



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:16 PM GMT

PDB ID : 1914
Title : SIGNAL RECOGNITION PARTICLE ALU RNA BINDING HET-
ERODIMER, SRP9/14
Authors : Birse, D.; Kapp, U.; Strub, K.; Cusack, S.; Aberg, A.
Deposited on : 1997-11-13
Resolution : 2.53 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (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

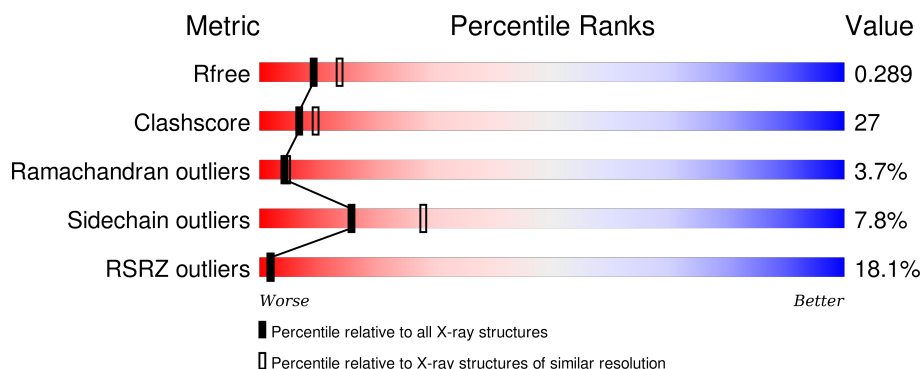
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	232	

2 Entry composition [i](#)

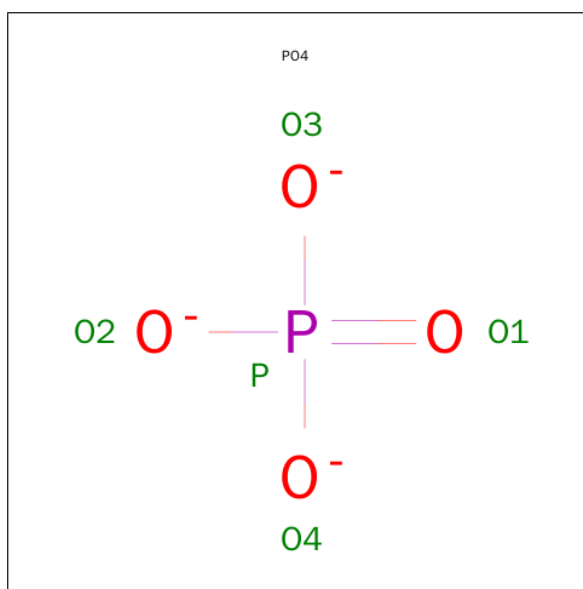
There are 4 unique types of molecules in this entry. The entry contains 1409 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SIGNAL RECOGNITION PARTICLE 9/14 FUSION PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	171	Total	C	N	O	S	0	0	0
			1383	873	246	254	10			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		

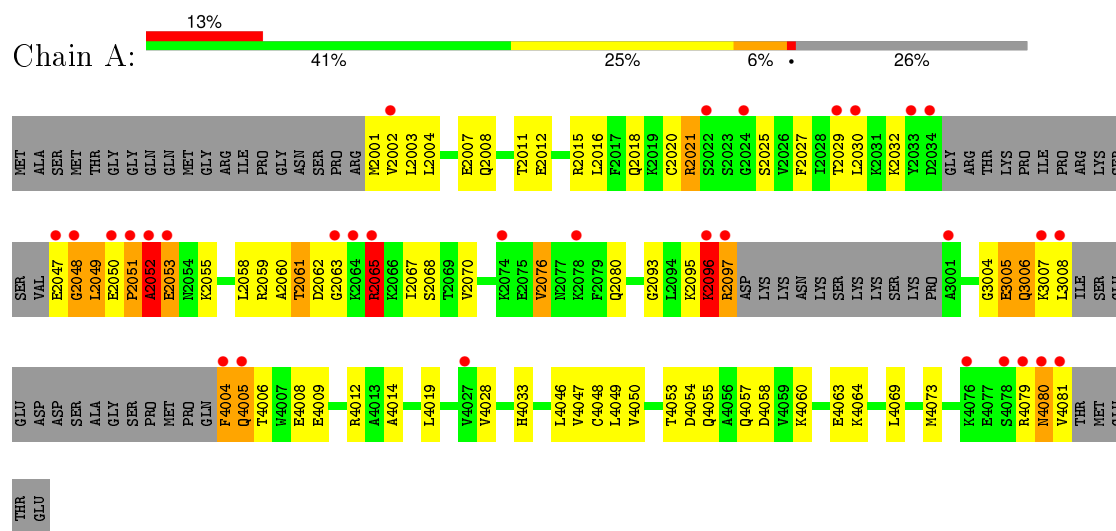
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		

