Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 12:57 PM EDT

PDB ID	:	3ZX7
Title	:	Complex of lysenin with phosphocholine
Authors	:	De Colibus, L.; Sonnen, A.F.P.; Morris, K.J.; Siebert, C.A.; Abrusci, P.; Plitzko, J.; Hodnik, V.; Leippe, M.; Volpi, E.; Anderluh, G.; Gilbert, R.J.C.
Deposited on	:	2011-08-08
Resolution	:	2.84 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:

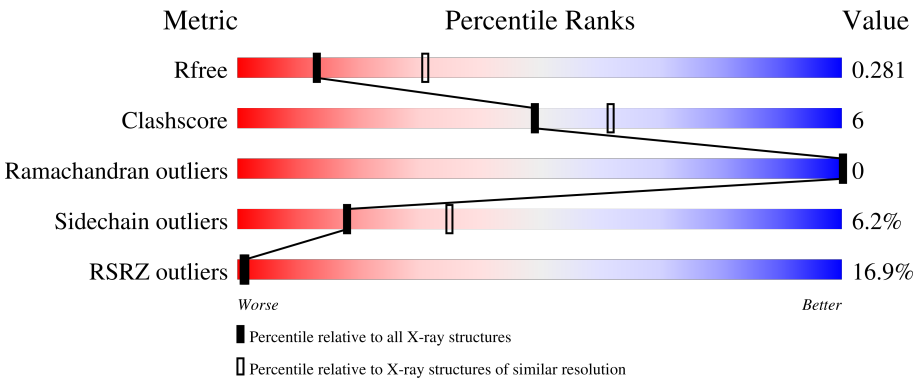
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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

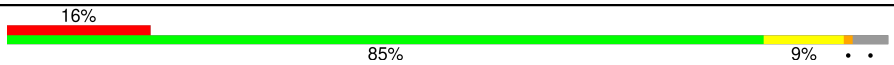
The reported resolution of this entry is 2.84 Å.

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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	309	

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
2	PO4	A	888	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PC	A	992	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2451 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.

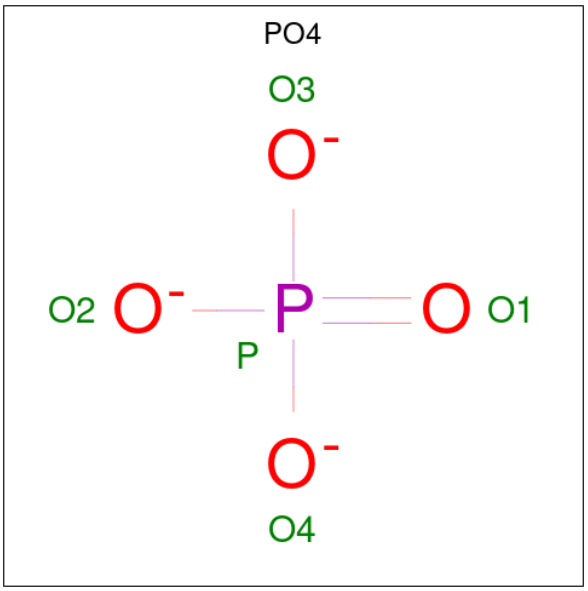
- Molecule 1 is a protein called LYSENIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	296	2355	1492	396	459	2	6	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

