



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 11:55 pm BST

PDB ID : 4BA2
Title : Archaeal exosome (Rrp4-Rrp41(D182A)-Rrp42) bound to inorganic phosphate
Authors : Lorentzen, E.; Conti, E.
Deposited on : 2012-09-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

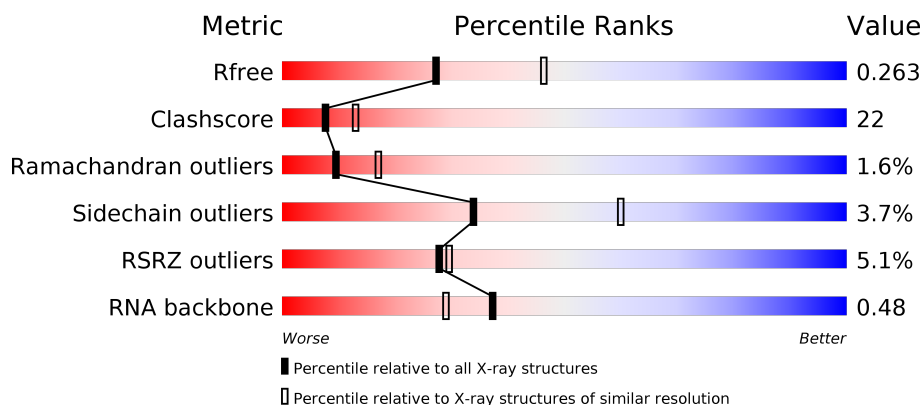
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	277	<div> <div>3%</div> <div>66% 31% ..</div> </div>
2	B	250	<div> <div>%</div> <div>70% 22% • 6%</div> </div>
3	I	251	<div> <div>10%</div> <div>50% 31% • 15%</div> </div>
4	R	4	<div> <div>25% 75%</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
6	PO4	B	1242	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5717 atoms, of which 22 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 PROBABLE EXOSOME COMPLEX EXONUCLEASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	5	5	0
			2094	1335	339	415	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9UXC0
A	0	HIS	-	expression tag	UNP Q9UXC0

- Molecule 2 is a protein called PROBABLE EXOSOME COMPLEX EXONUCLEASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	5	0
			1809	1149	313	336	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q9UXC2
B	0	HIS	-	expression tag	UNP Q9UXC2
B	182	ALA	ASP	engineered mutation	UNP Q9UXC2

- Molecule 3 is a protein called PROBABLE EXOSOME COMPLEX RNA-BINDING PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	213	Total	C	N	O	S	0	2	0
			1572	1019	253	296	4			

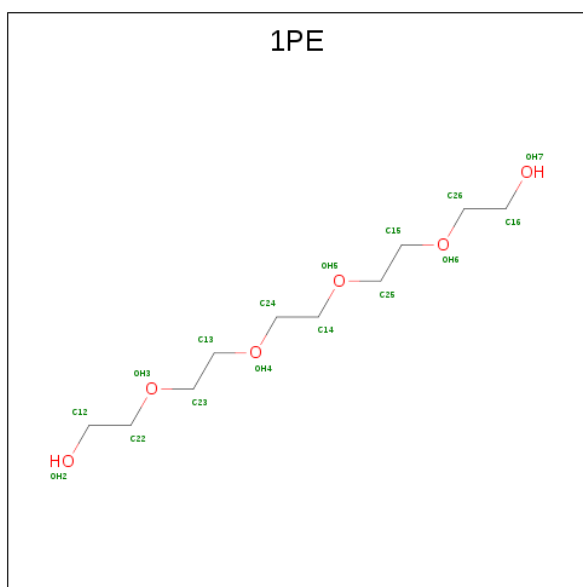
There are 3 discrepancies between the modelled and reference sequences:

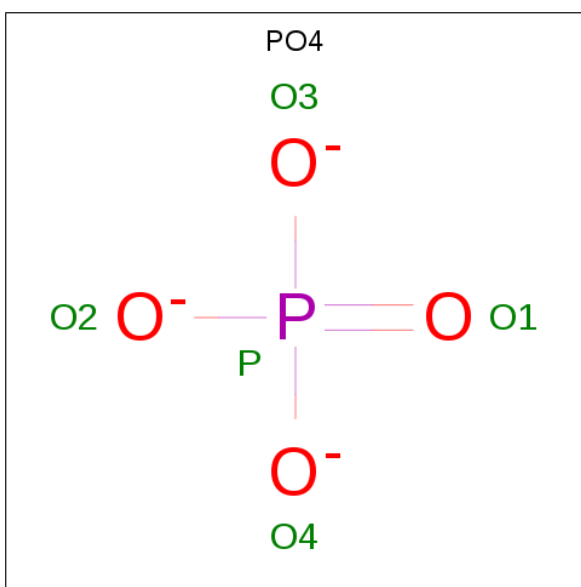
Chain	Residue	Modelled	Actual	Comment	Reference
I	-1	GLY	-	expression tag	UNP Q9UXC4
I	0	HIS	-	expression tag	UNP Q9UXC4
I	8	GLU	LYS	conflict	UNP Q9UXC4