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: SIGNAL RECOGNITION PARTICLE 9/14 FUSION PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α , β , γ	69.02Å 69.02Å 90.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.53 25.65 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.53) 95.3 (25.65-2.51)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.50Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.248 , 0.299 0.251 , 0.289	Depositor DCC
R_{free} test set	621 reflections (8.38%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.420	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 7811 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1409	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% 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, 0.375 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: PO4, BME

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	0.90	3/1397 (0.2%)	1.16	16/1863 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2061	THR	CB-CG2	-14.88	1.03	1.52
1	A	2048	GLY	N-CA	8.76	1.59	1.46
1	A	2097	ARG	C-O	5.80	1.34	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2047	GLU	O-C-N	-14.44	98.65	123.20
1	A	2047	GLU	CB-CA-C	13.92	138.24	110.40
1	A	2047	GLU	CA-C-N	11.92	140.04	116.20
1	A	2047	GLU	N-CA-C	-7.23	91.47	111.00
1	A	2065	ARG	C-N-CA	7.22	139.76	121.70
1	A	2096	LYS	C-N-CA	6.67	138.39	121.70
1	A	2021	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	A	4080	ASN	N-CA-C	6.35	128.14	111.00
1	A	2065	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	A	4004	PHE	O-C-N	6.09	132.45	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4079	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	2001	MET	CG-SD-CE	5.72	109.35	100.20
1	A	4004	PHE	C-N-CA	-5.63	107.61	121.70
1	A	2052	ALA	N-CA-C	5.36	125.48	111.00
1	A	2052	ALA	CB-CA-C	-5.28	102.18	110.10
1	A	2052	ALA	O-C-N	-5.01	114.68	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	2047	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2065	ARG	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1383	0	1432	76	1
2	A	5	0	0	0	0
3	A	4	0	5	0	0
4	A	17	0	0	0	0
All	All	1409	0	1437	76	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 27.