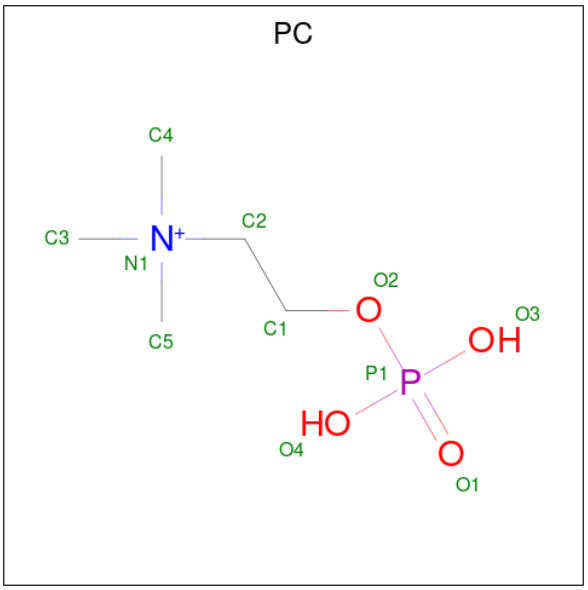
Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP O18423
A	299	VAL	-	expression tag	UNP O18423
A	300	PRO	-	expression tag	UNP O18423
A	301	ARG	-	expression tag	UNP O18423
A	302	GLY	-	expression tag	UNP O18423
A	303	SER	-	expression tag	UNP O18423
A	304	GLY	-	expression tag	UNP O18423
A	305	HIS	-	expression tag	UNP O18423
A	306	HIS	-	expression tag	UNP O18423
A	307	HIS	-	expression tag	UNP O18423
A	308	HIS	-	expression tag	UNP O18423
A	309	HIS	-	expression tag	UNP O18423
A	310	HIS	-	expression tag	UNP O18423

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is PHOSPHOCHOLINE (three-letter code: PC) (formula: $C_5H_{15}NO_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	11	5	1	4	1	0	0
			Total	C	N	O	P		
3	A	1	11	5	1	4	1	0	0
			Total	C	N	O	P		
3	A	1	11	5	1	4	1	0	0
			Total	C	N	O	P		
3	A	1	11	5	1	4	1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	3	3	3	0	0

- Molecule 5 is water.

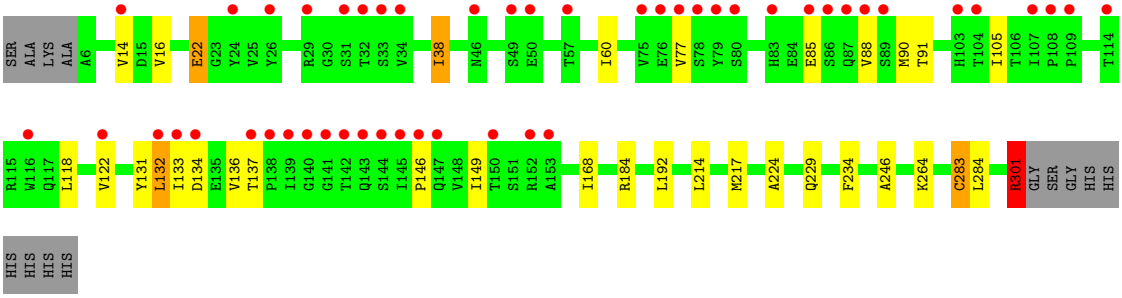
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	24	24	24	0	0

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: LYSENIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	98.11Å 98.11Å 184.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.70 – 2.84 32.11 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.6 (23.70-2.84) 100.0 (32.11-2.84)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 2.85Å)	Xtriage
Refinement program	BUSTER 2.11.1	Depositor
R, R_{free}	0.224 , 0.264 0.244 , 0.281	Depositor DCC
R_{free} test set	630 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	2451	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: NA, PO4, PC

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	0/2401	0.69	3/3245 (0.1%)

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	A	22	GLU	CA-CB-CG	7.11	129.03	113.40
1	A	22	GLU	CB-CG-CD	6.15	130.80	114.20
1	A	301	ARG	CG-CD-NE	5.82	124.02	111.80

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	2355	0	2308	26	0
2	A	25	0	0	0	0
3	A	44	0	52	14	0
4	A	3	0	0	0	0
5	A	24	0	0	1	0
All	All	2451	0	2360	28	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 6.