- Molecule 4 is a RNA chain called 5'-R(*AP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	4	Total	C	N	O	P	0	0	0
			88	40	20	24	4			

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	I	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Na	0	0
			1	1		

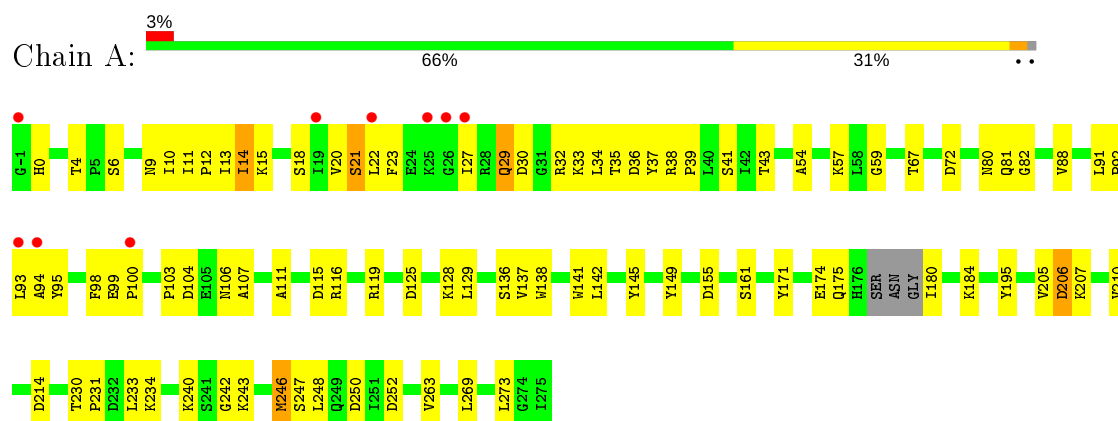
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	57	Total	O	0	0
			57	57		
8	B	35	Total	O	0	0
			35	35		
8	I	9	Total	O	0	0
			9	9		
8	R	4	Total	O	0	0
			4	4		

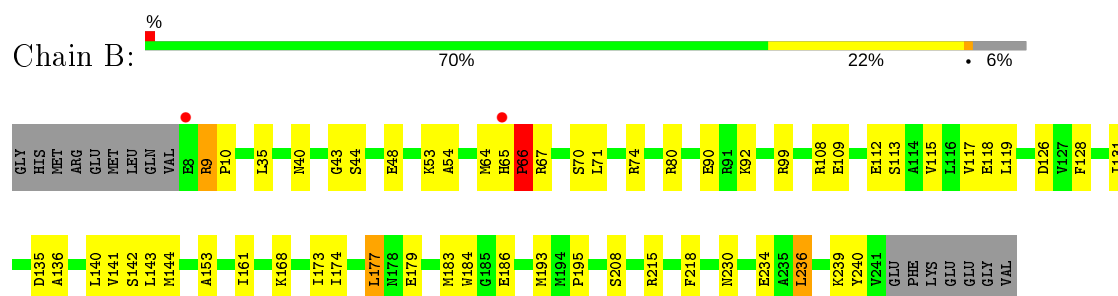
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

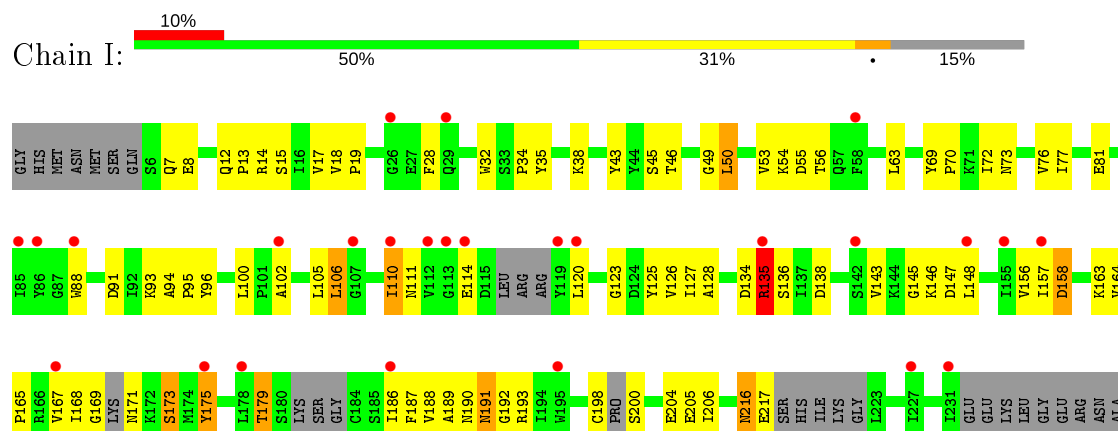
• Molecule 1: PROBABLE EXOSOME COMPLEX EXONUCLEASE 2



