Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 04:15 pm GMT

PDB ID	:	5A0T
Title	:	Catalysis and 5' end sensing by ribonuclease RNase J of the metallo- beta-lactamase family
Authors	:	Pei, X.Y.; Bralley, P.; Jones, G.H.; Luisi, B.F.
Deposited on	:	2015-04-22
Resolution	:	2.28 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:

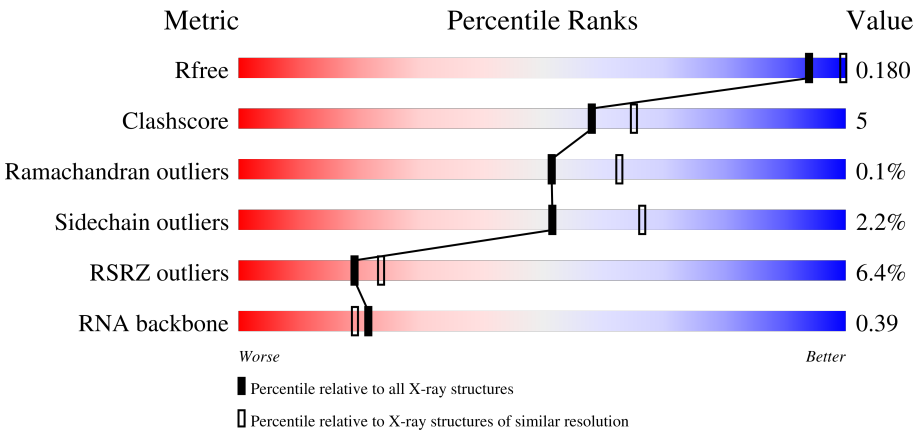
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.28 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)
RNA backbone	3102	1121 (2.70-1.86)

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	561	5% 71% 9% • 19%
1	B	561	5% 73% 7% • 20%
2	E	6	17% 33% 50% 17%
2	F	6	17% 50% 33% 17%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7742 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.

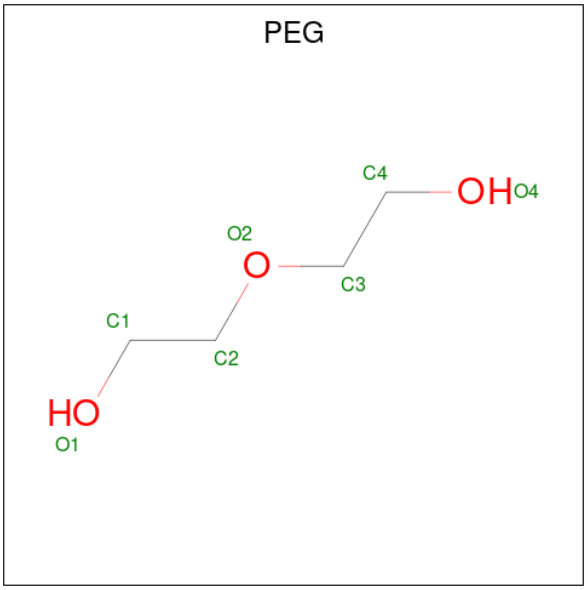
- Molecule 1 is a protein called RIBONUCLEASE J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	454	3482	2201	634	635	12	0	0	0
1	B	451	3468	2193	631	632	12	0	0	0

- Molecule 2 is a RNA chain called 5'-R(*CP*GP*CP*CP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	6	108	46	16	40	6	0	0	0
2	F	6	108	46	16	40	6	0	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	7	4	3	0	0
3	B	1	7	4	3	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
4	A	2	2	2	0	0
4	B	2	2	2	0	0

- Molecule 5 is water.