All (28) 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:284:LEU:HD22	3:A:992:PC:H51	1.28	1.08
1:A:284:LEU:HA	3:A:992:PC:H52	1.36	1.06
1:A:133:ILE:O	3:A:991:PC:H41	1.58	1.02
1:A:284:LEU:CD2	3:A:992:PC:H51	1.94	0.96
1:A:284:LEU:CD2	3:A:992:PC:C5	2.52	0.87
1:A:284:LEU:HD22	3:A:992:PC:C5	2.11	0.80
1:A:284:LEU:HD23	3:A:992:PC:C5	2.13	0.77
1:A:184:ARG:NH2	3:A:900:PC:H11	2.03	0.73
1:A:283:CYS:O	3:A:992:PC:O3	2.09	0.70
1:A:133:ILE:CD1	1:A:146:PRO:HG3	2.23	0.69
1:A:229:GLN:HB3	3:A:900:PC:H52	1.85	0.58
1:A:132:LEU:C	1:A:132:LEU:HD22	2.25	0.57
1:A:284:LEU:CA	3:A:992:PC:H52	2.24	0.56
1:A:77:VAL:HG11	1:A:118:LEU:HD21	1.87	0.55
1:A:38:ILE:HD11	1:A:105:ILE:HG23	1.89	0.54
1:A:88:VAL:HG11	1:A:131:TYR:CE2	2.45	0.52
1:A:88:VAL:HG11	1:A:131:TYR:CD2	2.45	0.51
1:A:301:ARG:HH11	1:A:301:ARG:HG3	1.75	0.50
1:A:184:ARG:NH1	5:A:2021:HOH:O	2.46	0.49
1:A:184:ARG:HH21	3:A:900:PC:H11	1.78	0.49
1:A:133:ILE:CD1	1:A:146:PRO:CG	2.89	0.48
1:A:16:VAL:HG11	1:A:122:VAL:HG22	1.97	0.47
1:A:133:ILE:HD11	1:A:146:PRO:CG	2.46	0.46
1:A:246:ALA:HB2	1:A:264:LYS:HE3	1.98	0.45
1:A:224:ALA:HB2	1:A:234:PHE:CE2	2.51	0.45
1:A:14:VAL:CG2	1:A:60:ILE:HG22	2.50	0.42
3:A:990:PC:H12	3:A:990:PC:H42	1.74	0.41
3:A:992:PC:H52	3:A:992:PC:H12	1.70	0.41

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	294/309 (95%)	275 (94%)	19 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	259/262 (99%)	243 (94%)	16 (6%)	18	35

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

Mol	Chain	Res	Type
1	A	22	GLU
1	A	38	ILE
1	A	85	GLU
1	A	90	MSE
1	A	91	THR
1	A	132	LEU
1	A	134	ASP
1	A	136	VAL
1	A	137	THR
1	A	149	ILE
1	A	168	ILE
1	A	192	LEU
1	A	214	LEU
1	A	217	MSE
1	A	283	CYS
1	A	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
2	PO4	A	883	-	4,4,4	2.13	1 (25%)	6,6,6	0.39	0
3	PC	A	992	-	10,10,10	1.27	0	15,15,15	1.31	1 (6%)
2	PO4	A	888	-	4,4,4	2.04	1 (25%)	6,6,6	0.48	0
2	PO4	A	884	4	4,4,4	2.12	1 (25%)	6,6,6	0.49	0
3	PC	A	990	-	10,10,10	1.01	0	15,15,15	1.30	1 (6%)
2	PO4	A	882	-	4,4,4	2.07	1 (25%)	6,6,6	0.52	0
3	PC	A	991	-	10,10,10	1.63	1 (10%)	15,15,15	1.25	1 (6%)
3	PC	A	900	-	10,10,10	1.57	1 (10%)	15,15,15	1.36	1 (6%)
2	PO4	A	881	-	4,4,4	2.02	1 (25%)	6,6,6	0.44	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
3	PC	A	900	-	-	4/8/8/8	-
3	PC	A	990	-	-	4/8/8/8	-
3	PC	A	992	-	-	4/8/8/8	-
3	PC	A	991	-	-	3/8/8/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	991	PC	P1-O1	3.76	1.62	1.50
2	A	883	PO4	P-O1	3.59	1.58	1.50
2	A	884	PO4	P-O1	3.51	1.58	1.50
3	A	900	PC	P1-O1	3.49	1.61	1.50
2	A	881	PO4	P-O1	3.39	1.58	1.50
2	A	882	PO4	P-O1	3.36	1.58	1.50
2	A	888	PO4	P-O1	3.33	1.58	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	900	PC	P1-O2-C1	-4.36	106.34	118.21
3	A	990	PC	P1-O2-C1	-4.11	107.03	118.21
3	A	992	PC	P1-O2-C1	-4.09	107.09	118.21
3	A	991	PC	P1-O2-C1	-3.73	108.06	118.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	900	PC	O2-C1-C2-N1
3	A	990	PC	C1-O2-P1-O1
3	A	990	PC	C1-O2-P1-O3
3	A	990	PC	C1-O2-P1-O4
3	A	990	PC	O2-C1-C2-N1
3	A	991	PC	C1-O2-P1-O1
3	A	991	PC	C1-O2-P1-O3
3	A	991	PC	C1-O2-P1-O4
3	A	900	PC	C1-C2-N1-C3
3	A	900	PC	C1-C2-N1-C4
3	A	900	PC	C1-C2-N1-C5
3	A	992	PC	C1-C2-N1-C4
3	A	992	PC	C1-C2-N1-C5

