



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:36 AM GMT

PDB ID : 2R8X
Title : Crystal structure of YrbI phosphatase from Escherichia coli
Authors : Tsodikov, O.V.; Aggarwal, P.; Rubin, J.R.; Stuckey, J.A.; Woodard, R.W.; Biswas, T.
Deposited on : 2007-09-11
Resolution : 2.60 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

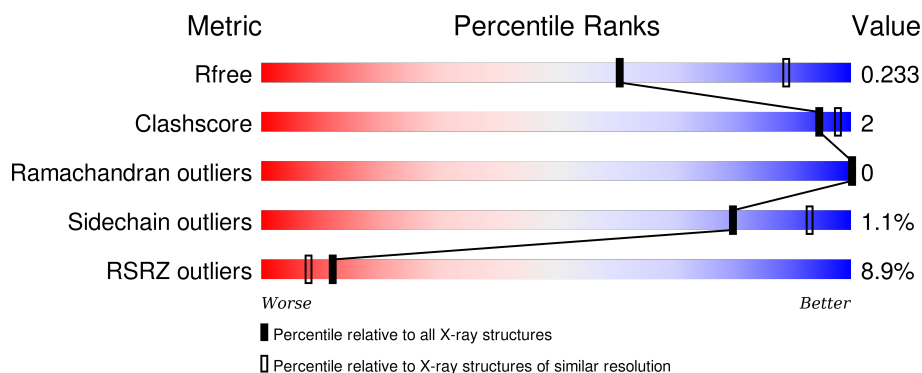
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	188	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>...</div> </div> </div>
1	B	188	<div> <div></div> <div>90%</div> <div>6% ..</div> </div>
1	C	188	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>...</div> </div> </div>
1	D	188	<div> <div>4%</div> <div> <div></div> <div>93%</div> <div>...</div> </div> </div>
1	E	188	<div> <div>%</div> <div> <div></div> <div>91%</div> <div>5% ..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	188	
1	G	188	
1	H	188	
1	I	188	
1	J	188	
1	K	188	
1	L	188	
1	M	188	
1	N	188	
1	O	188	
1	P	188	

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	CL	B	189	-	-	-	X
2	CL	G	189	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22256 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 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	B	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	C	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	D	181	Total	C	N	O	S	0	0	0
			1356	856	232	261	7			
1	E	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	F	172	Total	C	N	O	S	0	0	0
			1285	814	221	243	7			
1	G	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	H	183	Total	C	N	O	S	0	0	0
			1365	863	234	261	7			
1	I	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	J	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	K	181	Total	C	N	O	S	0	0	0
			1346	851	229	259	7			
1	L	181	Total	C	N	O	S	0	0	0
			1346	851	229	259	7			
1	M	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	N	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			
1	O	181	Total	C	N	O	S	0	0	0
			1344	849	231	257	7			
1	P	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	7			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	A	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	78	Total O 78 78	0	0
3	B	85	Total O 85 85	0	0
3	C	91	Total O 91 91	0	0
3	D	62	Total O 62 62	0	0
3	E	72	Total O 72 72	0	0
3	F	69	Total O 69 69	0	0
3	G	84	Total O 84 84	0	0
3	H	70	Total O 70 70	0	0
3	I	1	Total O 1 1	0	0
3	J	6	Total O 6 6	0	0
3	K	5	Total O 5 5	0	0
3	L	1	Total O 1 1	0	0
3	M	9	Total O 9 9	0	0
3	N	24	Total O 24 24	0	0
3	O	11	Total O 11 11	0	0

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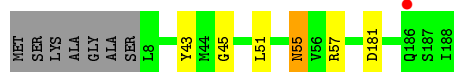
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	18	Total	O	0	0
			18	18		

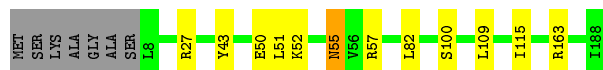
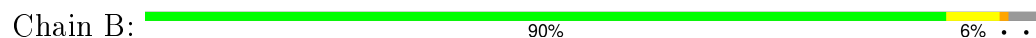
3 Residue-property plots [i](#)

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: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



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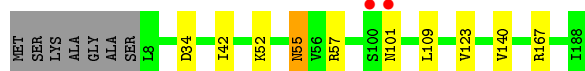
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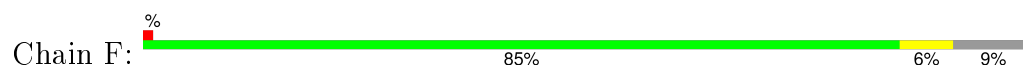
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