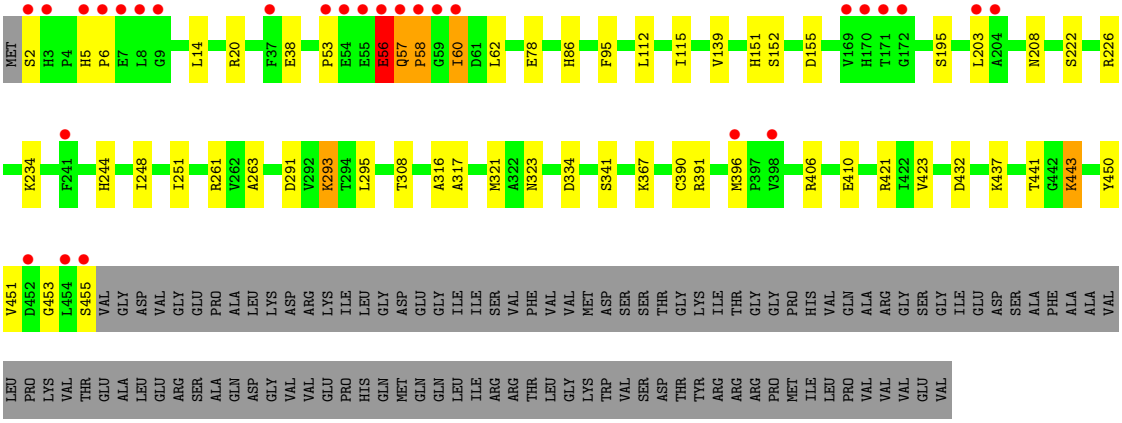
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	291	291	291	0	0
5	B	263	263	263	0	0
5	E	3	3	3	0	0
5	F	1	1	1	0	0

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.

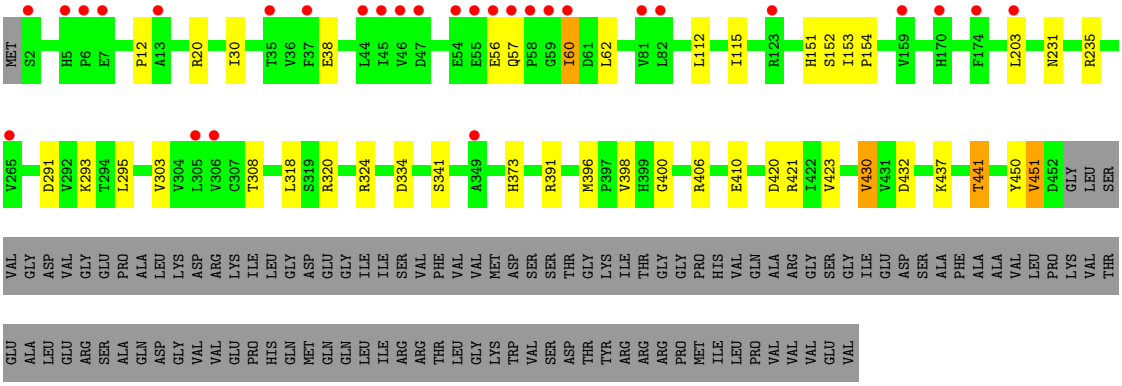
• Molecule 1: RIBONUCLEASE J

Chain A:



• Molecule 1: RIBONUCLEASE J

Chain B:



• Molecule 2: 5'-R(*CP*GP*CP*CP*UP)-3'

Chain E:

• Molecule 2: 5'-R(*CP*GP*CP*CP*UP)-3'

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	186.19Å 186.19Å 113.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.34 – 2.28 29.55 – 2.28	Depositor EDS
% Data completeness (in resolution range)	97.0 (29.34-2.28) 97.8 (29.55-2.28)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.145 , 0.177 0.149 , 0.180	Depositor DCC
R_{free} test set	4440 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	51.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.23 , 50.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	7742	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: PEG, ZN