• Molecule 2: PROBABLE EXOSOME COMPLEX EXONUCLEASE 1

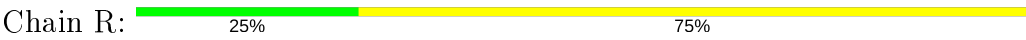


• Molecule 3: PROBABLE EXOSOME COMPLEX RNA-BINDING PROTEIN 1



SER
SER
GLY
THR
LYS
THR
ASN
SER

● Molecule 4: 5'-R(*AP*AP*AP*AP)-3'



A2
A3
A4
A5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	134.83Å 134.83Å 134.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 2.50 47.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.50) 100.0 (47.67-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.51Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8 _1069)	Depositor
R, R_{free}	0.185 , 0.259 0.190 , 0.263	Depositor DCC
R_{free} test set	1425 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 67.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.044 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5717	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, PO4, 1PE

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	0.42	0/2141	0.58	0/2912
2	B	0.43	0/1853	0.60	0/2505
3	I	0.37	0/1607	0.53	0/2196
4	R	0.60	0/99	1.08	0/152
All	All	0.41	0/5700	0.59	0/7765

There are no bond length outliers.

There are no bond angle outliers.

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	2094	0	2130	95	1
2	B	1809	0	1853	55	1
3	I	1572	0	1463	106	0
4	R	88	0	45	5	0
5	A	16	22	22	0	0
6	B	5	0	0	3	0
6	I	5	0	0	0	0
7	B	1	0	0	0	0
8	A	57	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	35	0	0	2	0
8	I	9	0	0	1	0
8	R	4	0	0	0	0
All	All	5695	22	5513	243	1

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 22.