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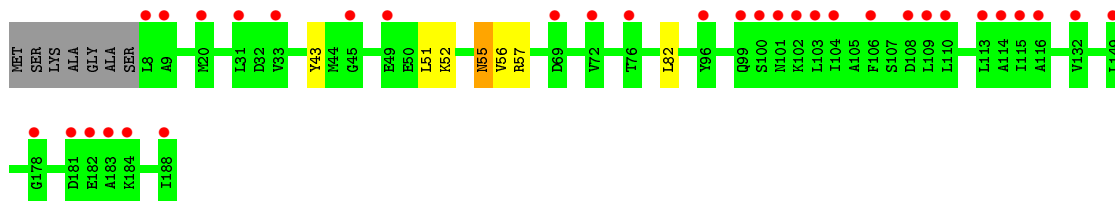
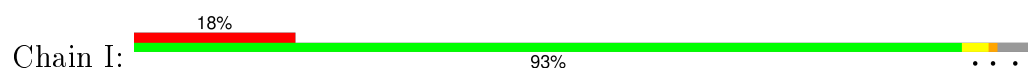
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



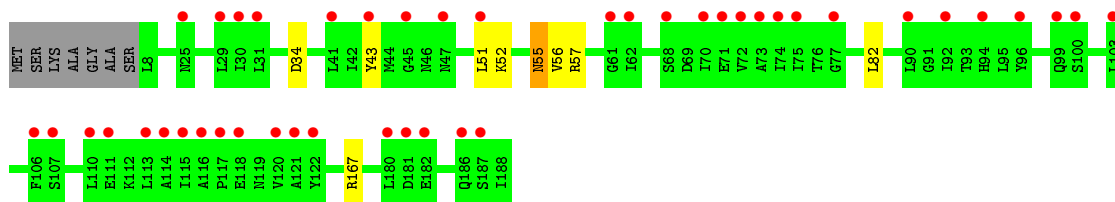
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



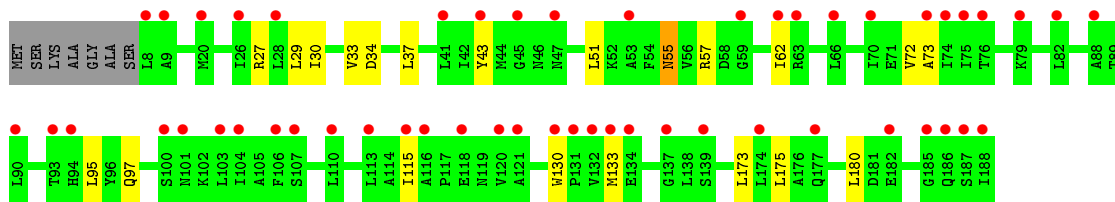
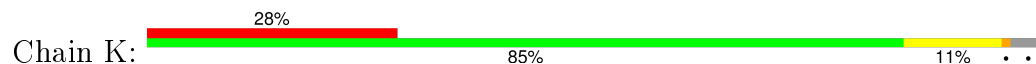
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



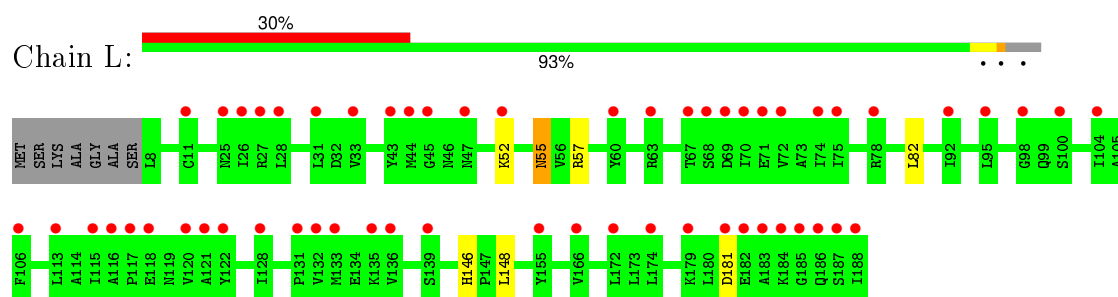
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



