Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 04:59 AM EDT

PDB ID	:	5JNB
Title	:	structure of GLD-2/RNP-8 complex
Authors	:	Nakel, K.; Bonneau, F.; Basquin, C.; Eckmann, C.R.; Conti, E.
Deposited on	:	2016-04-29
Resolution	:	2.49 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 (i) 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 (i)) were used in the production of this report:

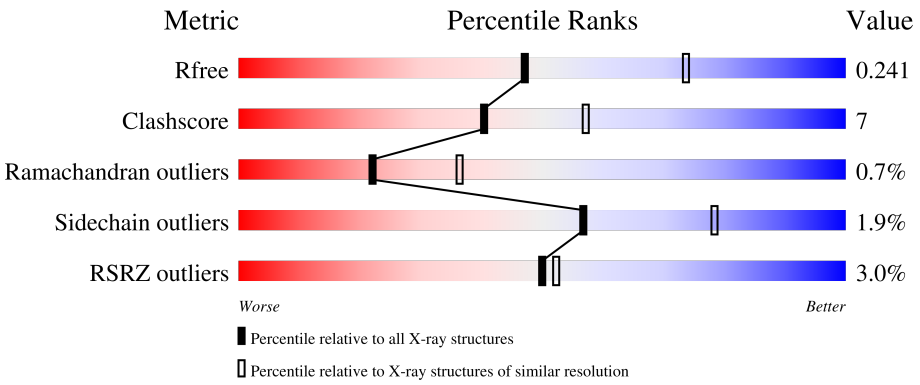
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.49 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 <=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	338	.% 76% 20% • •
1	B	338	81% 14% •
1	C	338	2% 73% 12% • 14%
1	D	338	7% 67% 11% • 22%
2	E	74	50% 11% • 38%

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Mol	Chain	Length	Quality of chain
2	F	74	% 51% 9% 38%
2	G	74	% 34% 62%
2	H	74	4% 28% 5% 66%

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	EDO	A	1003	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10776 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 Poly(A) RNA polymerase gld-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2623	1669	451	489	14	0	0	0
1	B	324	2590	1650	444	481	15	0	0	0
1	C	289	2259	1440	380	425	14	0	0	0
1	D	263	2004	1287	330	378	9	0	0	0

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	544	GLY	-	expression tag	UNP O17087
A	545	ALA	-	expression tag	UNP O17087
A	668	ALA	ASP	engineered mutation	UNP O17087
A	?	-	ALA	deletion	UNP O17087
A	?	-	LEU	deletion	UNP O17087
A	?	-	ALA	deletion	UNP O17087
A	?	-	VAL	deletion	UNP O17087
A	?	-	ARG	deletion	UNP O17087
A	?	-	PRO	deletion	UNP O17087
A	?	-	LYS	deletion	UNP O17087
A	?	-	ILE	deletion	UNP O17087
A	?	-	HIS	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	ASN	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	GLU	deletion	UNP O17087
A	?	-	GLY	deletion	UNP O17087
A	?	-	ASP	deletion	UNP O17087
A	?	-	LYS	deletion	UNP O17087
A	?	-	GLU	deletion	UNP O17087
A	?	-	THR	deletion	UNP O17087

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	PRO	deletion	UNP O17087
A	?	-	PRO	deletion	UNP O17087
A	?	-	PRO	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	ALA	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	THR	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	SER	deletion	UNP O17087
A	?	-	ILE	deletion	UNP O17087
A	?	-	HIS	deletion	UNP O17087
A	?	-	ASN	deletion	UNP O17087
A	?	-	GLY	deletion	UNP O17087
A	?	-	GLY	deletion	UNP O17087
A	?	-	THR	deletion	UNP O17087
A	?	-	PRO	deletion	UNP O17087
A	?	-	GLY	deletion	UNP O17087
A	?	-	ILE	deletion	UNP O17087
A	?	-	PRO	deletion	UNP O17087
A	?	-	MET	deletion	UNP O17087
A	?	-	HIS	deletion	UNP O17087
A	?	-	HIS	deletion	UNP O17087
B	544	GLY	-	expression tag	UNP O17087
B	545	ALA	-	expression tag	UNP O17087
B	668	ALA	ASP	engineered mutation	UNP O17087
B	?	-	ALA	deletion	UNP O17087
B	?	-	LEU	deletion	UNP O17087
B	?	-	ALA	deletion	UNP O17087
B	?	-	VAL	deletion	UNP O17087
B	?	-	ARG	deletion	UNP O17087
B	?	-	PRO	deletion	UNP O17087
B	?	-	LYS	deletion	UNP O17087
B	?	-	ILE	deletion	UNP O17087
B	?	-	HIS	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	ASN	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	GLU	deletion	UNP O17087
B	?	-	GLY	deletion	UNP O17087
B	?	-	ASP	deletion	UNP O17087