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Mol	Chain	Res	Type	Atoms
3	A	992	PC	C1-C2-N1-C3
3	A	992	PC	O2-C1-C2-N1

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	992	PC	9	0
3	A	990	PC	1	0
3	A	991	PC	1	0
3	A	900	PC	3	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	290/309 (93%)	0.56	49 (16%) 1 1	31, 70, 129, 157	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	SER	7.8
1	A	31	SER	6.8
1	A	87	GLN	6.2
1	A	77	VAL	6.1
1	A	143	GLN	6.1
1	A	24	TYR	5.1
1	A	139	ILE	5.0
1	A	153	ALA	4.7
1	A	145	ILE	4.6
1	A	46	ASN	4.4
1	A	147	GLN	4.1
1	A	33	SER	4.0
1	A	88	VAL	3.9
1	A	138	PRO	3.9
1	A	79	TYR	3.8
1	A	140	GLY	3.7
1	A	32	THR	3.6
1	A	146	PRO	3.3
1	A	14	VAL	3.3
1	A	109	PRO	3.3
1	A	34	VAL	3.3
1	A	144	SER	3.0
1	A	50	GLU	3.0
1	A	29	ARG	2.9
1	A	137	THR	2.8
1	A	116	TRP	2.8
1	A	80	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	108	PRO	2.8
1	A	107	ILE	2.7
1	A	150	THR	2.7
1	A	83	HIS	2.6
1	A	26	TYR	2.6
1	A	57	THR	2.6
1	A	104	THR	2.5
1	A	141	GLY	2.5
1	A	133	ILE	2.5
1	A	132	LEU	2.5
1	A	86	SER	2.5
1	A	142	THR	2.4
1	A	134	ASP	2.4
1	A	103	HIS	2.4
1	A	89	SER	2.4
1	A	49	SER	2.3
1	A	85	GLU	2.3
1	A	122	VAL	2.2
1	A	152	ARG	2.1
1	A	76	GLU	2.1
1	A	114	THR	2.0
1	A	75	VAL	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
2	PO4	A	881	5/5	0.73	0.31	156,157,158,160	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PC	A	991	11/11	0.73	0.33	111,116,118,119	0
2	PO4	A	888	5/5	0.79	0.42	66,66,68,73	5
3	PC	A	900	11/11	0.86	0.33	41,48,63,64	11
4	NA	A	904	1/1	0.86	0.09	66,66,66,66	0
4	NA	A	903	1/1	0.89	0.17	52,52,52,52	0
3	PC	A	992	11/11	0.90	0.30	44,48,55,55	11
2	PO4	A	883	5/5	0.91	0.31	79,80,84,85	5
2	PO4	A	884	5/5	0.91	0.45	92,93,96,98	0
3	PC	A	990	11/11	0.93	0.24	63,74,91,92	11
2	PO4	A	882	5/5	0.94	0.16	100,101,104,105	0
4	NA	A	905	1/1	0.98	0.14	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.