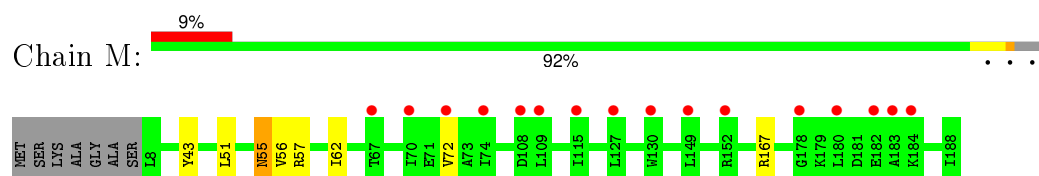
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



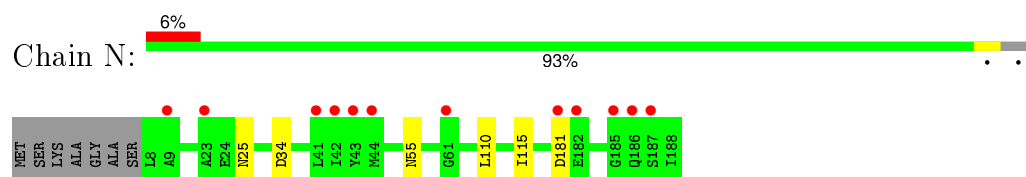
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



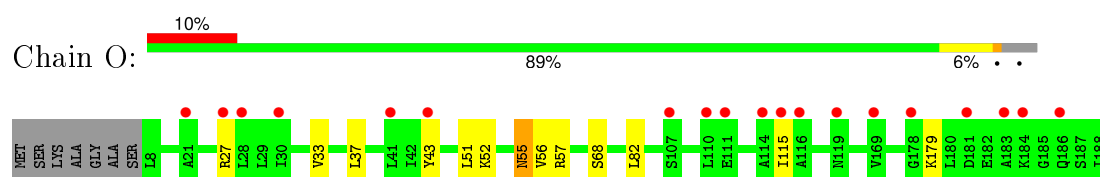
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



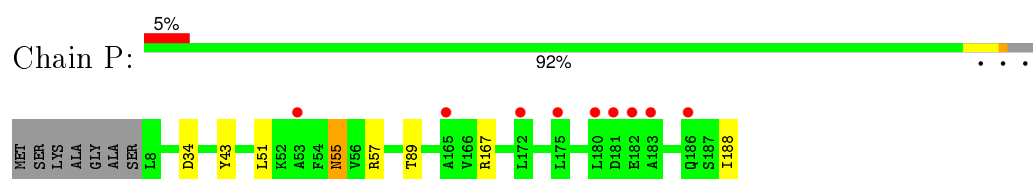
- Molecule 1: 3-deoxy-D-manno-octulosonate 8-phosphate phosphatase



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.07Å 156.96Å 114.41Å 90.00° 96.54° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 39.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-2.60) 96.1 (39.82-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.236 0.199 , 0.233	Depositor DCC
R_{free} test set	4532 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 54.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 111860 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22256	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: CL

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	0.30	0/1372	0.47	0/1858
1	B	0.32	0/1368	0.48	0/1853
1	C	0.37	0/1368	0.48	0/1853
1	D	0.30	0/1372	0.47	0/1858
1	E	0.31	0/1368	0.48	0/1853
1	F	0.31	0/1301	0.47	0/1765
1	G	0.31	0/1368	0.47	0/1853
1	H	0.31	0/1381	0.47	0/1871
1	I	0.30	0/1368	0.44	0/1853
1	J	0.30	0/1368	0.44	0/1853
1	K	0.30	0/1362	0.44	0/1846
1	L	0.30	0/1362	0.44	0/1846
1	M	0.30	0/1368	0.45	0/1853
1	N	0.30	0/1368	0.45	0/1853
1	O	0.30	0/1360	0.45	0/1844
1	P	0.30	0/1368	0.45	0/1853
All	All	0.31	0/21822	0.46	0/29565