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP O17087
B	?	-	GLU	deletion	UNP O17087
B	?	-	THR	deletion	UNP O17087
B	?	-	PRO	deletion	UNP O17087
B	?	-	PRO	deletion	UNP O17087
B	?	-	PRO	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	ALA	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	THR	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	SER	deletion	UNP O17087
B	?	-	ILE	deletion	UNP O17087
B	?	-	HIS	deletion	UNP O17087
B	?	-	ASN	deletion	UNP O17087
B	?	-	GLY	deletion	UNP O17087
B	?	-	GLY	deletion	UNP O17087
B	?	-	THR	deletion	UNP O17087
B	?	-	PRO	deletion	UNP O17087
B	?	-	GLY	deletion	UNP O17087
B	?	-	ILE	deletion	UNP O17087
B	?	-	PRO	deletion	UNP O17087
B	?	-	MET	deletion	UNP O17087
B	?	-	HIS	deletion	UNP O17087
B	?	-	HIS	deletion	UNP O17087
C	544	GLY	-	expression tag	UNP O17087
C	545	ALA	-	expression tag	UNP O17087
C	668	ALA	ASP	engineered mutation	UNP O17087
C	?	-	ALA	deletion	UNP O17087
C	?	-	LEU	deletion	UNP O17087
C	?	-	ALA	deletion	UNP O17087
C	?	-	VAL	deletion	UNP O17087
C	?	-	ARG	deletion	UNP O17087
C	?	-	PRO	deletion	UNP O17087
C	?	-	LYS	deletion	UNP O17087
C	?	-	ILE	deletion	UNP O17087
C	?	-	HIS	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	ASN	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP O17087
C	?	-	GLY	deletion	UNP O17087
C	?	-	ASP	deletion	UNP O17087
C	?	-	LYS	deletion	UNP O17087
C	?	-	GLU	deletion	UNP O17087
C	?	-	THR	deletion	UNP O17087
C	?	-	PRO	deletion	UNP O17087
C	?	-	PRO	deletion	UNP O17087
C	?	-	PRO	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	ALA	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	THR	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	SER	deletion	UNP O17087
C	?	-	ILE	deletion	UNP O17087
C	?	-	HIS	deletion	UNP O17087
C	?	-	ASN	deletion	UNP O17087
C	?	-	GLY	deletion	UNP O17087
C	?	-	GLY	deletion	UNP O17087
C	?	-	THR	deletion	UNP O17087
C	?	-	PRO	deletion	UNP O17087
C	?	-	GLY	deletion	UNP O17087
C	?	-	ILE	deletion	UNP O17087
C	?	-	PRO	deletion	UNP O17087
C	?	-	MET	deletion	UNP O17087
C	?	-	HIS	deletion	UNP O17087
C	?	-	HIS	deletion	UNP O17087
D	544	GLY	-	expression tag	UNP O17087
D	545	ALA	-	expression tag	UNP O17087
D	668	ALA	ASP	engineered mutation	UNP O17087
D	?	-	ALA	deletion	UNP O17087
D	?	-	LEU	deletion	UNP O17087
D	?	-	ALA	deletion	UNP O17087
D	?	-	VAL	deletion	UNP O17087
D	?	-	ARG	deletion	UNP O17087
D	?	-	PRO	deletion	UNP O17087
D	?	-	LYS	deletion	UNP O17087
D	?	-	ILE	deletion	UNP O17087
D	?	-	HIS	deletion	UNP O17087

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP O17087
D	?	-	ASN	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	GLU	deletion	UNP O17087
D	?	-	GLY	deletion	UNP O17087
D	?	-	ASP	deletion	UNP O17087
D	?	-	LYS	deletion	UNP O17087
D	?	-	GLU	deletion	UNP O17087
D	?	-	THR	deletion	UNP O17087
D	?	-	PRO	deletion	UNP O17087
D	?	-	PRO	deletion	UNP O17087
D	?	-	PRO	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	ALA	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	THR	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	SER	deletion	UNP O17087
D	?	-	ILE	deletion	UNP O17087
D	?	-	HIS	deletion	UNP O17087
D	?	-	ASN	deletion	UNP O17087
D	?	-	GLY	deletion	UNP O17087
D	?	-	GLY	deletion	UNP O17087
D	?	-	THR	deletion	UNP O17087
D	?	-	PRO	deletion	UNP O17087
D	?	-	GLY	deletion	UNP O17087
D	?	-	ILE	deletion	UNP O17087
D	?	-	PRO	deletion	UNP O17087
D	?	-	MET	deletion	UNP O17087
D	?	-	HIS	deletion	UNP O17087
D	?	-	HIS	deletion	UNP O17087

- Molecule 2 is a protein called RNP (RRM RNA binding domain) containing.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	E	46	360	230	60	70	0	0	0
			Total	C	N	O			
2	F	46	364	232	60	72	0	0	0
			Total	C	N	O			
2	G	28	201	128	30	43	0	0	0

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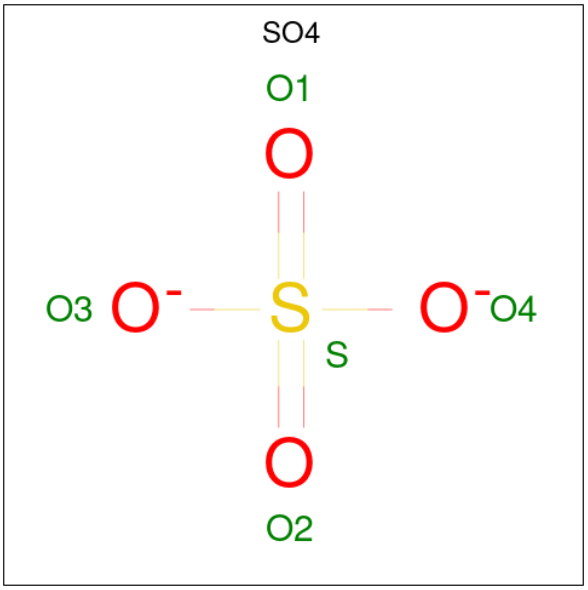
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	H	25	187	121	28	38	0	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

