: RNA 3'-terminal phosphate cyclase

Chain B:



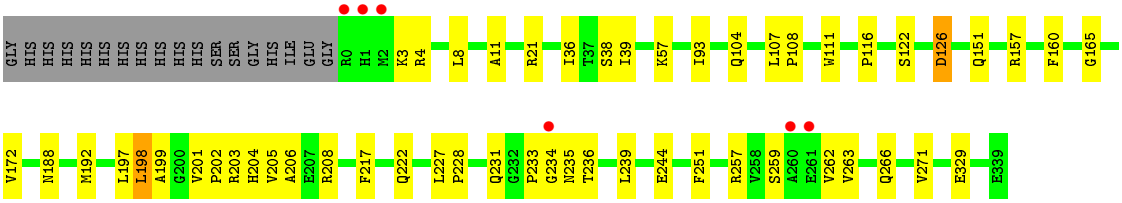
- Molecule 1: RNA 3'-terminal phosphate cyclase

Chain C:



- Molecule 1: RNA 3'-terminal phosphate cyclase

Chain D:


GLY HIS HIS HIS HIS HIS HIS HIS HIS HIS SER SER GLY HIS ILE GLU GLY R0 H1 M2 K3 R4 L8 A11 R21 I36 T37 S38 I39 K57 I93 Q104 L107 P108 W111 P116 S122 D126 Q151 R157 F160 G165
V172 N188 M192 L197 L198 A199 G200 V201 P202 R203 H204 V205 A206 E207 R208 F217 Q222 L227 P228 Q231 G232 P233 G234 N235 T236 L239 E244 F251 R257 V258 S259 A260 E261 V262 V263 Q266 V271 E329 E339

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.73Å 81.93Å 105.18Å 90.00° 103.44° 90.00°	Depositor
Resolution (Å)	35.14 – 1.68 48.71 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.14-1.68) 98.4 (48.71-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.4_125	Depositor
R, R_{free}	0.168 , 0.207 0.164 , 0.203	Depositor DCC
R_{free} test set	7840 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 179099 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12204	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.39 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.7110e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: GOL, SO4, NA, AMP

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	0.58	0/2709	0.72	0/3681
1	B	0.57	0/2752	0.72	2/3736 (0.1%)
1	C	0.56	0/2680	0.70	0/3636
1	D	0.56	0/2694	0.71	1/3656 (0.0%)
All	All	0.57	0/10835	0.71	3/14709 (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})
1	B	186	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	B	319	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	D	198	LEU	CA-CB-CG	5.03	126.88	115.30

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	2615	0	2717	41	0
1	B	2658	0	2725	26	0
1	C	2605	0	2683	55	0
1	D	2620	0	2683	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	22	0	12	0	0
2	B	22	0	12	0	0
2	C	22	0	12	0	0
2	D	22	0	12	1	0
3	A	12	0	16	1	0
3	B	12	0	16	0	0
3	C	18	0	24	9	0
3	D	18	0	24	7	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	15	0	0	0	0
5	B	10	0	0	0	0
5	C	10	0	0	0	0
5	D	5	0	0	0	0
6	A	376	0	0	10	0
6	B	413	0	0	9	0
6	C	364	0	0	11	0
6	D	360	0	0	12	0
All	All	12204	0	10936	177	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 8.

The worst 5 of 177 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:85:ARG:HH22	1:C:339[B]:GLU:HG2	0.98	1.15
1:A:85:ARG:NH2	1:C:339[B]:GLU:HG2	1.78	0.98
1:D:11[A]:ALA:HA	6:D:766:HOH:O	1.66	0.92
1:D:197:LEU:HD11	1:D:227:LEU:HD23	1.52	0.92
1:D:227:LEU:HD13	1:D:231:GLN:HB2	1.56	0.85

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	355/358 (99%)	351 (99%)	4 (1%)	0	100	100
1	B	359/358 (100%)	353 (98%)	6 (2%)	0	100	100
1	C	351/358 (98%)	343 (98%)	8 (2%)	0	100	100
1	D	354/358 (99%)	347 (98%)	7 (2%)	0	100	100
All	All	1419/1432 (99%)	1394 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	283/283 (100%)	280 (99%)	3 (1%)	80	67
1	B	283/283 (100%)	282 (100%)	1 (0%)	93	90
1	C	278/283 (98%)	274 (99%)	4 (1%)	74	57
1	D	278/283 (98%)	276 (99%)	2 (1%)	88	81
All	All	1122/1132 (99%)	1112 (99%)	10 (1%)	84	75