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

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	1356	0	1385	4	0
1	B	1352	0	1381	6	0
1	C	1352	0	1381	4	0
1	D	1356	0	1385	3	0
1	E	1352	0	1381	7	0
1	F	1285	0	1315	6	0
1	G	1352	0	1381	4	0
1	H	1365	0	1397	3	0
1	I	1352	0	1381	4	0
1	J	1352	0	1381	6	0
1	K	1346	0	1370	11	0
1	L	1346	0	1370	4	0
1	M	1352	0	1381	5	0
1	N	1352	0	1381	2	0
1	O	1344	0	1366	7	0
1	P	1352	0	1381	5	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	G	1	0	0	0	0
3	A	78	0	0	0	0
3	B	85	0	0	1	0
3	C	91	0	0	0	0
3	D	62	0	0	0	0
3	E	72	0	0	1	0
3	F	69	0	0	0	0
3	G	84	0	0	0	0
3	H	70	0	0	0	0
3	I	1	0	0	0	0
3	J	6	0	0	0	0
3	K	5	0	0	0	0
3	L	1	0	0	0	0
3	M	9	0	0	0	0
3	N	24	0	0	0	0
3	O	11	0	0	0	0
3	P	18	0	0	0	0
All	All	22256	0	22017	75	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 2.

All (75) 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:G:55:ASN:HD22	1:G:57:ARG:H	1.33	0.75
1:E:34:ASP:HB3	1:F:56:VAL:HG21	1.74	0.69
1:O:55:ASN:HD22	1:O:57:ARG:H	1.43	0.65
1:B:55:ASN:HD22	1:B:57:ARG:H	1.45	0.64
1:J:56:VAL:HG21	1:K:34:ASP:HB3	1.80	0.62
1:A:55:ASN:HD22	1:A:57:ARG:H	1.49	0.61
1:K:43:TYR:HB2	1:K:51:LEU:HB2	1.81	0.60
1:E:101:ASN:O	3:E:212:HOH:O	2.16	0.60
1:J:55:ASN:HD22	1:J:57:ARG:H	1.49	0.60
1:J:52:LYS:HE2	1:J:82:LEU:HD11	1.85	0.58
1:E:55:ASN:HD22	1:E:57:ARG:H	1.52	0.56
1:C:27:ARG:HB2	1:C:115:ILE:HD11	1.88	0.55
1:K:95:LEU:HD21	1:K:97:GLN:HE21	1.71	0.55
1:J:57:ARG:HG2	1:J:167:ARG:HG2	1.88	0.55
1:C:55:ASN:HD22	1:C:57:ARG:H	1.53	0.54
1:M:57:ARG:HG2	1:M:167:ARG:HG2	1.90	0.54
1:M:55:ASN:HD22	1:M:57:ARG:H	1.54	0.54
1:K:33:VAL:HA	1:K:37:LEU:HD12	1.90	0.54
1:F:43:TYR:HB2	1:F:51:LEU:HB2	1.89	0.54
1:I:55:ASN:HD22	1:I:57:ARG:H	1.55	0.54
1:H:27:ARG:HB2	1:H:115:ILE:HD11	1.90	0.53
1:H:55:ASN:HD22	1:H:57:ARG:H	1.56	0.52
1:O:52:LYS:HE2	1:O:82:LEU:HD11	1.92	0.52
1:O:27:ARG:HB2	1:O:115:ILE:HD11	1.90	0.52
1:L:52:LYS:HE2	1:L:82:LEU:HD11	1.94	0.50
1:I:43:TYR:HB2	1:I:51:LEU:HB2	1.94	0.49
1:K:27:ARG:HB2	1:K:115:ILE:HD11	1.95	0.49
1:H:43:TYR:HB2	1:H:51:LEU:HB2	1.95	0.48
1:K:55:ASN:HD22	1:K:57:ARG:H	1.60	0.48
1:C:43:TYR:HB2	1:C:51:LEU:HB2	1.95	0.47
1:P:55:ASN:HD22	1:P:57:ARG:H	1.60	0.47
1:M:43:TYR:HB2	1:M:51:LEU:HB2	1.96	0.47
1:K:62:ILE:HG23	1:K:72:VAL:HG21	1.96	0.47
1:P:43:TYR:HB2	1:P:51:LEU:HB2	1.97	0.47
1:O:43:TYR:HB2	1:O:51:LEU:HB2	1.96	0.47
1:G:68:SER:HB3	1:G:179:LYS:HD2	1.96	0.47
1:O:56:VAL:HG21	1:P:34:ASP:HB3	1.97	0.47
1:D:55:ASN:HD22	1:D:57:ARG:H	1.62	0.46
1:I:56:VAL:HG21	1:J:34:ASP:HB3	1.98	0.46
1:O:33:VAL:HA	1:O:37:LEU:HD12	1.98	0.46
1:M:62:ILE:HG23	1:M:72:VAL:HG21	1.98	0.45
1:P:89:THR:HG22	1:P:188:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:LYS:HE2	1:B:82:LEU:HD11	1.98	0.45
1:E:42:ILE:HD12	1:E:52:LYS:HZ1	1.81	0.45
1:F:52:LYS:HE2	1:F:82:LEU:HD11	1.98	0.44
1:L:55:ASN:ND2	1:L:57:ARG:HG2	2.33	0.44
1:I:52:LYS:HE2	1:I:82:LEU:HD11	1.99	0.44