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	0.46	2/3555 (0.1%)	0.59	1/4831 (0.0%)
1	B	0.49	4/3541 (0.1%)	0.60	3/4812 (0.1%)
2	E	1.21	1/118 (0.8%)	1.31	1/180 (0.6%)
2	F	1.14	1/118 (0.8%)	1.23	1/180 (0.6%)
All	All	0.51	8/7332 (0.1%)	0.63	6/10003 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	0	C	OP3-P	-11.00	1.48	1.61
2	F	0	C	OP3-P	-10.44	1.48	1.61
1	B	56	GLU	CG-CD	-9.53	1.37	1.51
1	B	56	GLU	CD-OE2	9.35	1.35	1.25
1	B	56	GLU	CD-OE1	9.17	1.35	1.25
1	B	56	GLU	CB-CG	8.13	1.67	1.52
1	A	57	GLN	CB-CG	5.41	1.67	1.52
1	A	56	GLU	CD-OE2	5.09	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	60	ILE	CG1-CB-CG2	-11.81	85.42	111.40
2	E	0	C	OP1-P-O3'	5.62	117.57	105.20
1	B	56	GLU	CG-CD-OE1	-5.61	107.08	118.30
2	F	3	C	C6-N1-C2	-5.11	118.26	120.30
1	A	60	ILE	CG1-CB-CG2	-5.10	100.19	111.40
1	B	56	GLU	CB-CG-CD	-5.03	100.63	114.20

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	3482	0	3505	41	0
1	B	3468	0	3498	28	0
2	E	108	0	54	4	0
2	F	108	0	54	1	0
3	A	7	0	10	0	0
3	B	7	0	10	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	291	0	0	4	0
5	B	263	0	0	2	0
5	E	3	0	0	0	0
5	F	1	0	0	0	0
All	All	7742	0	7131	69	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 5.

