



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 6J1K / pdb_00006j1k
Title : Crystal structure of ribose-5-phosphate isomerase A from Ochrobactrum sp. CSL1
Authors : Xu, X.Q.; Mo, X.B.; Ju, X.; Shen, M.; Li, L.Z.; Yuan, A.Y.
Deposited on : 2018-12-28
Resolution : 2.82 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

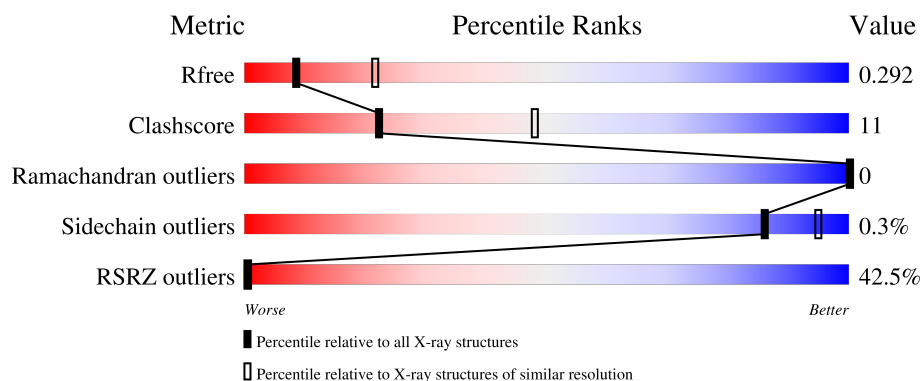
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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 $\leq 5\%$. 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	50% 73% 26% .
1	B	232	34% 80% 17% .

2 Entry composition [i](#)

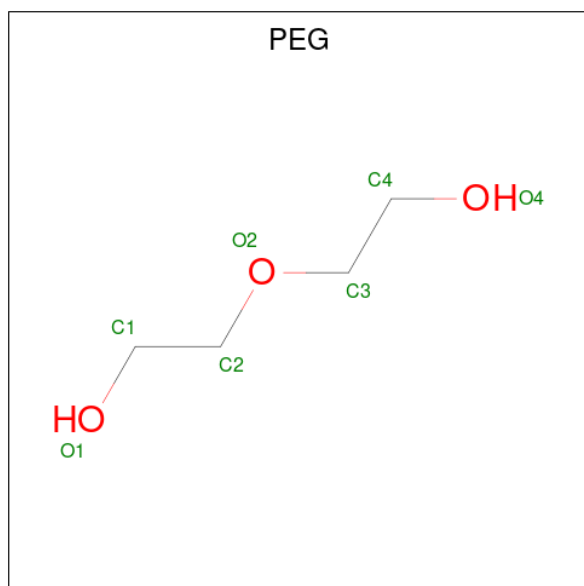
There are 3 unique types of molecules in this entry. The entry contains 3351 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribose-5-phosphate isomerase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	0	0
			1678	1057	295	320	6			
1	B	226	Total	C	N	O	S	0	0	0
			1647	1040	288	313	6			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 3 is water.

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

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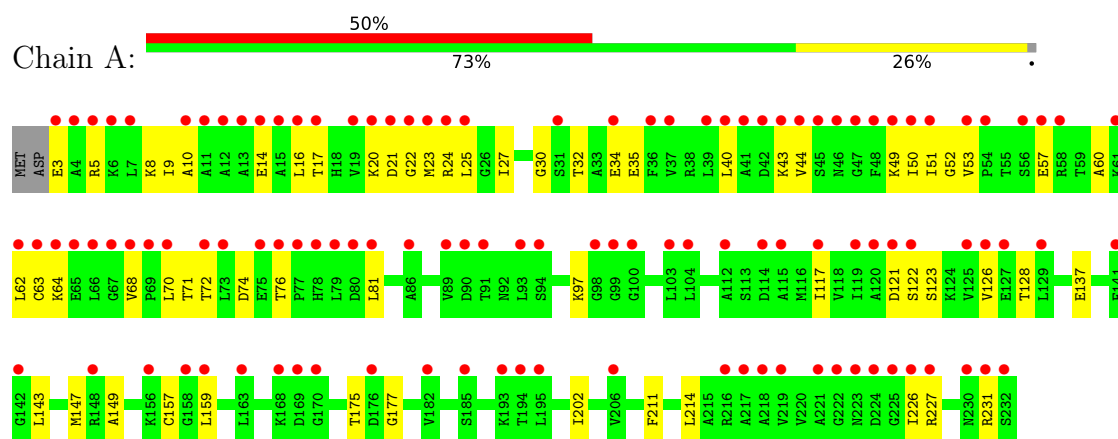
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	15	Total	O	0	0
			15	15		