1:E:57:ARG:HG2	1:E:167:ARG:HG2	2.00	0.43
1:F:55:ASN:HD22	1:F:58:ASP:H	1.65	0.43
1:A:45:GLY:HA2	1:B:50:GLU:O	2.18	0.43
1:K:130:TRP:HA	1:K:133:MET:HB2	2.00	0.43
1:G:74:ILE:HD12	1:G:87:CYS:SG	2.59	0.43
1:F:68:SER:HB3	1:F:179:LYS:HD3	1.99	0.43
1:L:55:ASN:HD22	1:L:57:ARG:H	1.65	0.43
1:B:163:ARG:HD3	3:B:274:HOH:O	2.18	0.43
1:J:43:TYR:HB2	1:J:51:LEU:HB2	2.00	0.43
1:A:55:ASN:ND2	1:A:57:ARG:H	2.14	0.42
1:D:27:ARG:HB2	1:D:115:ILE:HD11	2.01	0.42
1:A:43:TYR:HB2	1:A:51:LEU:HB2	2.00	0.42
1:B:43:TYR:HB2	1:B:51:LEU:HB2	2.00	0.42
1:E:42:ILE:CD1	1:E:52:LYS:NZ	2.82	0.42
1:K:175:LEU:HB2	1:K:180:LEU:HD22	2.01	0.42
1:O:68:SER:HB3	1:O:179:LYS:HD3	2.02	0.42
1:K:30:ILE:HG12	1:K:73:ALA:HB3	2.02	0.42
1:E:123:VAL:HG22	1:E:140:VAL:HB	2.02	0.42
1:G:64:CYS:HB3	1:G:174:LEU:HD11	2.01	0.42
1:L:146:HIS:HE1	1:L:148:LEU:HD12	1.85	0.41
1:P:57:ARG:HG2	1:P:167:ARG:HG2	2.03	0.41
1:N:110:LEU:HD23	1:N:115:ILE:HG23	2.03	0.41
1:K:29:LEU:HD13	1:K:173:LEU:HD11	2.02	0.41
1:F:74:ILE:HD12	1:F:87:CYS:SG	2.61	0.41
1:D:52:LYS:HE2	1:D:82:LEU:HD11	2.02	0.41
1:B:27:ARG:HB2	1:B:115:ILE:HD12	2.03	0.41
1:M:56:VAL:HG21	1:N:34:ASP:HB3	2.04	0.40
1:C:27:ARG:HB2	1:C:115:ILE:CD1	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	B	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	C	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	D	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	E	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
1	F	170/188 (90%)	166 (98%)	4 (2%)	0	100	100
1	G	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	H	181/188 (96%)	177 (98%)	4 (2%)	0	100	100
1	I	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	J	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	K	179/188 (95%)	175 (98%)	4 (2%)	0	100	100
1	L	179/188 (95%)	174 (97%)	5 (3%)	0	100	100
1	M	179/188 (95%)	175 (98%)	4 (2%)	0	100	100
1	N	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	O	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	P	179/188 (95%)	175 (98%)	4 (2%)	0	100	100
All	All	2857/3008 (95%)	2804 (98%)	53 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	142/147 (97%)	140 (99%)	2 (1%)	74	90
1	B	141/147 (96%)	138 (98%)	3 (2%)	61	85
1	C	141/147 (96%)	140 (99%)	1 (1%)	88	96
1	D	142/147 (97%)	141 (99%)	1 (1%)	88	96
1	E	141/147 (96%)	139 (99%)	2 (1%)	74	90
1	F	134/147 (91%)	133 (99%)	1 (1%)	88	96
1	G	141/147 (96%)	139 (99%)	2 (1%)	74	90
1	H	142/147 (97%)	140 (99%)	2 (1%)	74	90
1	I	141/147 (96%)	140 (99%)	1 (1%)	88	96
1	J	141/147 (96%)	140 (99%)	1 (1%)	88	96
1	K	140/147 (95%)	139 (99%)	1 (1%)	88	96
1	L	140/147 (95%)	138 (99%)	2 (1%)	74	90
1	M	141/147 (96%)	140 (99%)	1 (1%)	88	96
1	N	141/147 (96%)	138 (98%)	3 (2%)	61	85
1	O	139/147 (95%)	138 (99%)	1 (1%)	88	96
1	P	141/147 (96%)	140 (99%)	1 (1%)	88	96
All	All	2248/2352 (96%)	2223 (99%)	25 (1%)	80	93