All (69) 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:451:VAL:HG22	1:A:453:GLY:H	1.48	0.79
1:B:154:PRO:O	5:B:2121:HOH:O	2.05	0.73
1:A:57:GLN:HB3	1:A:58:PRO:HD2	1.71	0.71
1:A:308:THR:HG21	2:E:4:U:OP1	1.93	0.69
1:B:57:GLN:HG2	1:B:60:ILE:HD12	1.76	0.67
1:A:53:PRO:HB2	1:A:56:GLU:HB2	1.76	0.67
1:B:420:ASP:O	1:B:437:LYS:NZ	2.29	0.66
1:B:295:LEU:HD13	1:B:303:VAL:HG13	1.83	0.61
1:A:334:ASP:OD1	5:A:2196:HOH:O	2.16	0.61
1:B:57:GLN:OE1	1:B:60:ILE:HD11	2.02	0.59
1:B:151:HIS:CG	1:B:152:SER:H	2.22	0.57
1:A:60:ILE:HG23	1:A:450:TYR:HD1	1.69	0.57
1:A:308:THR:HG23	1:A:316:ALA:HB1	1.86	0.56
1:B:308:THR:HB	2:F:3:C:H5"	1.87	0.56
1:B:62:LEU:HB2	1:B:451:VAL:HG23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HB2	1:A:451:VAL:CG1	2.36	0.55
1:B:57:GLN:OE1	1:B:60:ILE:CD1	2.55	0.55
1:A:62:LEU:HB2	1:A:451:VAL:HG13	1.89	0.54
1:A:323:ASN:ND2	5:A:2244:HOH:O	2.29	0.54
1:B:430:VAL:HG22	1:B:441:THR:HG22	1.89	0.53
1:A:57:GLN:CB	1:A:58:PRO:HD2	2.37	0.52
1:B:60:ILE:HG23	1:B:450:TYR:HD1	1.75	0.51
1:A:20:ARG:HB3	1:A:38:GLU:HB3	1.93	0.51
1:A:222:SER:O	1:A:226:ARG:HG3	2.10	0.50
1:B:30:ILE:HD13	1:B:400:GLY:HA2	1.94	0.50
1:B:60:ILE:HG23	1:B:450:TYR:CD1	2.47	0.50
1:B:432:ASP:OD2	1:B:441:THR:HG21	2.13	0.49
1:A:151:HIS:CG	1:A:152:SER:H	2.31	0.48
1:A:396:MET:HG2	1:A:423:VAL:HG22	1.96	0.48
1:B:421:ARG:HD3	1:B:437:LYS:NZ	2.29	0.47
1:A:317:ALA:O	1:A:321:MET:HG3	2.16	0.46
1:A:234:LYS:HB3	5:A:2196:HOH:O	2.15	0.46
1:A:244:HIS:HE1	5:A:2201:HOH:O	1.99	0.46
1:A:112:LEU:HA	1:A:115:ILE:HG22	1.98	0.45
1:A:57:GLN:HB3	1:A:58:PRO:CD	2.45	0.45
1:A:341:SER:HB3	2:E:0:C:OP3	2.15	0.45
1:B:291:ASP:OD2	1:B:293:LYS:HG2	2.16	0.45
1:B:406:ARG:O	1:B:410:GLU:HG2	2.16	0.45
1:A:451:VAL:HG23	1:A:455:SER:N	2.33	0.44
1:B:20:ARG:HB3	1:B:38:GLU:HB3	1.99	0.44
1:A:432:ASP:OD2	1:A:441:THR:HG21	2.18	0.44
1:A:86:HIS:CE1	2:E:1:G:H5"	2.53	0.44
1:A:451:VAL:HG22	1:A:453:GLY:N	2.26	0.44
1:A:443:LYS:HB2	1:A:443:LYS:HE2	1.68	0.44
1:A:60:ILE:HG23	1:A:450:TYR:CD1	2.52	0.43
1:B:12:PRO:HD2	1:B:441:THR:HG23	2.01	0.43
1:B:151:HIS:CG	1:B:152:SER:N	2.85	0.43
1:A:203:LEU:HA	1:A:396:MET:O	2.17	0.43
1:B:235:ARG:HB3	1:B:334:ASP:OD1	2.18	0.43
1:A:308:THR:HG21	2:E:4:U:P	2.59	0.43
1:A:60:ILE:HD13	1:A:60:ILE:HG21	1.79	0.43
1:A:95:PHE:CE1	1:A:451:VAL:HG21	2.54	0.43
1:A:406:ARG:O	1:A:410:GLU:HG2	2.19	0.43
1:B:153:ILE:HA	1:B:154:PRO:HD3	1.89	0.43
1:B:112:LEU:HA	1:B:115:ILE:HG22	2.00	0.42
1:B:203:LEU:HA	1:B:396:MET:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ALA:HB3	1:A:295:LEU:HD11	2.01	0.42
1:A:14:LEU:HD13	1:A:20:ARG:HB2	2.01	0.42
1:A:421:ARG:CZ	1:A:437:LYS:HG2	2.50	0.42
1:A:78:GLU:HB3	1:A:139:VAL:HG12	2.02	0.41
1:A:291:ASP:OD2	1:A:293:LYS:HB2	2.20	0.41
1:A:248:ILE:HA	1:A:251:ILE:HD12	2.01	0.41
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.93	0.41
1:B:231:ASN:OD1	3:B:1453:PEG:H41	2.20	0.41
1:A:195:SER:HB2	1:A:390:CYS:O	2.21	0.40
1:B:341:SER:HB3	1:B:373:HIS:NE2	2.36	0.40
1:A:151:HIS:CG	1:A:152:SER:N	2.89	0.40
1:A:5:HIS:CG	1:A:6:PRO:HD2	2.57	0.40
1:B:320:ARG:NE	5:B:2220:HOH:O	2.55	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	452/561 (81%)	437 (97%)	14 (3%)	1 (0%)	47 57
1	B	449/561 (80%)	436 (97%)	13 (3%)	0	100 100
All	All	901/1122 (80%)	873 (97%)	27 (3%)	1 (0%)	51 63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	PRO

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	371/462 (80%)	362 (98%)	9 (2%)	49	63
1	B	371/462 (80%)	364 (98%)	7 (2%)	57	71
All	All	742/924 (80%)	726 (98%)	16 (2%)	52	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	56	GLU
1	A	155	ASP
1	A	208	ASN
1	A	261	ARG
1	A	293	LYS
1	A	367	LYS
1	A	391	ARG
1	A	443	LYS
1	B	324	ARG
1	B	391	ARG
1	B	398	VAL
1	B	423	VAL
1	B	430	VAL
1	B	441	THR
1	B	451	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	244	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	4/6 (66%)	1 (25%)	0
2	F	4/6 (66%)	1 (25%)	0
All	All	8/12 (66%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	C
2	F	2	C

There are no RNA pucker outliers to report.