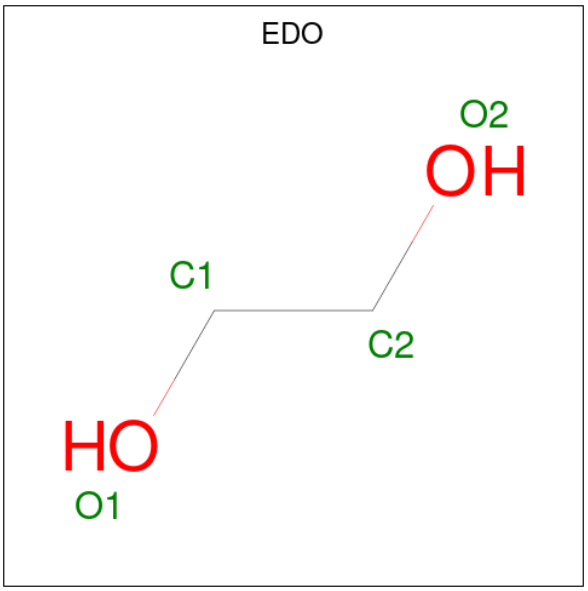


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	A	1	5	4	1		0	0
3	B	1	5	4	1		0	0
3	C	1	5	4	1		0	0
3	D	1	5	4	1		0	0

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

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	47	47	47	0	0
			Total	O		
6	B	37	37	37	0	0
			Total	O		
6	C	20	20	20	0	0

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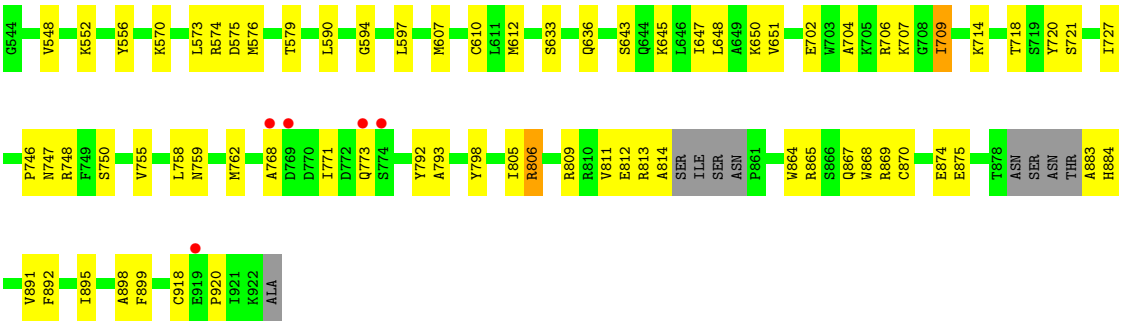
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	D	9	9	9	0	0
			Total	O		
6	E	9	9	9	0	0
			Total	O		
6	F	7	7	7	0	0
			Total	O		
6	G	1	1	1	0	0

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.

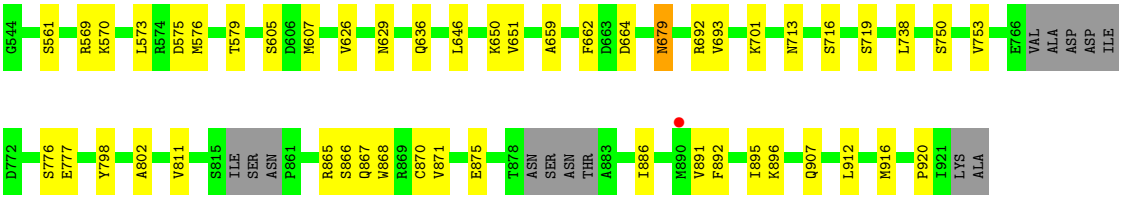
• Molecule 1: Poly(A) RNA polymerase gld-2

Chain A:



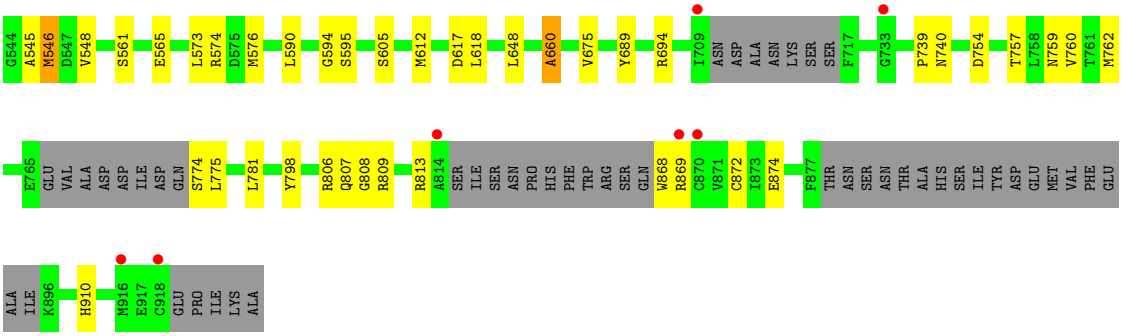
• Molecule 1: Poly(A) RNA polymerase gld-2

Chain B:



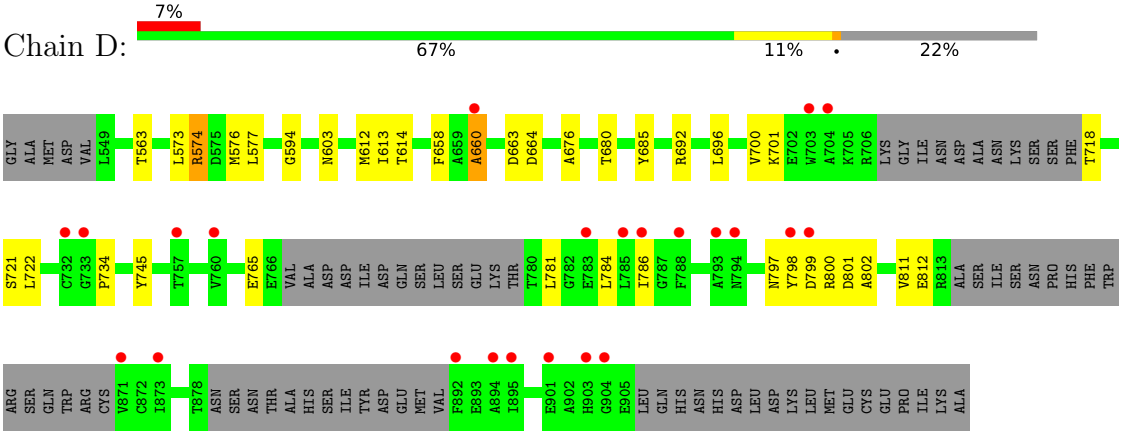
• Molecule 1: Poly(A) RNA polymerase gld-2

Chain C:



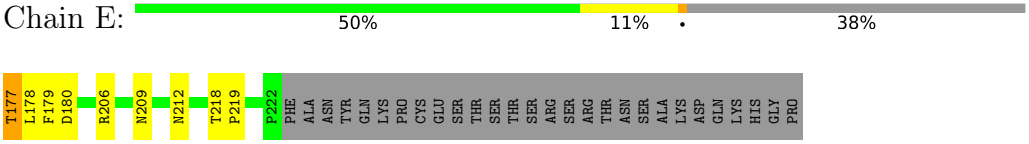
• Molecule 1: Poly(A) RNA polymerase gld-2

Chain D:



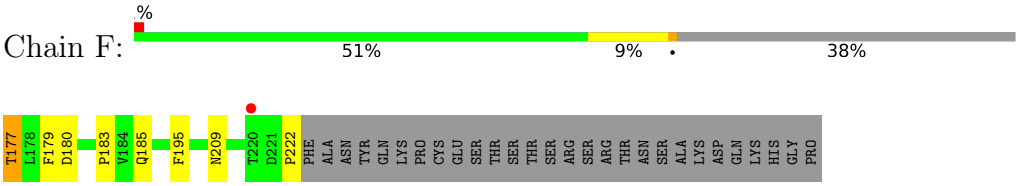
• Molecule 2: RNP (RRM RNA binding domain) containing

Chain E:



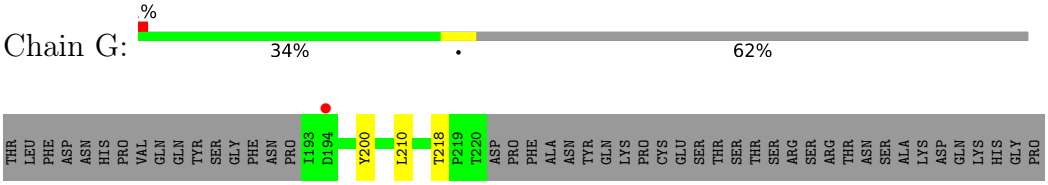
• Molecule 2: RNP (RRM RNA binding domain) containing

Chain F:



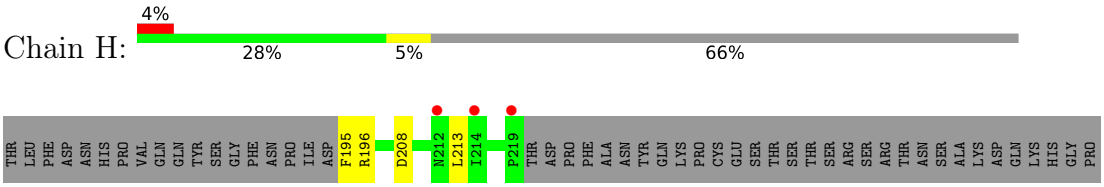
• Molecule 2: RNP (RRM RNA binding domain) containing

Chain G:



• Molecule 2: RNP (RRM RNA binding domain) containing

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	65.35Å 86.44Å 91.91Å 89.88° 93.13° 90.22°	Depositor
Resolution (Å)	46.25 – 2.49 46.25 – 2.49	Depositor EDS
% Data completeness (in resolution range)	95.6 (46.25-2.49) 95.4 (46.25-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.45 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.242 0.194 , 0.241	Depositor DCC
R_{free} test set	3383 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.358	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10776	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EDO, MG

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	0.47	0/2677	0.62	1/3630 (0.0%)
1	B	0.47	0/2643	0.58	0/3580
1	C	0.43	0/2300	0.59	1/3123 (0.0%)
1	D	0.34	0/2041	0.54	1/2785 (0.0%)
2	E	0.46	0/371	0.60	0/508
2	F	0.50	0/375	0.53	0/513
2	G	0.41	0/205	0.50	0/281
2	H	0.35	0/191	0.61	0/259
All	All	0.44	0/10803	0.58	3/14679 (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	D	660	ALA	C-N-CD	6.86	142.81	128.40
1	C	660	ALA	C-N-CD	6.57	142.21	128.40
1	A	806	ARG	NE-CZ-NH1	-5.80	117.40	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2570	55	0
1	B	2590	0	2547	37	0
1	C	2259	0	2191	27	0
1	D	2004	0	1908	28	0
2	E	360	0	316	6	0
2	F	364	0	320	6	0
2	G	201	0	161	5	0
2	H	187	0	158	5	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	5	0	0	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	12	0	18	6	0
5	B	12	0	18	6	0
5	C	8	0	12	1	0
5	D	4	0	6	1	0
6	A	47	0	0	2	0
6	B	37	0	0	2	0
6	C	20	0	0	0	0
6	D	9	0	0	1	0
6	E	9	0	0	2	0
6	F	7	0	0	1	0
6	G	1	0	0	0	0
All	All	10776	0	10225	151	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 7.