All (243) 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:14:ILE:H	1:A:14:ILE:HD12	1.13	1.14
1:A:10:ILE:HD11	3:I:81:GLU:HG2	1.04	1.01
1:A:10:ILE:CD1	3:I:81:GLU:HG2	1.93	0.99
1:A:91:LEU:HD11	1:A:145:TYR:HD2	1.38	0.88
3:I:77:ILE:O	3:I:191:ASN:ND2	2.09	0.86
1:A:10:ILE:HD11	3:I:81:GLU:CG	1.99	0.86
3:I:110:ILE:CD1	3:I:114:GLU:HB3	2.06	0.85
1:A:20:VAL:O	1:A:23:PHE:N	2.09	0.84
3:I:77:ILE:O	3:I:77:ILE:HG13	1.77	0.83
1:A:36:ASP:OD2	8:A:2004:HOH:O	1.98	0.81
2:B:64:MET:HE1	2:B:70:SER:HA	1.63	0.78
3:I:105:LEU:CD2	3:I:143:VAL:HG21	2.13	0.78
2:B:99:ARG:HG2	2:B:99:ARG:HH11	1.48	0.77
1:A:14:ILE:H	1:A:14:ILE:CD1	1.91	0.76
1:A:18:SER:O	1:A:21:SER:OG	2.01	0.75
1:A:248:LEU:CD2	2:B:218[A]:PHE:CZ	2.69	0.75
8:A:2029:HOH:O	4:R:4:A:OP1	2.04	0.74
2:B:64:MET:CE	2:B:70:SER:HA	2.17	0.74
3:I:77:ILE:HD11	3:I:193:ARG:HB3	1.70	0.74
3:I:77:ILE:HG12	3:I:193:ARG:HB2	1.69	0.73
3:I:105:LEU:HD23	3:I:143:VAL:HG21	1.70	0.72
3:I:157:ILE:N	3:I:157:ILE:HD12	2.04	0.72
3:I:120:LEU:HD13	3:I:126:VAL:HG21	1.72	0.72
1:A:128:LYS:HE3	8:A:2038:HOH:O	1.91	0.71
2:B:74[A]:ARG:NH1	2:B:118:GLU:OE2	2.23	0.71
1:A:37:TYR:OH	1:A:155:ASP:OD2	2.08	0.71
3:I:38:LYS:HB2	3:I:43:TYR:CE1	2.25	0.71
1:A:92:PRO:HA	1:A:98:PHE:O	1.89	0.70
1:A:115:ASP:O	8:A:2031:HOH:O	2.11	0.69
3:I:135[B]:ARG:HH11	3:I:135[B]:ARG:CG	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:LEU:HD22	2:B:218[A]:PHE:CZ	2.29	0.67
1:A:20:VAL:O	1:A:23:PHE:HB2	1.94	0.67
3:I:186:ILE:C	3:I:186:ILE:HD12	2.16	0.66
2:B:108:ARG:NH1	2:B:112:GLU:OE2	2.27	0.66
3:I:93:LYS:NZ	3:I:158:ASP:HB3	2.11	0.66
3:I:135[B]:ARG:NH1	3:I:135[B]:ARG:HG2	2.11	0.65
3:I:135[B]:ARG:HH11	3:I:135[B]:ARG:HG2	1.61	0.65
1:A:9:ASN:HB2	1:A:95:TYR:OH	1.96	0.64
2:B:183[A]:MET:SD	2:B:184:TRP:NE1	2.71	0.64
3:I:13:PRO:O	3:I:14:ARG:HB3	1.97	0.64
3:I:50:LEU:HD12	3:I:63:LEU:HD11	1.80	0.64
3:I:175:TYR:HE1	3:I:179:THR:HG21	1.63	0.63
1:A:6:SER:HA	2:B:71:LEU:HD21	1.79	0.63
1:A:104:ASP:OD2	1:A:106:ASN:ND2	2.29	0.62
1:A:12:PRO:HG2	1:A:15:LYS:HB2	1.80	0.62
3:I:18:VAL:HG13	3:I:19:PRO:HD2	1.80	0.62
1:A:119:ARG:HB2	8:A:2031:HOH:O	2.00	0.62
1:A:240:LYS:NZ	8:A:2053:HOH:O	2.32	0.62
1:A:91:LEU:HD11	1:A:145:TYR:CD2	2.28	0.62
3:I:105:LEU:HD22	3:I:143:VAL:HG21	1.82	0.62
1:A:20:VAL:HA	1:A:23:PHE:CD2	2.34	0.62
3:I:158:ASP:OD2	3:I:193:ARG:HD3	2.00	0.61
2:B:174:ILE:HG13	2:B:177:LEU:HD22	1.82	0.61
1:A:98:PHE:CE2	1:A:149:TYR:CD2	2.88	0.61
3:I:186:ILE:CD1	3:I:188:VAL:HG23	2.30	0.61
3:I:14:ARG:NH1	3:I:14:ARG:HG3	2.16	0.61
3:I:164:VAL:N	3:I:165:PRO:HD2	2.16	0.61
1:A:14:ILE:N	1:A:14:ILE:HD12	1.99	0.61
1:A:125:ASP:HB3	1:A:128:LYS:HD2	1.83	0.60