All (76) 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:4005:GLN:HG3	1:A:4006:THR:H	1.07	1.11
1:A:2052:ALA:O	1:A:2053:GLU:CB	2.04	0.98
1:A:4005:GLN:CG	1:A:4006:THR:H	1.76	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2052:ALA:O	1:A:2053:GLU:CG	2.16	0.93
1:A:4005:GLN:HG3	1:A:4006:THR:N	1.86	0.90
1:A:2052:ALA:O	1:A:2053:GLU:HG3	1.72	0.90
1:A:2052:ALA:O	1:A:2053:GLU:HB2	1.71	0.86
1:A:4053:THR:HG22	1:A:4055:GLN:H	1.41	0.86
1:A:2061:THR:HG22	1:A:2063:GLY:H	1.42	0.85
1:A:4004:PHE:O	1:A:4006:THR:N	2.10	0.83
1:A:3008:LEU:O	1:A:3008:LEU:HG	1.80	0.79
1:A:4004:PHE:O	1:A:4005:GLN:HG2	1.82	0.79
1:A:2051:PRO:O	1:A:2052:ALA:HB3	1.89	0.73
1:A:2048:GLY:C	1:A:2049:LEU:HG	2.05	0.71
1:A:2052:ALA:C	1:A:2053:GLU:HG3	2.11	0.70
1:A:4006:THR:OG1	1:A:4009:GLU:HG3	1.91	0.70
1:A:2002:VAL:CG1	1:A:2004:LEU:HD21	2.23	0.69
1:A:4053:THR:HG22	1:A:4054:ASP:N	2.08	0.67
1:A:2093:GLY:HA3	1:A:4033:HIS:CE1	2.31	0.65
1:A:2030:LEU:HD13	1:A:2058:LEU:HD13	1.79	0.64
1:A:2012:GLU:HG2	1:A:2067:ILE:HG21	1.78	0.64
1:A:4005:GLN:HG3	1:A:4006:THR:HG23	1.78	0.63
1:A:2015:ARG:HB2	1:A:2065:ARG:HH22	1.64	0.63
1:A:2012:GLU:CG	1:A:2067:ILE:HG21	2.30	0.62
1:A:4004:PHE:O	1:A:4005:GLN:CG	2.47	0.62
1:A:2048:GLY:C	1:A:2049:LEU:CG	2.69	0.61
1:A:2002:VAL:HG12	1:A:2004:LEU:HD21	1.81	0.60
1:A:2061:THR:HG22	1:A:2062:ASP:N	2.16	0.59
1:A:4053:THR:HG21	1:A:4058:ASP:OD2	2.03	0.59
1:A:2029:THR:HG22	1:A:4028:VAL:HG22	1.85	0.58
1:A:4014:ALA:HA	1:A:4049:LEU:HD12	1.84	0.58
1:A:2050:GLU:OE1	1:A:2050:GLU:HA	2.01	0.58
1:A:4004:PHE:O	1:A:4005:GLN:C	2.40	0.58
1:A:4004:PHE:C	1:A:4005:GLN:HG2	2.25	0.57
1:A:4005:GLN:CG	1:A:4006:THR:N	2.48	0.57
1:A:2002:VAL:HG12	1:A:2004:LEU:CD2	2.35	0.56
1:A:3005:GLU:HB2	1:A:4050:VAL:HG22	1.87	0.56
1:A:2051:PRO:O	1:A:2052:ALA:CB	2.53	0.56
1:A:4055:GLN:HB3	1:A:4057:GLN:HG2	1.88	0.56
1:A:2015:ARG:CB	1:A:2065:ARG:HH22	2.18	0.55
1:A:4060:LYS:O	1:A:4064:LYS:HG3	2.07	0.54
1:A:2016:LEU:HD21	1:A:2065:ARG:HE	1.72	0.54
1:A:4053:THR:HG22	1:A:4055:GLN:N	2.18	0.54
1:A:2004:LEU:HD22	1:A:2008:GLN:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3006:GLN:OE1	1:A:4004:PHE:CZ	2.61	0.54
1:A:4053:THR:CG2	1:A:4054:ASP:N	2.71	0.53
1:A:4053:THR:CG2	1:A:4055:GLN:H	2.16	0.53
1:A:2016:LEU:CD2	1:A:2065:ARG:HE	2.23	0.52
1:A:4004:PHE:HB3	1:A:4009:GLU:HB2	1.90	0.52
1:A:4006:THR:OG1	1:A:4009:GLU:CG	2.58	0.51
1:A:2007:GLU:O	1:A:2011:THR:HG23	2.11	0.51
1:A:3007:LYS:HB3	1:A:4048:CYS:HB3	1.92	0.50
1:A:3004:GLY:O	1:A:4004:PHE:N	2.45	0.49
1:A:4080:ASN:O	1:A:4080:ASN:CG	2.50	0.49
1:A:2020:CYS:SG	1:A:2062:ASP:HB2	2.53	0.49
1:A:4008:GLU:O	1:A:4012:ARG:HG2	2.13	0.48
1:A:2059:ARG:HG2	1:A:2068:SER:HB3	1.93	0.48
1:A:3007:LYS:CG	1:A:3008:LEU:N	2.76	0.48
1:A:4048:CYS:O	1:A:4049:LEU:HD23	2.14	0.47
1:A:2076:VAL:O	1:A:2080:GLN:HG3	2.14	0.47
1:A:2016:LEU:HD23	1:A:2065:ARG:HH21	1.79	0.47
1:A:2061:THR:CG2	1:A:2063:GLY:H	2.22	0.47
1:A:3008:LEU:HD13	1:A:4047:VAL:HG12	1.97	0.47
1:A:2048:GLY:O	1:A:2049:LEU:HD12	2.15	0.47
1:A:2050:GLU:OE1	1:A:2051:PRO:HD2	2.16	0.45
1:A:4069:LEU:O	1:A:4073:MET:HG3	2.16	0.45
1:A:2058:LEU:O	1:A:2068:SER:HA	2.16	0.45
1:A:3006:GLN:OE1	1:A:4004:PHE:CE1	2.70	0.44
1:A:2055:LYS:HD3	1:A:2070:VAL:CG1	2.48	0.44
1:A:2027:PHE:O	1:A:2060:ALA:HA	2.17	0.43
1:A:2061:THR:CG2	1:A:2062:ASP:N	2.78	0.42
1:A:2012:GLU:HG3	1:A:2067:ILE:HG21	2.01	0.42
1:A:3004:GLY:C	1:A:4004:PHE:N	2.73	0.42
1:A:2097:ARG:HG3	1:A:2097:ARG:O	2.19	0.42
1:A:3005:GLU:O	1:A:4049:LEU:HA	2.20	0.41
1:A:2003:LEU:HA	1:A:2003:LEU:HD12	1.85	0.41

