



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 AM GMT

PDB ID : 2R8Y
Title : Crystal structure of YrbI phosphatase from Escherichia coli in a complex with Ca
Authors : Tsodikov, O.V.; Aggarwal, P.; Rubin, J.R.; Stuckey, J.A.; Woodard, R.W.; Biswas, T.
Deposited on : 2007-09-11
Resolution : 1.85 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

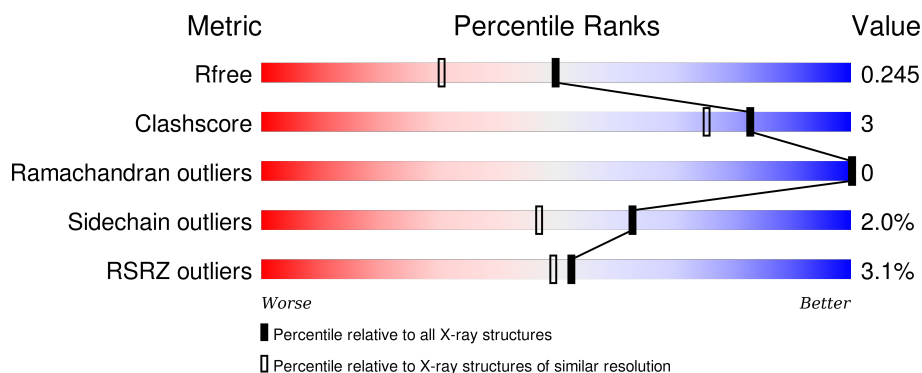
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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>90%</div> <div>5% . .</div> </div>
1	B	188	<div> <div>89%</div> <div>5% . .</div> </div>
1	C	188	<div> <div>92%</div> <div>. . .</div> </div>
1	D	188	<div> <div>2%</div> <div>95%</div> <div>. . .</div> </div>
1	E	188	<div> <div>2%</div> <div>84%</div> <div>11% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	188	<div><div>%</div><div><div></div><div>82%</div><div>9%</div><div>9%</div></div></div>
1	G	188	<div><div></div><div>90%</div><div>6%</div><div></div></div>
1	H	188	<div><div>%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	I	188	<div><div>4%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	J	188	<div><div>7%</div><div><div></div><div>92%</div><div></div><div></div></div></div>
1	K	188	<div><div>7%</div><div><div></div><div>87%</div><div>9%</div><div></div></div></div>
1	L	188	<div><div>9%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	M	188	<div><div>2%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	N	188	<div><div>2%</div><div><div></div><div>92%</div><div></div><div></div></div></div>
1	O	188	<div><div>7%</div><div><div></div><div>93%</div><div></div><div></div></div></div>
1	P	188	<div><div>3%</div><div><div></div><div>89%</div><div>7%</div><div></div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22566 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 YrbI from Escherichia coli.

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
			1352	854	232	259	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	181	Total	C	N	O	S	0	0	0
			1352	854	232	259	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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	P	1	Total Ca 1 1	0	0
2	G	1	Total Ca 1 1	0	0
2	J	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	N	1	Total Ca 1 1	0	0
2	O	1	Total Ca 1 1	0	0
2	L	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0
2	M	1	Total Ca 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	P	1	Total Cl 1 1	0	0
3	G	1	Total Cl 1 1	0	0
3	J	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total 1	Cl 1	0	0
3	K	1	Total 1	Cl 1	0	0
3	E	1	Total 1	Cl 1	0	0
3	H	1	Total 1	Cl 1	0	0
3	B	1	Total 1	Cl 1	0	0
3	I	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0
3	N	1	Total 1	Cl 1	0	0
3	O	1	Total 1	Cl 1	0	0
3	L	1	Total 1	Cl 1	0	0
3	F	1	Total 1	Cl 1	0	0
3	M	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total 95	O 95	0	0
4	B	105	Total 105	O 105	0	0
4	C	111	Total 111	O 111	0	0
4	D	75	Total 75	O 75	0	0
4	E	106	Total 106	O 106	0	0
4	F	93	Total 93	O 93	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	106	Total 106	O 106	0	0
4	H	90	Total 90	O 90	0	0
4	I	28	Total 28	O 28	0	0
4	J	32	Total 32	O 32	0	0
4	K	10	Total 10	O 10	0	0
4	L	10	Total 10	O 10	0	0
4	M	23	Total 23	O 23	0	0
4	N	37	Total 37	O 37	0	0
4	O	29	Total 29	O 29	0	0
4	P	35	Total 35	O 35	0	0

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: YrbI from Escherichia coli

Chain A:  90% 5% . .