1:A:243:LYS:HE3	2:B:74[B]:ARG:NH1	2.16	0.60
1:A:33:LYS:HE3	1:A:36:ASP:OD2	2.01	0.60
2:B:48:GLU:HG2	2:B:53:LYS:HG3	1.83	0.60
3:I:14:ARG:HH11	3:I:14:ARG:HG3	1.65	0.60
1:A:33:LYS:O	1:A:35:THR:N	2.35	0.60
3:I:38:LYS:HB2	3:I:43:TYR:CD1	2.37	0.59
3:I:38:LYS:HD2	3:I:43:TYR:CE1	2.37	0.59
1:A:248:LEU:HD23	2:B:218[A]:PHE:HZ	1.68	0.58
2:B:99:ARG:HG2	2:B:99:ARG:NH1	2.16	0.58
1:A:38:ARG:HB3	1:A:39:PRO:HD2	1.84	0.58
3:I:88:TRP:HE3	3:I:100:LEU:O	1.87	0.58
2:B:35:LEU:CD1	2:B:236:LEU:HD12	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:O	1:A:21:SER:C	2.43	0.56
1:A:248:LEU:HD23	2:B:218[A]:PHE:CZ	2.41	0.56
3:I:55[B]:ASP:OD1	3:I:56:THR:HG22	2.06	0.56
6:B:1242:PO4:O1	4:R:5:A:H5"	2.06	0.56
1:A:98:PHE:HE2	1:A:149:TYR:CD2	2.23	0.56
1:A:174:GLU:O	1:A:180:ILE:HA	2.06	0.55
3:I:204:GLU:O	3:I:206:ILE:N	2.39	0.55
3:I:157:ILE:H	3:I:157:ILE:HD12	1.71	0.55
2:B:239:LYS:HE2	2:B:240:TYR:CZ	2.42	0.55
3:I:128:ALA:HA	3:I:148:LEU:HD22	1.88	0.55
1:A:205:VAL:O	1:A:206:ASP:HB2	2.07	0.54
3:I:93:LYS:HZ1	3:I:158:ASP:HB3	1.72	0.54
2:B:80:ARG:HD3	8:B:2014:HOH:O	2.07	0.54
1:A:125:ASP:HB3	1:A:128:LYS:CD	2.37	0.54
3:I:12:GLN:O	3:I:15:SER:OG	2.12	0.54
3:I:127:ILE:HG22	3:I:148:LEU:HD23	1.90	0.54
3:I:198:CYS:O	3:I:200:SER:HA	2.08	0.54
3:I:175:TYR:HE1	3:I:179:THR:CG2	2.20	0.54
2:B:99:ARG:NH2	6:B:1242:PO4:O1	2.38	0.53
2:B:35:LEU:HD11	2:B:236:LEU:HD12	1.90	0.53
2:B:174:ILE:HG13	2:B:177:LEU:CD2	2.38	0.53
2:B:109:GLU:HA	2:B:112:GLU:HG3	1.90	0.53
1:A:80:ASN:O	1:A:81:GLN:HG3	2.08	0.53
1:A:94:ALA:HB1	1:A:149:TYR:HB2	1.91	0.52
3:I:110:ILE:HD12	3:I:111:ASN:N	2.24	0.52
3:I:135[B]:ARG:HD2	8:I:2005:HOH:O	2.08	0.52
1:A:171:TYR:CD1	1:A:184:LYS:HA	2.44	0.52
2:B:140:LEU:O	2:B:144:MET:HG3	2.09	0.52
3:I:204:GLU:C	3:I:206:ILE:H	2.13	0.52
3:I:77:ILE:HD11	3:I:193:ARG:CB	2.37	0.52
3:I:7:GLN:NE2	3:I:28:PHE:CE2	2.77	0.52
1:A:11:ILE:HG13	1:A:12:PRO:HD2	1.91	0.52
1:A:29:GLN:NE2	1:A:214:ASP:OD2	2.41	0.52
2:B:66:PRO:HB2	2:B:67:ARG:HA	1.91	0.52
3:I:94:ALA:HB1	3:I:95:PRO:HD2	1.91	0.52
3:I:94:ALA:HB1	3:I:95:PRO:CD	2.39	0.51
3:I:186:ILE:CD1	3:I:188:VAL:CG2	2.89	0.51
3:I:18:VAL:HG13	3:I:19:PRO:CD	2.41	0.51
3:I:54:LYS:O	3:I:55[B]:ASP:CG	2.49	0.51
1:A:243:LYS:HE3	2:B:74[B]:ARG:HH12	1.74	0.51
1:A:38:ARG:HB3	1:A:39:PRO:CD	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:ASP:HB3	2:B:128:PHE:CE2	2.46	0.51
3:I:163:LYS:HE3	3:I:217:GLU:CB	2.40	0.51
3:I:77:ILE:HG23	3:I:189:ALA:HB2	1.93	0.51
1:A:10:ILE:O	1:A:10:ILE:HG13	2.10	0.51
2:B:168:LYS:HG3	2:B:173:ILE:HD13	1.93	0.51
3:I:105:LEU:HD13	3:I:105:LEU:O	2.10	0.51
3:I:76:VAL:HA	3:I:189:ALA:HB1	1.92	0.51
2:B:66:PRO:HB2	2:B:67:ARG:CA	2.41	0.50