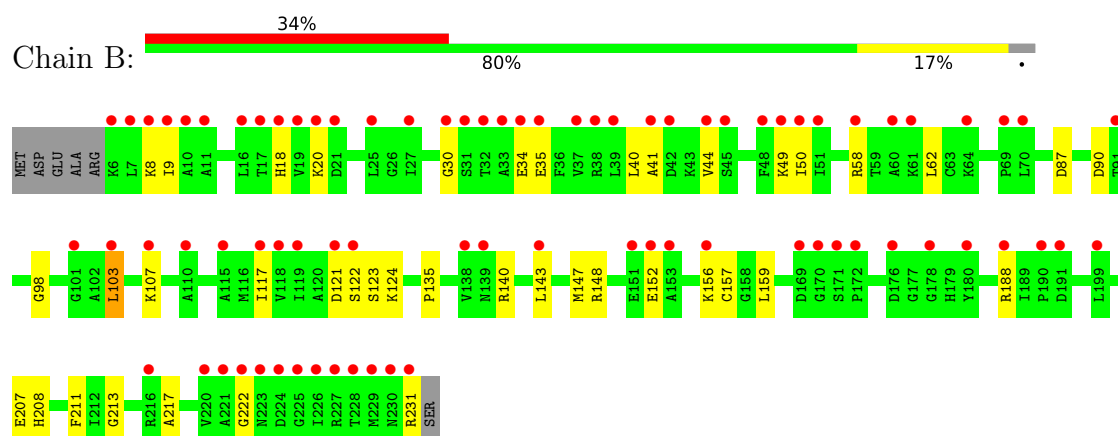
3 Residue-property plots [i](#)

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: Ribose-5-phosphate isomerase A



• Molecule 1: Ribose-5-phosphate isomerase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.82Å 169.26Å 41.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.06 – 2.82 30.06 – 2.82	Depositor EDS
% Data completeness (in resolution range)	93.6 (30.06-2.82) 95.1 (30.06-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.26 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.236 , 0.287 0.246 , 0.292	Depositor DCC
R_{free} test set	617 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	3351	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% 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: PEG

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	0.49	0/1700	0.83	4/2300 (0.2%)
1	B	0.48	0/1669	0.81	4/2259 (0.2%)
All	All	0.49	0/3369	0.82	8/4559 (0.2%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLU	CA-CB-CG	-8.28	97.55	114.10
1	A	24	ARG	CB-CG-CD	-6.79	95.69	111.30
1	B	140	ARG	CA-CB-CG	6.54	127.19	114.10
1	A	231	ARG	NE-CZ-NH1	6.06	127.56	121.50
1	B	140	ARG	NE-CZ-NH1	-5.96	115.54	121.50
1	B	103	LEU	CA-CB-CG	5.66	136.09	116.30
1	A	231	ARG	NE-CZ-NH2	-5.16	114.55	119.20
1	B	140	ARG	NE-CZ-NH2	5.10	123.79	119.20

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	1678	0	1735	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1647	0	1706	29	0
2	A	7	0	10	2	0
3	A	4	0	0	0	0
3	B	15	0	0	0	0
All	All	3351	0	3451	72	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 11.