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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	PEG	B	1453	-	6,6,6	1.36	1 (16%)	5,5,5	1.36	1 (20%)
3	PEG	A	1456	-	6,6,6	1.33	1 (16%)	5,5,5	1.49	1 (20%)

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	PEG	B	1453	-	-	2/4/4/4	-
3	PEG	A	1456	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1453	PEG	C2-C1	-2.75	1.34	1.49
3	A	1456	PEG	C2-C1	-2.69	1.35	1.49

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1456	PEG	O2-C2-C1	2.72	122.02	110.07
3	B	1453	PEG	O2-C2-C1	2.40	120.61	110.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1456	PEG	O2-C3-C4-O4
3	B	1453	PEG	O2-C3-C4-O4
3	A	1456	PEG	C4-C3-O2-C2
3	A	1456	PEG	C1-C2-O2-C3
3	B	1453	PEG	C4-C3-O2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1453	PEG	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	454/561 (80%)	0.08	28 (6%)	20	25	34, 50, 71, 108	295 (64%)
1	B	451/561 (80%)	0.26	29 (6%)	19	23	39, 57, 80, 107	310 (68%)
2	E	6/6 (100%)	1.04	1 (16%)	1	2	56, 66, 84, 102	6 (100%)
2	F	6/6 (100%)	1.40	1 (16%)	1	2	69, 73, 98, 117	6 (100%)
All	All	917/1134 (80%)	0.18	59 (6%)	19	23	34, 54, 79, 117	617 (67%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	PRO	10.1
1	A	58	PRO	9.5
1	A	59	GLY	9.4
1	A	57	GLN	8.4
1	B	60	ILE	7.8
1	B	57	GLN	7.7
1	B	56	GLU	6.4
1	A	6	PRO	6.4
1	A	60	ILE	6.2
1	A	454	LEU	6.0
1	B	55	GLU	5.9
1	A	2	SER	5.7
1	A	455	SER	5.4
1	B	59	GLY	5.0
1	A	452	ASP	4.9
1	A	56	GLU	4.9
1	B	7	GLU	4.7
1	A	7	GLU	4.4
2	F	0	C	4.3
1	B	6	PRO	4.1
1	A	203	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	2	SER	4.1
1	B	35	THR	3.8
1	A	55	GLU	3.7
1	B	5	HIS	3.7
1	B	44	LEU	3.7
1	A	3	HIS	3.6
1	B	123	ARG	3.5
1	A	54	GLU	3.4
1	A	53	PRO	3.3
1	B	82	LEU	3.3
1	B	46	VAL	3.2
1	B	306	VAL	3.2
1	A	5	HIS	3.1
1	B	45	ILE	2.9
1	A	169	VAL	2.8
1	A	396	MET	2.8
1	B	81	VAL	2.8
1	B	203	LEU	2.7
1	B	170	HIS	2.7
1	A	8	LEU	2.7
1	A	204	ALA	2.6
1	A	9	GLY	2.6
1	A	170	HIS	2.6
1	B	265	VAL	2.5
1	B	54	GLU	2.5
1	A	171	THR	2.5
1	B	174	PHE	2.3
1	B	159	VAL	2.3
1	A	398	VAL	2.2
1	A	172	GLY	2.2
1	B	47	ASP	2.2
1	A	241	PHE	2.2
1	B	305	LEU	2.2
1	A	37	PHE	2.1
1	B	349	ALA	2.1
2	E	0	C	2.0
1	B	37	PHE	2.0
1	B	13	ALA	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
3	PEG	A	1456	7/7	0.69	0.28	80,89,103,106	0
3	PEG	B	1453	7/7	0.77	0.27	87,94,99,100	0
4	ZN	A	1457	1/1	0.98	0.04	49,49,49,49	1
4	ZN	A	1458	1/1	0.99	0.05	61,61,61,61	0
4	ZN	B	1454	1/1	0.99	0.07	53,53,53,53	1
4	ZN	B	1455	1/1	0.99	0.03	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.