All (151) 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)
2:E:177:THR:HG23	2:E:179:PHE:H	1.40	0.86
2:F:177:THR:HG23	2:F:179:PHE:H	1.41	0.85
1:B:692:ARG:NH2	1:B:777:GLU:OE1	2.10	0.85
1:A:574:ARG:NE	6:A:1101:HOH:O	2.16	0.79
1:C:573:LEU:HA	1:C:576:MET:HE3	1.65	0.79
1:D:594:GLY:H	1:D:680:THR:HG21	1.48	0.79
1:B:659:ALA:O	6:B:1101:HOH:O	2.00	0.78
2:E:206:ARG:NH1	6:E:401:HOH:O	2.18	0.76
1:B:679:ASN:HD22	5:B:1003:EDO:H12	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:HIS:HD1	1:A:892:PHE:HE2	1.41	0.67
1:C:740:ASN:ND2	1:C:808:GLY:H	1.93	0.67
1:D:718:THR:HG23	1:D:721:SER:HB2	1.77	0.66
1:C:798:TYR:O	1:C:813:ARG:NH2	2.28	0.66
1:A:792:TYR:O	1:A:798:TYR:OH	2.12	0.65
1:D:797:ASN:OD1	1:D:798:TYR:N	2.30	0.64
2:E:209:ASN:OD1	2:E:212:ASN:ND2	2.30	0.64
1:A:870:CYS:HB3	1:A:892:PHE:CE1	2.33	0.63
1:A:643:SER:HB2	1:B:713:ASN:HB3	1.80	0.63
1:A:594:GLY:HA2	5:A:1005:EDO:H22	1.80	0.63
1:A:771:ILE:HG22	1:A:773:GLN:HG2	1.81	0.63
1:B:629:ASN:HB3	5:B:1002:EDO:H22	1.81	0.62
1:D:573:LEU:HA	1:D:576:MET:HE3	1.81	0.62
1:B:626:VAL:HA	5:B:1002:EDO:H11	1.81	0.61
1:D:563:THR:HG23	1:D:603:ASN:HD21	1.66	0.61
1:A:574:ARG:HH11	1:A:574:ARG:HG2	1.66	0.60
1:B:650:LYS:NZ	2:E:180:ASP:OD1	2.32	0.58
1:C:648:LEU:HD12	2:F:195:PHE:HE2	1.69	0.57
1:D:676:ALA:O	1:D:680:THR:HG23	2.04	0.57
1:D:594:GLY:H	1:D:680:THR:CG2	2.18	0.57
1:A:748:ARG:NH2	1:A:762:MET:O	2.39	0.56
1:D:799:ASP:N	1:D:799:ASP:OD1	2.38	0.56
1:B:870:CYS:HB3	1:B:892:PHE:CZ	2.42	0.55
1:A:721:SER:OG	1:A:865:ARG:NH1	2.39	0.55
1:A:812:GLU:O	1:A:814:ALA:N	2.39	0.55
1:A:891:VAL:O	1:A:895:ILE:HG12	2.07	0.54
1:B:866:SER:H	5:B:1004:EDO:H11	1.72	0.54
1:A:650:LYS:NZ	2:F:180:ASP:OD2	2.39	0.53
1:A:714:LYS:HB3	5:A:1003:EDO:H21	1.91	0.53
1:D:800:ARG:O	1:D:812:GLU:HB2	2.09	0.53
1:A:707:LYS:HD3	1:A:898:ALA:HB1	1.90	0.53
1:B:575:ASP:O	1:B:579:THR:HG23	2.09	0.53
1:D:802:ALA:N	1:D:811:VAL:O	2.41	0.52
1:B:891:VAL:O	1:B:895:ILE:HG12	2.09	0.52
1:C:605:SER:OG	3:C:1001:SO4:O2	2.26	0.52
1:B:750:SER:HB3	1:B:753:VAL:HG23	1.92	0.51
1:B:802:ALA:HB3	1:B:811:VAL:HG23	1.92	0.51
1:A:575:ASP:O	1:A:579:THR:HG23	2.10	0.51
1:D:696:LEU:O	1:D:700:VAL:HG23	2.10	0.51
1:A:755:VAL:HA	1:A:758:LEU:HG	1.93	0.51
1:A:867:GLN:HG3	1:A:868:TRP:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ASN:HD21	1:A:762:MET:HB2	1.75	0.50
1:B:605:SER:OG	3:B:1001:SO4:O3	2.27	0.49
5:A:1003:EDO:C2	1:B:636:GLN:HB2	2.42	0.49