All (72) 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:B:107:LYS:NZ	1:B:208:HIS:O	1.94	1.00
1:A:175:THR:HG22	1:A:177:GLY:H	1.42	0.82
1:A:34:GLU:OE1	1:A:62:LEU:HD22	1.80	0.81
1:A:72:THR:HG22	1:A:74:ASP:H	1.44	0.81
1:A:157:CYS:HB2	1:A:159:LEU:HD23	1.70	0.73
1:A:157:CYS:HB2	1:A:159:LEU:CD2	2.20	0.72
1:A:72:THR:HG22	1:A:74:ASP:N	2.05	0.70
1:B:213:GLY:HA2	1:B:231:ARG:HH22	1.57	0.70
1:A:9:ILE:HD13	1:A:35:GLU:HG3	1.74	0.69
1:B:207:GLU:HG3	1:B:208:HIS:H	1.58	0.69
1:A:122:SER:OG	1:A:227:ARG:NH2	2.27	0.67
1:A:40:LEU:O	1:A:44:VAL:HG23	1.94	0.67
1:A:157:CYS:O	1:A:159:LEU:HD22	1.95	0.66
1:A:8:LYS:HB3	1:A:32:THR:HG23	1.82	0.61
1:A:5:ARG:O	1:A:9:ILE:HG12	2.01	0.61
1:B:143:LEU:O	1:B:147:MET:HG2	2.03	0.59
1:A:9:ILE:CD1	1:A:35:GLU:HG3	2.32	0.59
1:A:81:LEU:HD11	1:A:117:ILE:HG13	1.85	0.58
1:A:16:LEU:HD21	1:A:43:LYS:HD3	1.85	0.58
1:A:143:LEU:O	1:A:147:MET:HG2	2.04	0.58
1:A:25:LEU:HD13	1:A:50:ILE:HD11	1.85	0.57
1:A:126:VAL:HG12	1:A:128:THR:N	2.20	0.57
1:A:137:GLU:OE2	1:A:175:THR:HG21	2.05	0.56
1:A:126:VAL:HG12	1:A:128:THR:H	1.71	0.55
1:B:30:GLY:O	1:B:34:GLU:HG3	2.07	0.54
1:A:9:ILE:HD13	1:A:35:GLU:CG	2.36	0.54
1:A:9:ILE:CD1	1:A:35:GLU:CG	2.86	0.53
1:B:157:CYS:HB2	1:B:159:LEU:HD12	1.91	0.52
1:A:60:ALA:O	1:A:64:LYS:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LYS:NZ	2:A:301:PEG:H11	2.24	0.51
1:B:107:LYS:HD3	1:B:211:PHE:CD1	2.46	0.51
1:A:20:LYS:HB2	1:A:23:MET:HE3	1.93	0.51
1:A:211:PHE:CD2	1:A:214:LEU:HD12	2.47	0.50
1:B:103:LEU:CD1	1:B:135:PRO:HB2	2.41	0.50
1:B:152:GLU:O	1:B:156:LYS:HG3	2.13	0.49
1:B:121:ASP:OD1	1:B:123:SER:HB3	2.12	0.49
1:A:22:GLY:HA2	1:A:49:LYS:HD2	1.95	0.48
1:B:117:ILE:HD13	1:B:217:ALA:HB3	1.95	0.48
1:B:9:ILE:HD13	1:B:35:GLU:CG	2.44	0.48
1:A:53:VAL:HG22	1:A:71:THR:HG23	1.96	0.47
1:A:157:CYS:C	1:A:159:LEU:HD22	2.40	0.47
1:B:103:LEU:HD21	1:B:208:HIS:C	2.40	0.47
1:B:107:LYS:HD3	1:B:211:PHE:CE1	2.50	0.47
1:A:157:CYS:CB	1:A:159:LEU:CD2	2.90	0.46
1:A:14:GLU:O	1:A:17:THR:HB	2.16	0.46
1:A:97:LYS:HZ2	2:A:301:PEG:H11	1.78	0.46
1:B:207:GLU:HG3	1:B:208:HIS:N	2.29	0.46
1:B:40:LEU:HD21	1:B:50:ILE:HG21	1.99	0.45
1:B:41:ALA:O	1:B:44:VAL:HG22	2.18	0.44
1:B:148:ARG:O	1:B:152:GLU:HG3	2.18	0.44
1:A:68:VAL:O	1:A:70:LEU:HD13	2.18	0.44
1:B:62:LEU:HD12	1:B:62:LEU:HA	1.89	0.44
1:B:58:ARG:O	1:B:58:ARG:HD2	2.17	0.44
1:A:63:CYS:HB3	1:A:70:LEU:HD11	2.01	0.43
1:A:3:GLU:OE1	1:A:3:GLU:N	2.52	0.43
1:B:18:HIS:O	1:B:20:LYS:HE2	2.18	0.43
1:B:49:LYS:HD3	1:B:49:LYS:HA	1.73	0.43
1:A:25:LEU:HD23	1:A:27:ILE:CD1	2.48	0.42
1:A:121:ASP:OD1	1:A:123:SER:OG	2.35	0.42
1:B:122:SER:OG	1:B:222:GLY:HA2	2.19	0.42
1:B:107:LYS:HG2	1:B:211:PHE:CE1	2.55	0.42
1:A:10:ALA:HB1	1:A:226:ILE:HD11	2.02	0.42
1:B:159:LEU:HD23	1:B:188:ARG:O	2.19	0.41
1:A:72:THR:O	1:A:76:THR:N	2.52	0.41
1:B:98:GLY:HA3	1:B:103:LEU:HD12	2.03	0.41
1:A:30:GLY:O	1:A:34:GLU:HG2	2.20	0.41
1:A:51:ILE:HD12	1:A:52:GLY:H	1.85	0.41
1:A:21:ASP:OD1	1:A:49:LYS:HB3	2.21	0.41
1:A:149:ALA:HB1	1:A:202:ILE:HG12	2.01	0.41
1:B:90:ASP:OD1	1:B:90:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HD13	1:B:35:GLU:CD	2.46	0.41
1:B:87:ASP:O	1:B:124:LYS:HD2	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	228/232 (98%)	224 (98%)	4 (2%)	0	100	100
1	B	224/232 (97%)	222 (99%)	2 (1%)	0	100	100
All	All	452/464 (97%)	446 (99%)	6 (1%)	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	174/176 (99%)	174 (100%)	0	100	100
1	B	171/176 (97%)	170 (99%)	1 (1%)	78	92
All	All	345/352 (98%)	344 (100%)	1 (0%)	86	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	8	LYS