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	181	ASP
1	B	55	ASN
1	B	100	SER
1	B	109	LEU
1	C	55	ASN
1	D	55	ASN
1	E	55	ASN
1	E	109	LEU
1	F	100	SER
1	G	55	ASN
1	G	125	ASP
1	H	24	GLU
1	H	55	ASN
1	I	55	ASN
1	J	55	ASN

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Mol	Chain	Res	Type
1	K	55	ASN
1	L	55	ASN
1	L	181	ASP
1	M	55	ASN
1	N	25	ASN
1	N	55	ASN
1	N	181	ASP
1	O	55	ASN
1	P	55	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	119	ASN
1	B	47	ASN
1	B	55	ASN
1	C	47	ASN
1	C	55	ASN
1	C	94	HIS
1	C	101	ASN
1	C	119	ASN
1	D	55	ASN
1	D	119	ASN
1	E	55	ASN
1	F	55	ASN
1	F	119	ASN
1	G	47	ASN
1	G	55	ASN
1	H	55	ASN
1	I	55	ASN
1	J	55	ASN
1	K	25	ASN
1	K	55	ASN
1	L	55	ASN
1	L	119	ASN
1	M	25	ASN
1	M	47	ASN
1	M	55	ASN
1	N	25	ASN
1	N	55	ASN
1	O	55	ASN