- Molecule 1: YrbI from Escherichia coli

Chain B:  89% 5% . .



- Molecule 1: YrbI from Escherichia coli

Chain C:  92% . . .




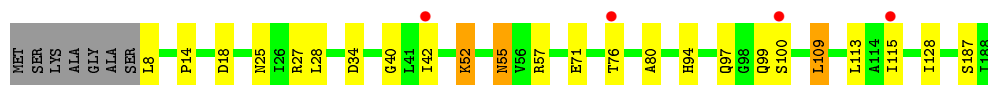
- Molecule 1: YrbI from Escherichia coli

Chain D:  2% 95% . .




- Molecule 1: YrbI from Escherichia coli

Chain E:  2% 84% 11% . .



- Molecule 1: YrbI from Escherichia coli

Chain F:  % 82% 9% 9%



- Molecule 1: YrbI from Escherichia coli

Chain G: 90% 6% . .



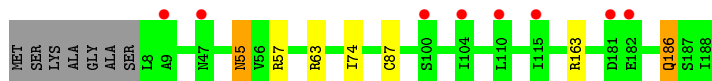
- Molecule 1: YrbI from Escherichia coli

Chain H: 93% . . .



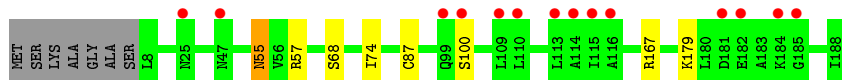
- Molecule 1: YrbI from Escherichia coli

Chain I: 93% . . .



- Molecule 1: YrbI from Escherichia coli

Chain J: 92% . . .



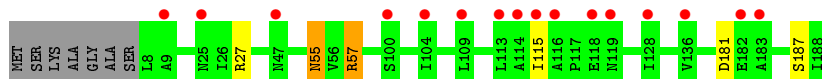
- Molecule 1: YrbI from Escherichia coli

Chain K: 87% 9% . .



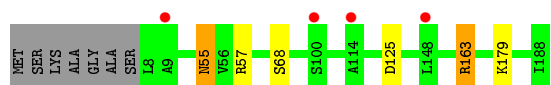
- Molecule 1: YrbI from Escherichia coli

Chain L: 93% . . .

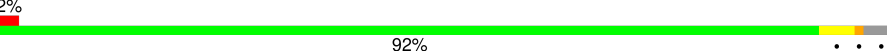


- Molecule 1: YrbI from Escherichia coli

Chain M:  2% 93% ..

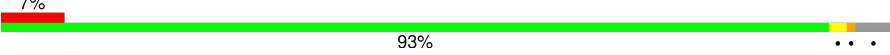


• Molecule 1: YrbI from Escherichia coli

Chain N:  2% 92% ..




• Molecule 1: YrbI from Escherichia coli

Chain O:  7% 93% ..



• Molecule 1: YrbI from Escherichia coli

Chain P:  3% 89% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.58Å 156.95Å 113.99Å 90.00° 96.72° 90.00°	Depositor
Resolution (Å)	36.61 – 1.85 37.07 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.2 (36.61-1.85) 96.2 (37.07-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.213 , 0.244 0.213 , 0.245	Depositor DCC
R_{free} test set	12231 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 243323 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22566	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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: CA, 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	0.49	0/1372	0.60	0/1858
1	B	0.53	0/1368	0.62	0/1853
1	C	0.51	0/1368	0.57	0/1853
1	D	0.48	0/1368	0.57	0/1853
1	E	0.54	0/1368	0.60	0/1853
1	F	0.50	0/1301	0.59	0/1765
1	G	0.53	0/1368	0.60	0/1853
1	H	0.51	0/1368	0.59	0/1853
1	I	0.39	0/1368	0.51	0/1853
1	J	0.38	0/1368	0.52	0/1853
1	K	0.36	0/1362	0.51	0/1846
1	L	0.37	0/1362	0.50	0/1846
1	M	0.38	0/1368	0.51	0/1853
1	N	0.40	0/1368	0.50	0/1853
1	O	0.38	0/1360	0.52	0/1844
1	P	0.39	0/1368	0.53	0/1853
All	All	0.45	0/21805	0.55	0/29542