1:A:648:LEU:HB2	1:B:646:LEU:HB3	1.95	0.49
1:B:867:GLN:HG3	1:B:868:TRP:CD2	2.48	0.49
1:C:759:ASN:CG	1:C:762:MET:HB3	2.32	0.49
1:D:701:LYS:HA	1:D:722:LEU:HD23	1.93	0.49
1:A:869:ARG:NH2	2:F:185:GLN:OE1	2.45	0.48
1:A:870:CYS:HB3	1:A:892:PHE:CZ	2.49	0.48
1:D:685:TYR:CE1	2:H:213:LEU:HD11	2.49	0.48
1:D:614:THR:HG22	2:H:196:ARG:O	2.14	0.48
1:A:806:ARG:HH12	1:A:874:GLU:CD	2.17	0.47
5:A:1003:EDO:H22	1:B:636:GLN:HB2	1.97	0.47
1:B:865:ARG:HD2	1:B:875:GLU:OE2	2.13	0.47
1:C:694:ARG:HH12	2:G:218:THR:HG22	1.79	0.47
1:B:679:ASN:ND2	5:B:1003:EDO:H12	2.24	0.47
1:B:798:TYR:CD2	1:B:896:LYS:HE3	2.50	0.47
1:D:797:ASN:O	1:D:801:ASP:HB2	2.15	0.46
1:A:574:ARG:HD2	1:A:590:LEU:O	2.15	0.46
1:A:709:ILE:HD13	1:A:709:ILE:HA	1.72	0.46
2:E:206:ARG:NH2	6:E:402:HOH:O	2.35	0.46
1:A:570:LYS:HB3	1:A:607:MET:SD	2.56	0.46
1:A:718:THR:HG22	1:A:720:TYR:N	2.31	0.46
1:C:612:MET:HG2	2:G:200:TYR:CE1	2.51	0.46
1:D:811:VAL:HG22	1:D:812:GLU:H	1.81	0.46
1:A:793:ALA:HB2	1:A:899:PHE:HB3	1.98	0.46
1:B:573:LEU:HA	1:B:576:MET:HE2	1.97	0.46
1:B:646:LEU:HD12	2:F:183:PRO:HG2	1.98	0.46
1:B:870:CYS:HB3	1:B:892:PHE:CE1	2.50	0.46
1:A:610:CYS:SG	1:A:612:MET:CE	3.04	0.46
1:C:807:GLN:O	1:C:809:ARG:N	2.49	0.46
1:A:718:THR:HG22	1:A:720:TYR:H	1.81	0.45
1:B:867:GLN:HG3	1:B:868:TRP:CE3	2.51	0.45
1:C:694:ARG:HH12	2:G:218:THR:CG2	2.28	0.45
1:C:694:ARG:NH1	2:G:218:THR:HG22	2.32	0.45
1:A:610:CYS:SG	1:A:612:MET:HE1	2.55	0.45
1:A:612:MET:HE3	1:A:612:MET:HB2	1.72	0.45
1:A:702:GLU:O	1:A:706:ARG:HG3	2.16	0.45
1:C:740:ASN:HD22	1:C:808:GLY:H	1.60	0.45
1:D:685:TYR:CZ	2:H:213:LEU:HD11	2.52	0.45
1:A:556:TYR:OH	1:A:702:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:MET:HE1	1:B:662:PHE:CZ	2.52	0.45
1:A:727:ILE:HG22	1:A:805:ILE:HD12	1.99	0.45
1:B:693:VAL:HG21	1:B:738:LEU:HD21	1.98	0.44
1:A:643:SER:CB	1:B:713:ASN:HB3	2.47	0.44
1:D:574:ARG:HH12	2:H:208:ASP:CG	2.20	0.44
1:A:720:TYR:HD2	1:A:865:ARG:CZ	2.30	0.44
1:B:569:ARG:NH2	1:B:664:ASP:OD2	2.51	0.44
1:D:573:LEU:HD21	1:D:658:PHE:CE2	2.52	0.44
1:A:574:ARG:NH1	1:A:575:ASP:OD1	2.46	0.44
1:A:883:ALA:HA	1:A:884:HIS:HD2	1.83	0.44
1:A:884:HIS:N	1:A:884:HIS:CD2	2.86	0.44
1:C:868:TRP:O	1:C:869:ARG:HG3	2.18	0.44
1:D:612:MET:HE3	6:D:1109:HOH:O	2.16	0.44
1:A:645:LYS:HD2	1:A:647:ILE:HD11	1.99	0.43
1:D:786:ILE:H	1:D:786:ILE:HG13	1.68	0.43
1:B:912:LEU:O	1:B:916:MET:HG2	2.18	0.43
1:A:875:GLU:HB3	6:A:1131:HOH:O	2.17	0.43