1:A:82:GLY:HA3	1:A:129:LEU:HB2	1.94	0.49
3:I:55[B]:ASP:CG	3:I:56:THR:H	2.08	0.49
1:A:91:LEU:HB3	1:A:93:LEU:CD1	2.42	0.49
1:A:98:PHE:HE2	1:A:149:TYR:HD2	1.61	0.49
3:I:125:TYR:CD2	3:I:156:VAL:HG21	2.48	0.49
3:I:134:ASP:O	3:I:136:SER:N	2.45	0.49
3:I:32:TRP:CZ3	3:I:34:PRO:HD3	2.48	0.49
1:A:4:THR:HG21	2:B:74[B]:ARG:CZ	2.43	0.49
1:A:13:ILE:HD12	3:I:123:GLY:C	2.33	0.49
3:I:38:LYS:HD2	3:I:43:TYR:CZ	2.47	0.48
3:I:145:GLY:HA3	3:I:148:LEU:HD12	1.95	0.48
1:A:103:PRO:HB3	1:A:107:ALA:HB3	1.95	0.48
1:A:92:PRO:HB3	1:A:98:PHE:O	2.14	0.48
3:I:102:ALA:O	3:I:106:LEU:HB2	2.14	0.48
1:A:129:LEU:HB3	1:A:138:TRP:HB2	1.94	0.48
3:I:164:VAL:N	3:I:165:PRO:CD	2.75	0.48
3:I:186:ILE:HD13	3:I:188:VAL:CG2	2.43	0.48
3:I:88:TRP:CZ3	3:I:102:ALA:HA	2.49	0.48
1:A:38:ARG:HD2	1:A:59:GLY:HA3	1.96	0.48
3:I:120:LEU:CD1	3:I:126:VAL:HG21	2.41	0.48
2:B:43:GLY:HA3	2:B:153:ALA:HB2	1.96	0.48
2:B:136:ALA:HB2	2:B:179:GLU:HA	1.96	0.47
2:B:239:LYS:HE2	2:B:240:TYR:CE2	2.50	0.47
1:A:13:ILE:H	1:A:13:ILE:HD12	1.79	0.47
1:A:175:GLN:CB	8:A:2045:HOH:O	2.61	0.47
3:I:190:ASN:O	3:I:192:GLY:N	2.47	0.47
3:I:72:ILE:O	3:I:73:ASN:HB2	2.13	0.47
3:I:35:TYR:HA	3:I:46:THR:OG1	2.14	0.47
1:A:92:PRO:CA	1:A:98:PHE:O	2.60	0.47
3:I:49:GLY:HA2	3:I:63:LEU:HG	1.96	0.47
1:A:29:GLN:H	1:A:29:GLN:HG3	1.45	0.47
1:A:206:ASP:HB3	1:A:207:LYS:H	1.41	0.46
3:I:110:ILE:HD12	3:I:114:GLU:HB3	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LEU:CD2	1:A:27:ILE:CD1	2.93	0.46
3:I:146:LYS:O	3:I:147:ASP:HB2	2.15	0.46
3:I:91:ASP:O	3:I:193:ARG:NH2	2.49	0.46
2:B:135:ASP:O	2:B:136:ALA:HB3	2.16	0.46
2:B:193:MET:O	2:B:195:PRO:HD3	2.16	0.46
3:I:7:GLN:HG2	3:I:28:PHE:CE1	2.51	0.46
3:I:186:ILE:HD13	3:I:188:VAL:HG22	1.98	0.46
3:I:175:TYR:CE1	3:I:179:THR:HG21	2.48	0.45
3:I:216:ASN:O	3:I:217:GLU:C	2.54	0.45
3:I:7:GLN:HG2	3:I:28:PHE:CZ	2.52	0.45
2:B:64:MET:CG	2:B:66:PRO:HD2	2.46	0.45
2:B:35:LEU:HD13	2:B:236:LEU:HD12	1.98	0.45
2:B:65:HIS:N	2:B:66:PRO:HD2	2.32	0.45
3:I:17:VAL:HG13	3:I:45:SER:CB	2.47	0.45
2:B:131:ILE:HD11	2:B:142:SER:HB2	1.98	0.45
3:I:77:ILE:CD1	3:I:193:ARG:HB3	2.42	0.45
3:I:96:TYR:HB3	3:I:138:ASP:OD1	2.17	0.45
1:A:30:ASP:OD1	1:A:32:ARG:HG2	2.16	0.45
1:A:33:LYS:C	1:A:35:THR:H	2.20	0.45
3:I:168:ILE:HG22	3:I:169:GLY:N	2.32	0.45
1:A:11:ILE:O	1:A:11:ILE:HG23	2.17	0.45
3:I:77:ILE:CG1	3:I:193:ARG:HB2	2.42	0.45
1:A:41:SER:HB3	1:A:57:LYS:HB2	1.99	0.45
3:I:50:LEU:HD13	3:I:63:LEU:HD21	1.99	0.45
3:I:110:ILE:HD11	3:I:114:GLU:HB3	1.93	0.44
8:B:2031:HOH:O	4:R:4:A:H5''	2.17	0.44
1:A:72:ASP:O	1:A:136:SER:HA	2.17	0.44
1:A:13:ILE:HD12	3:I:123:GLY:HA3	1.99	0.44
1:A:33:LYS:HE3	1:A:33:LYS:HB2	1.83	0.44