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	154	THR
1	C	329	GLU
1	C	339[B]	GLU

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Mol	Chain	Res	Type
1	B	231	GLN
1	C	339[A]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	1	HIS
1	D	204	HIS
1	D	18	GLN
1	C	18	GLN
1	D	104	GLN

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 27 ligands modelled in this entry, 5 are monoatomic - leaving 22 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	GOL	A	340	-	5,5,5	0.40	0	5,5,5	0.45	0
3	GOL	A	341	-	5,5,5	0.30	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	A	343	-	4,4,4	0.34	0	6,6,6	0.21	0
5	SO4	A	344	-	4,4,4	0.22	0	6,6,6	0.37	0
5	SO4	A	345	-	4,4,4	0.17	0	6,6,6	0.17	0
2	AMP	A	501	1	15,24,25	1.04	1 (6%)	16,35,38	2.67	3 (18%)
3	GOL	B	340	-	5,5,5	0.38	0	5,5,5	0.16	0
3	GOL	B	341	-	5,5,5	0.35	0	5,5,5	0.24	0
5	SO4	B	343	4	4,4,4	0.34	0	6,6,6	0.68	0
5	SO4	B	344	-	4,4,4	0.17	0	6,6,6	0.13	0
2	AMP	B	501	1	15,24,25	1.17	1 (6%)	16,35,38	2.78	4 (25%)
3	GOL	C	340	-	5,5,5	0.34	0	5,5,5	0.29	0
3	GOL	C	341	-	5,5,5	0.33	0	5,5,5	0.25	0
3	GOL	C	342	-	5,5,5	0.24	0	5,5,5	0.79	0
5	SO4	C	345	-	4,4,4	0.26	0	6,6,6	0.24	0
5	SO4	C	346	-	4,4,4	0.09	0	6,6,6	0.43	0
2	AMP	C	501	1	15,24,25	1.07	1 (6%)	16,35,38	2.19	6 (37%)
3	GOL	D	340	-	5,5,5	0.38	0	5,5,5	0.37	0
3	GOL	D	341	-	5,5,5	0.45	0	5,5,5	0.69	0
3	GOL	D	342	-	5,5,5	0.35	0	5,5,5	0.17	0
5	SO4	D	344	4	4,4,4	0.45	0	6,6,6	0.38	0
2	AMP	D	501	1	15,24,25	1.00	1 (6%)	16,35,38	2.49	4 (25%)

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	GOL	A	340	-	-	0/4/4/4	0/0/0/0
3	GOL	A	341	-	-	0/4/4/4	0/0/0/0
5	SO4	A	343	-	-	0/0/0/0	0/0/0/0
5	SO4	A	344	-	-	0/0/0/0	0/0/0/0
5	SO4	A	345	-	-	0/0/0/0	0/0/0/0
2	AMP	A	501	1	-	0/3/25/26	0/3/3/3
3	GOL	B	340	-	-	0/4/4/4	0/0/0/0
3	GOL	B	341	-	-	0/4/4/4	0/0/0/0
5	SO4	B	343	4	-	0/0/0/0	0/0/0/0
5	SO4	B	344	-	-	0/0/0/0	0/0/0/0
2	AMP	B	501	1	-	0/3/25/26	0/3/3/3
3	GOL	C	340	-	-	0/4/4/4	0/0/0/0
3	GOL	C	341	-	-	0/4/4/4	0/0/0/0
3	GOL	C	342	-	-	0/4/4/4	0/0/0/0
5	SO4	C	345	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	C	346	-	-	0/0/0/0	0/0/0/0
2	AMP	C	501	1	-	0/3/25/26	0/3/3/3
3	GOL	D	340	-	-	0/4/4/4	0/0/0/0
3	GOL	D	341	-	-	0/4/4/4	0/0/0/0
3	GOL	D	342	-	-	0/4/4/4	0/0/0/0
5	SO4	D	344	4	-	0/0/0/0	0/0/0/0
2	AMP	D	501	1	-	0/3/25/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	AMP	C5-C4	2.70	1.46	1.40
2	C	501	AMP	C5-C4	2.72	1.46	1.40
2	D	501	AMP	C5-C4	2.76	1.46	1.40
2	A	501	AMP	C5-C4	2.84	1.46	1.40