1:C:594:GLY:HA2	5:C:1002:EDO:H12	2.00	0.43
1:C:760:VAL:HG22	2:G:210:LEU:HG	2.00	0.43
1:C:618:LEU:HD12	1:C:618:LEU:HA	1.83	0.43
1:A:747:ASN:ND2	1:A:748:ARG:HG2	2.34	0.43
1:B:662:PHE:HB2	6:B:1101:HOH:O	2.18	0.43
1:B:701:LYS:HE2	1:B:719:SER:HB2	2.00	0.43
1:D:701:LYS:NZ	3:D:1001:SO4:O1	2.45	0.43
1:C:813:ARG:NH1	1:C:872:CYS:HB2	2.34	0.43
1:A:633:SER:O	1:A:636:GLN:HG2	2.19	0.43
1:B:798:TYR:HD1	1:B:871:VAL:HG22	1.84	0.43
1:D:577:LEU:HD23	1:D:577:LEU:HA	1.89	0.43
1:D:664:ASP:OD1	1:D:664:ASP:N	2.48	0.43
1:D:692:ARG:HE	1:D:784:LEU:HD11	1.84	0.43
1:A:865:ARG:HA	5:A:1004:EDO:H11	2.01	0.43
1:A:573:LEU:HA	1:A:576:MET:HE3	2.00	0.42
1:C:774:SER:OG	1:C:775:LEU:N	2.52	0.42
2:F:209:ASN:ND2	6:F:301:HOH:O	2.45	0.42
1:A:714:LYS:CB	5:A:1003:EDO:H21	2.49	0.42
1:A:809:ARG:NH1	1:A:811:VAL:HG12	2.34	0.42
1:C:806:ARG:HD3	1:C:874:GLU:CD	2.40	0.42
1:B:886:ILE:HG21	2:H:195:PHE:CE1	2.55	0.42
1:C:574:ARG:O	1:C:574:ARG:HG2	2.19	0.42
1:A:864:TRP:CZ3	1:A:874:GLU:HB2	2.54	0.42
1:C:689:TYR:CE2	1:C:739:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:ILE:HD13	1:A:805:ILE:HA	1.90	0.41
1:D:745:TYR:OH	1:D:765:GLU:O	2.21	0.41
1:B:798:TYR:CD1	1:B:871:VAL:HG22	2.56	0.41
1:A:809:ARG:CZ	1:A:811:VAL:HG12	2.50	0.41
1:A:704:ALA:HB1	1:A:709:ILE:HG22	2.02	0.41
1:C:590:LEU:HD12	1:C:590:LEU:HA	1.94	0.41
1:D:680:THR:HG22	5:D:1002:EDO:O1	2.21	0.41
1:B:679:ASN:HB3	5:B:1003:EDO:H12	2.01	0.41
1:A:707:LYS:HG3	1:A:918:CYS:SG	2.60	0.41
1:A:746:PRO:O	1:A:750:SER:HB2	2.20	0.41
1:C:754:ASP:O	1:C:757:THR:HB	2.20	0.41
1:C:781:LEU:HD23	1:C:781:LEU:HA	1.86	0.41
2:E:218:THR:HA	2:E:219:PRO:HD2	1.93	0.41
1:D:613:ILE:HG22	1:D:614:THR:HG23	2.02	0.40
1:A:870:CYS:HB3	1:A:892:PHE:CD1	2.56	0.40
1:C:545:ALA:O	1:C:548:VAL:HB	2.21	0.40
1:B:570:LYS:HB3	1:B:607:MET:SD	2.61	0.40
1:C:546:MET:HG3	1:C:910:HIS:CD2	2.56	0.40
1:C:813:ARG:O	1:C:813:ARG:HG3	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	323/338 (96%)	309 (96%)	11 (3%)	3 (1%)	17 29
1	B	316/338 (94%)	306 (97%)	9 (3%)	1 (0%)	41 59
1	C	279/338 (82%)	265 (95%)	13 (5%)	1 (0%)	34 52
1	D	253/338 (75%)	243 (96%)	7 (3%)	3 (1%)	13 22
2	E	44/74 (60%)	40 (91%)	3 (7%)	1 (2%)	6 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	44/74 (60%)	41 (93%)	3 (7%)	0	100	100
2	G	26/74 (35%)	24 (92%)	2 (8%)	0	100	100
2	H	23/74 (31%)	23 (100%)	0	0	100	100
All	All	1308/1648 (79%)	1251 (96%)	48 (4%)	9 (1%)	22	36