1:A:67:THR:HA	1:A:141:TRP:O	2.17	0.44
3:I:171:ASN:C	3:I:173:SER:H	2.19	0.44
3:I:204:GLU:C	3:I:206:ILE:N	2.71	0.44
1:A:99:GLU:HB3	1:A:100:PRO:HD2	1.98	0.44
1:A:246:MET:HG2	1:A:250:ASP:HB3	2.00	0.44
1:A:82:GLY:HA2	1:A:137:VAL:HB	2.00	0.44
3:I:175:TYR:C	3:I:175:TYR:CD1	2.89	0.44
3:I:53:VAL:O	3:I:53:VAL:HG12	2.17	0.44
2:B:143:LEU:HD21	2:B:161:ILE:HG21	1.99	0.44
4:R:3:A:O2'	4:R:4:A:H5'	2.17	0.43
3:I:88:TRP:CE3	3:I:100:LEU:O	2.69	0.43
3:I:186:ILE:HD12	3:I:187:PHE:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:GLU:CD	2:B:53:LYS:HE2	2.39	0.43
2:B:9:ARG:CB	2:B:10:PRO:CD	2.97	0.43
1:A:116:ARG:HD3	8:A:2029:HOH:O	2.19	0.43
1:A:230:THR:HB	1:A:231:PRO:CD	2.49	0.43
1:A:43:THR:O	1:A:54:ALA:HA	2.18	0.43
1:A:98:PHE:CZ	1:A:149:TYR:CD2	3.07	0.43
1:A:116:ARG:CG	8:A:2029:HOH:O	2.66	0.42
1:A:98:PHE:CD1	1:A:98:PHE:N	2.86	0.42
2:B:35:LEU:HD11	2:B:236:LEU:CD1	2.50	0.42
1:A:13:ILE:CD1	3:I:123:GLY:C	2.88	0.42
3:I:69:TYR:HA	3:I:70:PRO:HD3	1.93	0.42
1:A:20:VAL:O	1:A:23:PHE:CB	2.65	0.42
1:A:91:LEU:HA	1:A:92:PRO:HD2	1.75	0.42
3:I:186:ILE:HD11	3:I:188:VAL:HG23	2.01	0.42
1:A:234:LYS:HD3	2:B:208[A]:SER:OG	2.19	0.42
1:A:21:SER:OG	1:A:22:LEU:N	2.53	0.42
3:I:106:LEU:HA	3:I:106:LEU:HD12	1.79	0.42
3:I:77:ILE:HG23	3:I:189:ALA:CB	2.49	0.42
3:I:93:LYS:HD2	3:I:193:ARG:HH11	1.84	0.42
2:B:115:VAL:O	2:B:117:VAL:N	2.53	0.42
1:A:22:LEU:CD2	1:A:27:ILE:HD11	2.50	0.42
2:B:230:ASN:O	2:B:234:GLU:HG2	2.19	0.42
1:A:91:LEU:HB3	1:A:93:LEU:HD13	2.01	0.41
3:I:13:PRO:O	3:I:14:ARG:CB	2.64	0.41
2:B:64:MET:HG2	2:B:66:PRO:HD2	2.02	0.41
3:I:93:LYS:HZ2	3:I:158:ASP:HB3	1.83	0.41
3:I:167:VAL:HG12	3:I:167:VAL:O	2.20	0.41
3:I:8:GLU:HG3	3:I:8:GLU:O	2.18	0.41
1:A:233:LEU:HD11	1:A:263:VAL:HG22	2.03	0.41
1:A:247:SER:O	1:A:250:ASP:HB2	2.21	0.41
1:A:22:LEU:HB3	1:A:27:ILE:O	2.21	0.41
1:A:99:GLU:OE1	1:A:100:PRO:HD3	2.21	0.41
2:B:177:LEU:N	2:B:177:LEU:HD23	2.35	0.41
2:B:54:ALA:HB3	2:B:141:VAL:HG12	2.03	0.41
2:B:99:ARG:NH1	2:B:99:ARG:CG	2.83	0.41
3:I:93:LYS:HD2	3:I:193:ARG:NH1	2.36	0.41
6:B:1242:PO4:O2	4:R:5:A:H5'	2.20	0.41
1:A:252:ASP:OD1	2:B:215:ARG:NE	2.51	0.40
1:A:88:VAL:HG23	1:A:111:ALA:HB2	2.03	0.40
1:A:242:GLY:N	2:B:109:GLU:OE2	2.47	0.40
2:B:64:MET:HE3	2:B:70:SER:HA	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:14:ARG:CG	3:I:14:ARG:HH11	2.32	0.40
1:A:10:ILE:CD1	3:I:81:GLU:HA	2.51	0.40
3:I:186:ILE:C	3:I:186:ILE:CD1	2.84	0.40
1:A:142:LEU:HD21	1:A:161:SER:HB3	2.04	0.40
1:A:269:LEU:O	1:A:273:LEU:HG	2.21	0.40
2:B:71:LEU:HA	2:B:71:LEU:HD23	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:TYR:O	2:B:40:ASN:ND2[10_554]	2.17	0.03