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Mol	Chain	Res	Type
1	P	55	ASN
1	P	119	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	181/188 (96%)	0.13	1 (0%) 90 88	28, 37, 48, 60	0
1	B	181/188 (96%)	0.00	0 100 100	23, 31, 39, 47	0
1	C	181/188 (96%)	0.19	2 (1%) 82 79	25, 33, 44, 49	0
1	D	181/188 (96%)	0.32	7 (3%) 43 35	33, 43, 56, 56	0
1	E	181/188 (96%)	0.40	2 (1%) 82 79	34, 41, 57, 59	0
1	F	172/188 (91%)	0.13	1 (0%) 90 88	29, 39, 46, 48	0
1	G	181/188 (96%)	-0.02	1 (0%) 90 88	24, 31, 40, 46	0
1	H	183/188 (97%)	0.18	2 (1%) 82 79	29, 39, 51, 52	0
1	I	181/188 (96%)	1.10	33 (18%) 2 1	65, 76, 91, 91	0
1	J	181/188 (96%)	1.42	44 (24%) 1 0	63, 77, 94, 96	0
1	K	181/188 (96%)	1.42	52 (28%) 1 0	72, 89, 106, 107	0
1	L	181/188 (96%)	1.38	57 (31%) 1 0	72, 85, 98, 99	0
1	M	181/188 (96%)	0.56	16 (8%) 12 8	53, 64, 78, 79	0
1	N	181/188 (96%)	0.42	12 (6%) 22 16	50, 56, 64, 70	0
1	O	181/188 (96%)	0.67	19 (10%) 8 5	49, 63, 75, 76	0
1	P	181/188 (96%)	0.34	9 (4%) 32 26	50, 55, 66, 72	0
All	All	2889/3008 (96%)	0.54	258 (8%) 12 8	23, 52, 91, 107	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	73	ALA	9.9
1	J	110	LEU	7.8
1	L	183	ALA	7.1
1	J	114	ALA	6.6
1	I	114	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	O	183	ALA	6.4
1	L	100	SER	6.4
1	J	115	ILE	5.6
1	L	72	VAL	5.5
1	J	182	GLU	5.5
1	M	115	ILE	5.5
1	J	111	GLU	5.4
1	L	45	GLY	5.3
1	J	30	ILE	5.2
1	E	100	SER	5.2
1	K	100	SER	5.1
1	I	45	GLY	5.1
1	I	181	ASP	5.1
1	K	73	ALA	5.0
1	K	94	HIS	4.9
1	I	115	ILE	4.8
1	K	134	GLU	4.7
1	L	188	ILE	4.7
1	L	120	VAL	4.7
1	I	182	GLU	4.7
1	K	103	LEU	4.6
1	J	96	TYR	4.5
1	I	96	TYR	4.4
1	M	183	ALA	4.4
1	J	25	ASN	4.4
1	J	121	ALA	4.4
1	I	106	PHE	4.3
1	I	100	SER	4.3
1	O	110	LEU	4.3
1	J	116	ALA	4.3
1	P	183	ALA	4.3
1	K	74	ILE	4.1
1	L	116	ALA	4.1
1	J	71	GLU	4.1
1	L	68	SER	4.1
1	K	90	LEU	4.0
1	J	106	PHE	4.0
1	O	116	ALA	4.0
1	L	27	ARG	3.9
1	K	187	SER	3.9
1	J	92	ILE	3.8
1	P	181	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	L	117	PRO	3.8
1	L	121	ALA	3.8
1	K	121	ALA	3.8
1	K	188	ILE	3.7
1	L	106	PHE	3.7
1	L	182	GLU	3.7
1	N	186	GLN	3.7
1	D	25	ASN	3.7
1	L	174	LEU	3.7
1	J	94	HIS	3.7
1	L	25	ASN	3.6
1	I	99	GLN	3.6
1	K	106	PHE	3.6
1	J	29	LEU	3.6
1	J	181	ASP	3.6
1	K	115	ILE	3.5
1	K	62	ILE	3.5
1	K	186	GLN	3.4
1	O	30	ILE	3.4
1	E	101	ASN	3.4
1	K	93	THR	3.4
1	L	135	LYS	3.4
1	K	130	TRP	3.4
1	O	181	ASP	3.4
1	L	186	GLN	3.3
1	K	104	ILE	3.3
1	K	107	SER	3.3
1	J	180	LEU	3.3
1	K	182	GLU	3.3
1	K	133	MET	3.3
1	L	44	MET	3.3
1	J	77	GLY	3.2
1	P	172	LEU	3.2
1	L	185	GLY	3.2
1	J	99	GLN	3.2
1	O	119	ASN	3.2
1	I	110	LEU	3.1
1	K	110	LEU	3.1
1	L	95	LEU	3.1
1	I	72	VAL	3.1
1	I	104	ILE	3.1
1	K	131	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	L	98	GLY	3.1
1	I	183	ALA	3.1
1	K	9	ALA	3.1
1	M	182	GLU	3.1
1	N	23	ALA	3.1
1	P	180	LEU	3.1
1	K	75	ILE	3.1
1	L	184	LYS	3.0
1	C	41	LEU	3.0
1	K	43	TYR	3.0
1	O	114	ALA	3.0
1	J	41	LEU	3.0
1	I	109	LEU	3.0
1	N	181	ASP	3.0
1	J	118	GLU	3.0