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:2018:GLN:NE2	1:A:4008:GLU:OE1[3_654]	2.06	0.14

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	163/232 (70%)	148 (91%)	9 (6%)	6 (4%)	4 5

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2052	ALA
1	A	2053	GLU
1	A	2095	LYS
1	A	2096	LYS
1	A	4005	GLN
1	A	2051	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	154/207 (74%)	142 (92%)	12 (8%)	16 28

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2021	ARG
1	A	2025	SER
1	A	2032	LYS
1	A	2049	LEU
1	A	2076	VAL

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Mol	Chain	Res	Type
1	A	2096	LYS
1	A	3005	GLU
1	A	3006	GLN
1	A	4019	LEU
1	A	4046	LEU
1	A	4063	GLU
1	A	4081	VAL

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

Mol	Chain	Res	Type
1	A	2085	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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	$\# Z > 2$
2	PO4	A	5001	-	4,4,4	0.12	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BME	A	6000	1	3,3,3	0.28	0	2,2,2	0.63	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
2	PO4	A	5001	-	-	0/0/0/0	0/0/0/0
3	BME	A	6000	1	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	171/232 (73%)	0.97	31 (18%) 2 2	15, 33, 82, 100	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2048	GLY	18.0
1	A	2047	GLU	11.1
1	A	2097	ARG	7.9
1	A	2052	ALA	6.7
1	A	4080	ASN	6.2
1	A	4079	ARG	4.5
1	A	3001	ALA	4.5
1	A	2065	ARG	4.4
1	A	4005	GLN	4.2
1	A	4004	PHE	3.9
1	A	2078	LYS	3.7
1	A	2033	TYR	3.4
1	A	3008	LEU	3.0
1	A	2034	ASP	2.9
1	A	2063	GLY	2.9
1	A	2074	LYS	2.9
1	A	2051	PRO	2.7
1	A	3007	LYS	2.7
1	A	2096	LYS	2.6
1	A	2024	GLY	2.6
1	A	2029	THR	2.6
1	A	4076	LYS	2.5
1	A	2002	VAL	2.5
1	A	4081	VAL	2.5
1	A	4027	VAL	2.5
1	A	2022	SER	2.4
1	A	4078	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	2030	LEU	2.2
1	A	2050	GLU	2.1
1	A	2053	GLU	2.1
1	A	2064	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	PO4	A	5001	5/5	0.97	0.14	-1.50	73,75,80,83	0
3	BME	A	6000	4/4	0.95	0.11	-1.52	50,50,51,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.