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

Mol	Chain	Res	Type
1	B	46	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	PEG	A	301	-	6,6,6	0.65	0	5,5,5	0.65	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	PEG	A	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	PEG	O1-C1-C2-O2
2	A	301	PEG	O2-C3-C4-O4

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	PEG	2	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

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	230/232 (99%)	2.18	115 (50%) 0 0	18, 35, 69, 85	0
1	B	226/232 (97%)	1.79	79 (34%) 1 0	18, 30, 56, 73	0
All	All	456/464 (98%)	1.99	194 (42%) 0 0	18, 33, 65, 85	0

All (194) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	ASN	6.0
1	A	46	ASN	5.6
1	A	57	GLU	5.2
1	B	231	ARG	5.2
1	B	9	ILE	5.1
1	A	120	ALA	5.1
1	A	185	SER	5.1
1	A	232	SER	5.0
1	A	225	GLY	5.0
1	A	45	SER	4.9
1	A	12	ALA	4.8
1	A	223	ASN	4.7
1	A	67	GLY	4.6
1	A	3	GLU	4.6
1	A	66	LEU	4.5
1	A	50	ILE	4.5
1	A	49	LYS	4.4
1	A	91	THR	4.4
1	A	224	ASP	4.3
1	A	222	GLY	4.3
1	B	7	LEU	4.2
1	A	10	ALA	4.2
1	A	25	LEU	4.1
1	A	11	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	152	GLU	4.1
1	B	224	ASP	4.0
1	A	221	ALA	4.0
1	B	42	ASP	3.9
1	B	91	THR	3.9
1	A	42	ASP	3.9
1	B	50	ILE	3.9
1	A	122	SER	3.9
1	A	48	PHE	3.8
1	B	176	ASP	3.8
1	B	230	ASN	3.8
1	B	6	LYS	3.7
1	A	176	ASP	3.7
1	A	19	VAL	3.6
1	B	188	ARG	3.6
1	B	35	GLU	3.6
1	B	31	SER	3.6
1	A	86	ALA	3.5
1	A	53	VAL	3.5
1	A	56	SER	3.5
1	B	8	LYS	3.5
1	A	15	ALA	3.5
1	B	227	ARG	3.4
1	A	63	CYS	3.4
1	B	169	ASP	3.4
1	A	65	GLU	3.4
1	A	39	LEU	3.3
1	B	191	ASP	3.3
1	A	5	ARG	3.3
1	B	170	GLY	3.3
1	B	41	ALA	3.3
1	A	24	ARG	3.3
1	B	222	GLY	3.3
1	A	4	ALA	3.3
1	A	62	LEU	3.3
1	B	69	PRO	3.3
1	A	81	LEU	3.3
1	A	127	GLU	3.2
1	A	73	LEU	3.2
1	A	6	LYS	3.2
1	A	37	VAL	3.2
1	A	47	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	93	LEU	3.1
1	A	104	LEU	3.1
1	A	78	HIS	3.1
1	A	44	VAL	3.1
1	B	34	GLU	3.1
1	A	22	GLY	3.1
1	A	226	ILE	3.1
1	A	231	ARG	3.1
1	B	171	SER	3.0
1	A	89	VAL	3.0
1	A	20	LYS	3.0
1	A	51	ILE	3.0
1	A	99	GLY	3.0
1	B	216	ARG	2.9