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	AMP	N3-C2-N1	-9.17	121.88	128.89
2	A	501	AMP	N3-C2-N1	-8.21	122.61	128.89
2	D	501	AMP	N3-C2-N1	-7.84	122.89	128.89
2	C	501	AMP	N3-C2-N1	-4.99	125.08	128.89
2	A	501	AMP	C2'-C1'-N9	-4.75	107.04	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	340	GOL	1	0
3	C	341	GOL	8	0
3	C	342	GOL	1	0
3	D	340	GOL	3	0
3	D	341	GOL	4	0
2	D	501	AMP	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, 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	336/358 (93%)	-0.41	1 (0%)	94	95	16, 25, 45, 84	0
1	B	342/358 (95%)	-0.35	7 (2%)	68	72	16, 26, 49, 124	0
1	C	338/358 (94%)	-0.29	8 (2%)	62	65	15, 28, 53, 111	0
1	D	340/358 (94%)	-0.26	6 (1%)	71	75	15, 27, 75, 113	0
All	All	1356/1432 (94%)	-0.33	22 (1%)	74	78	15, 26, 55, 124	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	ASP	9.9
1	C	2	MET	5.9
1	B	-10	HIS	3.9
1	C	161	TYR	3.5
1	A	161	TYR	3.2

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	GOL	B	340	6/6	0.58	0.24	25.41	62,66,68,68	0
3	GOL	A	340	6/6	0.95	0.20	10.39	24,32,34,38	0
3	GOL	C	342	6/6	0.82	0.21	7.24	34,38,43,46	0
3	GOL	D	342	6/6	0.78	0.24	7.03	55,63,65,68	0
5	SO4	C	345	5/5	0.98	0.09	3.81	42,43,46,103	0
3	GOL	A	341	6/6	0.81	0.14	3.18	72,74,74,75	0
4	NA	D	343	1/1	0.96	0.12	1.95	32,32,32,32	0
5	SO4	D	344	5/5	0.97	0.09	1.41	52,53,72,74	0
3	GOL	C	340	6/6	0.67	0.20	1.19	73,74,76,77	0
5	SO4	A	345	5/5	0.94	0.17	1.18	36,38,38,41	5
5	SO4	A	343	5/5	0.98	0.09	1.18	51,53,60,67	0
4	NA	C	344	1/1	0.98	0.09	0.81	32,32,32,32	0
4	NA	B	342	1/1	0.96	0.10	0.75	32,32,32,32	0
5	SO4	B	343	5/5	0.96	0.10	0.74	63,67,70,83	0
3	GOL	D	341	6/6	0.89	0.19	0.64	43,46,50,53	0
5	SO4	B	344	5/5	0.88	0.10	0.47	45,47,49,50	5
3	GOL	C	341	6/6	0.84	0.13	0.31	49,51,55,59	0
2	AMP	D	501	22/23	0.97	0.07	-0.05	19,22,28,34	0
3	GOL	B	341	6/6	0.80	0.13	-0.29	80,83,84,85	0
2	AMP	C	501	22/23	0.98	0.07	-0.32	19,21,25,30	0
2	AMP	A	501	22/23	0.98	0.07	-0.96	17,21,25,27	0
2	AMP	B	501	22/23	0.98	0.05	-1.12	19,20,25,26	0
4	NA	C	343	1/1	0.95	0.07	-1.15	35,35,35,35	0
5	SO4	A	344	5/5	0.93	0.14	-	26,31,33,38	5
4	NA	A	342	1/1	0.98	0.07	-	43,43,43,43	0
3	GOL	D	340	6/6	0.84	0.15	-	58,66,68,69	0
5	SO4	C	346	5/5	0.94	0.14	-	30,32,34,35	5

6.5 Other polymers (i)

There are no such residues in this entry.