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	813	ARG
1	C	660	ALA
1	D	660	ALA
1	A	920	PRO
2	E	178	LEU
1	D	734	PRO
1	D	781	LEU
1	B	920	PRO
1	A	768	ALA

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	289/306 (94%)	284 (98%)	5 (2%)	60	81
1	B	287/306 (94%)	281 (98%)	6 (2%)	53	76
1	C	247/306 (81%)	241 (98%)	6 (2%)	49	72
1	D	212/306 (69%)	210 (99%)	2 (1%)	78	91
2	E	38/67 (57%)	37 (97%)	1 (3%)	46	70
2	F	39/67 (58%)	37 (95%)	2 (5%)	24	42
2	G	19/67 (28%)	19 (100%)	0	100	100
2	H	18/67 (27%)	18 (100%)	0	100	100
All	All	1149/1492 (77%)	1127 (98%)	22 (2%)	57	78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	548	VAL
1	A	552	LYS
1	A	597	LEU
1	A	651	VAL
1	A	709	ILE
1	B	561	SER
1	B	651	VAL
1	B	679	ASN
1	B	716	SER
1	B	776	SER
1	B	907	GLN
1	C	546	MET
1	C	561	SER
1	C	565	GLU
1	C	595	SER
1	C	617	ASP
1	C	675	VAL
1	D	574	ARG
1	D	663	ASP
2	E	177	THR
2	F	177	THR
2	F	222	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	HIS
1	B	679	ASN
1	C	740	ASN
2	E	209	ASN
2	E	212	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	EDO	B	1004	-	3,3,3	0.70	0	2,2,2	0.21	0
5	EDO	A	1004	-	3,3,3	0.48	0	2,2,2	0.40	0
5	EDO	A	1005	-	3,3,3	0.37	0	2,2,2	0.66	0
5	EDO	B	1002	-	3,3,3	0.55	0	2,2,2	0.24	0
3	SO4	B	1001	-	4,4,4	0.15	0	6,6,6	0.35	0
3	SO4	C	1001	-	4,4,4	0.13	0	6,6,6	0.23	0
5	EDO	B	1003	-	3,3,3	0.39	0	2,2,2	0.73	0
5	EDO	A	1003	-	3,3,3	0.74	0	2,2,2	0.52	0
5	EDO	D	1002	-	3,3,3	0.50	0	2,2,2	0.36	0
5	EDO	C	1002	-	3,3,3	0.52	0	2,2,2	0.27	0
5	EDO	C	1003	-	3,3,3	0.37	0	2,2,2	0.45	0
3	SO4	A	1001	-	4,4,4	0.13	0	6,6,6	0.35	0
3	SO4	D	1001	-	4,4,4	0.12	0	6,6,6	0.18	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
5	EDO	B	1004	-	-	0/1/1/1	-
5	EDO	A	1005	-	-	0/1/1/1	-
5	EDO	A	1004	-	-	0/1/1/1	-
5	EDO	B	1002	-	-	1/1/1/1	-
5	EDO	B	1003	-	-	1/1/1/1	-
5	EDO	A	1003	-	-	1/1/1/1	-
5	EDO	D	1002	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	C	1002	-	-	1/1/1/1	-
5	EDO	C	1003	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1003	EDO	O1-C1-C2-O2
5	C	1002	EDO	O1-C1-C2-O2
5	A	1003	EDO	O1-C1-C2-O2
5	B	1002	EDO	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1004	EDO	1	0
5	A	1004	EDO	1	0
5	A	1005	EDO	1	0
5	B	1002	EDO	2	0
3	B	1001	SO4	1	0
3	C	1001	SO4	1	0
5	B	1003	EDO	3	0
5	A	1003	EDO	4	0
5	D	1002	EDO	1	0
5	C	1002	EDO	1	0
3	D	1001	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	329/338 (97%)	0.03	5 (1%)	73	75	29, 45, 69, 90	0
1	B	324/338 (95%)	-0.08	1 (0%)	94	94	30, 45, 68, 89	0
1	C	289/338 (85%)	0.04	7 (2%)	59	61	28, 48, 73, 84	0
1	D	263/338 (77%)	0.48	23 (8%)	10	9	37, 72, 112, 118	0
2	E	46/74 (62%)	-0.03	0	100	100	33, 44, 69, 78	0
2	F	46/74 (62%)	0.06	1 (2%)	62	64	34, 44, 62, 77	0
2	G	28/74 (37%)	-0.05	1 (3%)	42	45	37, 52, 79, 87	0
2	H	25/74 (33%)	0.76	3 (12%)	4	3	53, 71, 94, 101	0
All	All	1350/1648 (81%)	0.10	41 (3%)	50	52	28, 49, 89, 118	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	895	ILE	5.2
1	D	732	CYS	5.1
1	D	786	ILE	4.6
1	A	774	SER	4.3
1	C	709	ILE	3.9
1	D	798	TYR	3.8
2	H	219	PRO	3.8
1	A	773	GLN	3.4
2	F	220	THR	3.4
1	D	799	ASP	3.2
1	D	871	VAL	3.1
2	H	214	ILE	3.1
1	D	901	GLU	3.1
1	D	894	ALA	3.1
1	D	903	HIS	3.0
1	D	733	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	703	TRP	3.0
1	D	793	ALA	2.9
2	H	212	ASN	2.9
1	D	892	PHE	2.7
1	D	783	GLU	2.5
1	D	788	PHE	2.5
1	C	870	CYS	2.4
1	D	785	LEU	2.4
1	A	769	ASP	2.4
1	A	768	ALA	2.4
1	C	918	CYS	2.3
1	C	916	MET	2.3
1	D	873	ILE	2.3
1	D	757	THR	2.3
1	D	794	ASN	2.2
1	A	919	GLU	2.2
1	D	660	ALA	2.2
1	C	814	ALA	2.2
1	C	869	ARG	2.2
1	C	733	GLY	2.1
1	D	904	GLY	2.1
2	G	194	ASP	2.1
1	D	704	ALA	2.1
1	D	760	VAL	2.0
1	B	890	MET	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 monosaccharides 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(Å^2)	Q<0.9
5	EDO	A	1003	4/4	0.76	0.26	49,51,53,59	0
5	EDO	B	1004	4/4	0.82	0.29	48,50,51,58	0
4	MG	A	1002	1/1	0.85	0.22	58,58,58,58	0
5	EDO	B	1002	4/4	0.89	0.19	44,49,53,57	0
5	EDO	A	1004	4/4	0.89	0.22	48,49,52,55	0
5	EDO	C	1003	4/4	0.90	0.34	35,46,48,54	0
5	EDO	B	1003	4/4	0.93	0.30	31,36,38,48	0
5	EDO	D	1002	4/4	0.93	0.30	57,59,61,71	0
5	EDO	A	1005	4/4	0.94	0.27	32,32,36,44	0
4	MG	B	1005	1/1	0.96	0.22	51,51,51,51	0
5	EDO	C	1002	4/4	0.96	0.22	41,43,48,48	0
3	SO4	D	1001	5/5	0.96	0.16	79,87,91,93	0
3	SO4	C	1001	5/5	0.96	0.13	59,62,72,73	0
3	SO4	B	1001	5/5	0.98	0.15	43,44,53,60	0
3	SO4	A	1001	5/5	0.99	0.15	46,46,54,55	0

6.5 Other polymers (i)

There are no such residues in this entry.