1	B	220	VAL	2.9
1	A	100	GLY	2.9
1	B	139	ASN	2.9
1	B	156	LYS	2.9
1	B	44	VAL	2.9
1	B	58	ARG	2.8
1	A	80	ASP	2.8
1	B	25	LEU	2.8
1	B	20	LYS	2.8
1	A	75	GLU	2.8
1	A	195	LEU	2.8
1	A	206	VAL	2.8
1	B	48	PHE	2.8
1	A	159	LEU	2.8
1	A	17	THR	2.8
1	B	30	GLY	2.8
1	A	68	VAL	2.7
1	A	40	LEU	2.7
1	A	36	PHE	2.7
1	A	119	ILE	2.7
1	A	169	ASP	2.7
1	A	13	ALA	2.6
1	A	41	ALA	2.6
1	B	11	ALA	2.6
1	A	79	LEU	2.6
1	A	103	LEU	2.6
1	B	32	THR	2.6
1	B	138	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	122	SER	2.6
1	A	58	ARG	2.6
1	A	219	VAL	2.6
1	B	21	ASP	2.6
1	B	39	LEU	2.6
1	B	103	LEU	2.6
1	B	117	ILE	2.6
1	B	228	THR	2.6
1	A	21	ASP	2.6
1	A	227	ARG	2.5
1	B	190	PRO	2.5
1	B	49	LYS	2.5
1	A	7	LEU	2.5
1	A	14	GLU	2.5
1	A	217	ALA	2.5
1	A	129	LEU	2.5
1	A	168	LYS	2.5
1	A	90	ASP	2.5
1	B	17	THR	2.5
1	B	33	ALA	2.5
1	A	54	PRO	2.4
1	A	194	THR	2.4
1	A	16	LEU	2.4
1	B	229	MET	2.4
1	A	114	ASP	2.4
1	A	142	GLY	2.4
1	A	148	ARG	2.4
1	A	193	LYS	2.4
1	A	141	PHE	2.4
1	B	64	LYS	2.4
1	A	218	ALA	2.4
1	B	143	LEU	2.4
1	A	43	LYS	2.3
1	B	221	ALA	2.3
1	A	94	SER	2.3
1	B	27	ILE	2.3
1	B	180	TYR	2.3
1	A	34	GLU	2.3
1	A	72	THR	2.3
1	A	77	PRO	2.3
1	A	126	VAL	2.3
1	B	178	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	112	ALA	2.3
1	B	151	GLU	2.3
1	B	70	LEU	2.3
1	A	31	SER	2.3
1	A	76	THR	2.3
1	A	64	LYS	2.2
1	B	18	HIS	2.2
1	A	182	VAL	2.2
1	B	225	GLY	2.2
1	A	23	MET	2.2
1	B	115	ALA	2.2
1	B	45	SER	2.2
1	B	16	LEU	2.2
1	B	118	VAL	2.2
1	B	107	LYS	2.2
1	B	121	ASP	2.2
1	B	101	GLY	2.2
1	B	153	ALA	2.2
1	A	163	LEU	2.1
1	A	117	ILE	2.1
1	A	230	ASN	2.1
1	A	69	PRO	2.1
1	A	61	LYS	2.1
1	A	156	LYS	2.1
1	A	70	LEU	2.1
1	A	115	ALA	2.1
1	B	119	ILE	2.1
1	B	226	ILE	2.1
1	B	19	VAL	2.1
1	B	37	VAL	2.1
1	B	199	LEU	2.1
1	B	38	ARG	2.1
1	B	10	ALA	2.1
1	B	51	ILE	2.1
1	B	110	ALA	2.1
1	B	172	PRO	2.1
1	A	98	GLY	2.1
1	A	158	GLY	2.1
1	B	61	LYS	2.0
1	A	125	VAL	2.0
1	A	216	ARG	2.0
1	A	121	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	2.0
1	B	60	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PEG	A	301	7/7	0.66	0.23	28,30,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.