1	I	178	GLY	3.0
1	L	67	THR	3.0
1	J	90	LEU	3.0
1	L	78	ARG	3.0
1	J	74	ILE	3.0
1	J	122	TYR	2.9
1	M	152	ARG	2.9
1	L	71	GLU	2.9
1	M	178	GLY	2.9
1	J	75	ILE	2.9
1	K	101	ASN	2.9
1	I	188	ILE	2.9
1	L	128	ILE	2.9
1	I	149	LEU	2.9
1	J	100	SER	2.9
1	J	113	LEU	2.9
1	I	184	LYS	2.9
1	P	186	GLN	2.9
1	I	76	THR	2.9
1	K	41	LEU	2.8
1	L	74	ILE	2.8
1	J	107	SER	2.8
1	N	182	GLU	2.8
1	O	27	ARG	2.8
1	O	21	ALA	2.8
1	K	174	LEU	2.8
1	K	59	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	139	SER	2.7
1	I	102	LYS	2.7
1	M	108	ASP	2.7
1	L	28	LEU	2.7
1	O	107	SER	2.7
1	M	109	LEU	2.7
1	L	118	GLU	2.7
1	L	43	TYR	2.7
1	K	70	ILE	2.7
1	I	113	LEU	2.6
1	N	42	ILE	2.6
1	O	169	VAL	2.6
1	A	186	GLN	2.6
1	N	41	LEU	2.6
1	J	120	VAL	2.6
1	L	104	ILE	2.6
1	M	127	LEU	2.6
1	P	175	LEU	2.6
1	K	45	GLY	2.6
1	J	187	SER	2.6
1	O	111	GLU	2.6
1	L	155	TYR	2.6
1	M	180	LEU	2.6
1	L	70	ILE	2.6
1	F	178	GLY	2.5
1	L	172	LEU	2.5
1	L	31	LEU	2.5
1	J	70	ILE	2.5
1	K	116	ALA	2.5
1	K	120	VAL	2.5
1	L	92	ILE	2.5
1	K	185	GLY	2.5
1	I	132	VAL	2.5
1	L	122	TYR	2.5
1	N	43	TYR	2.5
1	P	182	GLU	2.5
1	K	66	LEU	2.5
1	L	166	VAL	2.5
1	I	108	ASP	2.5
1	J	47	ASN	2.5
1	D	24	GLU	2.5
1	I	20	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	51	LEU	2.4
1	K	63	ARG	2.4
1	J	68	SER	2.4
1	N	44	MET	2.4
1	K	79	LYS	2.4
1	J	62	ILE	2.4
1	K	26	ILE	2.4
1	N	187	SER	2.4
1	L	113	LEU	2.4
1	L	132	VAL	2.4
1	N	9	ALA	2.4
1	K	137	GLY	2.4
1	L	60	TYR	2.4
1	L	133	MET	2.4
1	J	43	TYR	2.4
1	K	132	VAL	2.4
1	G	41	LEU	2.3
1	O	43	TYR	2.3
1	L	33	VAL	2.3
1	L	69	ASP	2.3
1	O	186	GLN	2.3
1	K	139	SER	2.3
1	L	187	SER	2.3
1	M	70	ILE	2.3
1	J	31	LEU	2.3
1	J	117	PRO	2.3
1	H	7	SER	2.3
1	K	20	MET	2.3
1	O	115	ILE	2.3
1	I	116	ALA	2.3
1	L	63	ARG	2.3
1	K	76	THR	2.3
1	O	178	GLY	2.3
1	N	61	GLY	2.2
1	I	69	ASP	2.2
1	K	53	ALA	2.2
1	L	136	VAL	2.2
1	J	61	GLY	2.2
1	I	31	LEU	2.2
1	I	49	GLU	2.2
1	M	184	LYS	2.2
1	C	181	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	28	LEU	2.2
1	D	182	GLU	2.2
1	I	8	LEU	2.2
1	I	103	LEU	2.2
1	M	130	TRP	2.2
1	K	177	GLN	2.2
1	I	33	VAL	2.2
1	K	118	GLU	2.2
1	L	52	LYS	2.1
1	L	47	ASN	2.1
1	M	72	VAL	2.1
1	L	131	PRO	2.1
1	I	9	ALA	2.1
1	M	67	THR	2.1
1	I	101	ASN	2.1
1	O	28	LEU	2.1
1	L	75	ILE	2.1
1	L	11	CYS	2.1
1	L	179	LYS	2.1
1	D	181	ASP	2.1
1	P	165	ALA	2.1
1	D	161	GLY	2.1
1	O	41	LEU	2.1
1	O	184	LYS	2.1
1	L	115	ILE	2.1
1	M	74	ILE	2.1
1	H	110	LEU	2.1
1	K	82	LEU	2.1
1	L	181	ASP	2.1
1	J	45	GLY	2.1
1	J	103	LEU	2.0
1	K	113	LEU	2.0
1	L	26	ILE	2.0
1	K	8	LEU	2.0
1	D	18	ASP	2.0
1	N	185	GLY	2.0
1	J	186	GLN	2.0
1	D	41	LEU	2.0
1	K	47	ASN	2.0
1	K	88	ALA	2.0
1	M	149	LEU	2.0
1	P	53	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	72	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 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	CL	G	189	1/1	0.90	0.27	3.55	82,82,82,82	0
2	CL	B	189	1/1	0.97	0.22	3.03	73,73,73,73	0
2	CL	C	189	1/1	0.97	0.20	0.08	77,77,77,77	0
2	CL	A	189	1/1	0.91	0.12	-2.19	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.