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	275/277 (99%)	258 (94%)	13 (5%)	4 (2%)	10	18
2	B	237/250 (95%)	227 (96%)	8 (3%)	2 (1%)	19	35
3	I	205/251 (82%)	183 (89%)	16 (8%)	6 (3%)	4	6
All	All	717/778 (92%)	668 (93%)	37 (5%)	12 (2%)	9	16

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	191	ASN
3	I	205	GLU
1	A	0	HIS
1	A	21	SER
1	A	34	LEU
2	B	66	PRO

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Mol	Chain	Res	Type
3	I	135[A]	ARG
3	I	135[B]	ARG
2	B	9	ARG
3	I	179	THR
1	A	206	ASP
3	I	216	ASN

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	235/243 (97%)	230 (98%)	5 (2%)	53	78
2	B	192/208 (92%)	182 (95%)	10 (5%)	23	44
3	I	155/223 (70%)	147 (95%)	8 (5%)	23	44
All	All	582/674 (86%)	559 (96%)	23 (4%)	34	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	29	GLN
1	A	195	TYR
1	A	210	VAL
1	A	246	MET
2	B	44	SER
2	B	66	PRO
2	B	90	GLU
2	B	92	LYS
2	B	113[A]	SER
2	B	113[B]	SER
2	B	119	LEU
2	B	177	LEU
2	B	186	GLU
2	B	236	LEU
3	I	50	LEU

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Mol	Chain	Res	Type
3	I	106	LEU
3	I	110	ILE
3	I	135[A]	ARG
3	I	135[B]	ARG
3	I	158	ASP
3	I	173	SER
3	I	175	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
2	B	199	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	3/4 (75%)	0	0

There are no RNA backbone outliers to report.

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	1PE	A	1276	-	15,15,15	0.47	0	14,14,14	1.78	3 (21%)
6	PO4	I	1232	-	4,4,4	0.92	0	6,6,6	0.41	0
6	PO4	B	1242	-	4,4,4	0.72	0	6,6,6	0.76	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	1PE	A	1276	-	-	2/13/13/13	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1276	1PE	OH4-C24-C14	2.39	121.18	110.39
5	A	1276	1PE	OH3-C22-C12	2.13	119.43	110.07
5	A	1276	1PE	OH5-C14-C24	2.10	119.86	110.39

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1276	1PE	C15-C25-OH5-C14
5	A	1276	1PE	OH6-C15-C25-OH5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1242	PO4	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	274/277 (98%)	-0.00	9 (3%) 46 50	28, 48, 109, 145	2 (0%)
2	B	234/250 (93%)	-0.26	2 (0%) 84 86	31, 45, 81, 106	0
3	I	213/251 (84%)	0.64	26 (12%) 4 3	53, 83, 117, 130	0
4	R	4/4 (100%)	-1.24	0 100 100	53, 56, 59, 61	0
All	All	725/782 (92%)	0.10	37 (5%) 28 29	28, 56, 108, 145	2 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	85	ILE	6.3
3	I	113	GLY	5.5
1	A	26	GLY	4.8
3	I	110	ILE	4.2
2	B	8	GLU	4.0
3	I	195	TRP	3.8
3	I	155	ILE	3.7
1	A	25	LYS	3.5
3	I	227	ILE	3.4
3	I	167	VAL	3.4
3	I	186	ILE	3.3
1	A	-1	GLY	3.1
1	A	27	ILE	3.0
3	I	175	TYR	2.9
1	A	94	ALA	2.9
3	I	120	LEU	2.9
1	A	93	LEU	2.7
3	I	26	GLY	2.7
1	A	100	PRO	2.7
1	A	22	LEU	2.6
3	I	231	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	107	GLY	2.5
3	I	29	GLN	2.5
3	I	58	PHE	2.5
3	I	135[A]	ARG	2.5
2	B	65	HIS	2.4
3	I	119	TYR	2.4
3	I	88	TRP	2.4
3	I	178	LEU	2.3
3	I	102	ALA	2.3
3	I	86	TYR	2.3
3	I	148	LEU	2.3
3	I	112	VAL	2.2
3	I	142	SER	2.1
1	A	19	ILE	2.1
3	I	157	ILE	2.1
3	I	114	GLU	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 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. 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
6	PO4	I	1232	5/5	0.86	0.25	192,193,193,193	5
5	1PE	A	1276	16/16	0.94	0.21	48,64,100,101	0
7	NA	B	1243	1/1	0.95	0.14	55,55,55,55	0
6	PO4	B	1242	5/5	0.98	0.09	48,56,61,68	0

6.5 Other polymers ⓘ

There are no such residues in this entry.