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	10	0
1	B	1352	0	1381	13	0
1	C	1352	0	1381	7	0
1	D	1352	0	1381	3	0
1	E	1352	0	1381	23	0
1	F	1285	0	1315	20	0
1	G	1352	0	1381	14	0
1	H	1352	0	1381	5	0
1	I	1352	0	1381	4	0
1	J	1352	0	1381	5	0
1	K	1346	0	1370	9	0
1	L	1346	0	1370	4	0
1	M	1352	0	1381	4	0
1	N	1352	0	1381	4	0
1	O	1344	0	1366	4	0
1	P	1352	0	1381	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
4	A	95	0	0	6	0
4	B	105	0	0	6	0
4	C	111	0	0	3	0
4	D	75	0	0	1	0
4	E	106	0	0	7	0
4	F	93	0	0	4	0
4	G	106	0	0	7	0
4	H	90	0	0	1	0
4	I	28	0	0	1	0
4	J	32	0	0	0	0
4	K	10	0	0	0	0
4	L	10	0	0	0	0
4	M	23	0	0	0	0
4	N	37	0	0	0	0
4	O	29	0	0	0	0
4	P	35	0	0	2	0
All	All	22566	0	21997	136	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 3.

All (136) 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:F:56:VAL:HB	4:F:387:HOH:O	1.31	1.22
1:I:163:ARG:HG2	4:I:858:HOH:O	1.76	0.85
1:C:99:GLN:HG2	4:C:359:HOH:O	1.78	0.83
1:B:99:GLN:HG3	4:B:326:HOH:O	1.79	0.82
1:E:42:ILE:HD12	1:E:52:LYS:HZ3	1.48	0.78
1:E:42:ILE:HD12	1:E:52:LYS:NZ	2.01	0.76
1:B:55:ASN:HD22	1:B:57:ARG:H	1.32	0.75
1:E:34:ASP:HB3	1:F:56:VAL:HG21	1.69	0.75
1:E:76:THR:HG21	1:E:97:GLN:OE1	1.88	0.73
1:C:55:ASN:HD22	1:C:57:ARG:H	1.38	0.71
1:P:55:ASN:HD22	1:P:57:ARG:H	1.37	0.70
1:G:99:GLN:HG3	4:G:327:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:ASN:HD22	1:G:57:ARG:H	1.38	0.69
1:C:163:ARG:NH2	4:C:382:HOH:O	2.27	0.68
1:E:40:GLY:O	1:F:56:VAL:HG22	1.95	0.67
1:A:55:ASN:HD22	1:A:57:ARG:H	1.42	0.67
1:P:99:GLN:HG3	4:P:880:HOH:O	1.95	0.66
1:N:55:ASN:HD22	1:N:57:ARG:H	1.43	0.66
1:E:42:ILE:CD1	1:E:52:LYS:NZ	2.59	0.65
1:D:55:ASN:HD22	1:D:57:ARG:H	1.44	0.65
1:O:27:ARG:HB2	1:O:115:ILE:HD11	1.78	0.65
1:J:57:ARG:HG2	1:J:167:ARG:HG2	1.79	0.65
1:F:99:GLN:CG	4:F:363:HOH:O	2.46	0.64
1:K:55:ASN:HD22	1:K:57:ARG:H	1.44	0.64
1:E:55:ASN:HD22	1:E:57:ARG:H	1.45	0.63
1:A:99:GLN:NE2	4:A:388:HOH:O	2.32	0.61
1:B:94:HIS:HD2	4:B:364:HOH:O	1.83	0.61
1:L:55:ASN:ND2	1:L:57:ARG:H	1.98	0.61
1:H:55:ASN:HD22	1:H:57:ARG:H	1.48	0.60
1:L:55:ASN:HD22	1:L:57:ARG:H	1.49	0.60
1:I:55:ASN:HD22	1:I:57:ARG:H	1.48	0.59
1:A:99:GLN:HG2	4:A:383:HOH:O	2.03	0.58
4:E:310:HOH:O	1:F:56:VAL:CG2	2.52	0.57
1:A:99:GLN:CG	4:A:383:HOH:O	2.52	0.57
1:F:68:SER:HB3	1:F:179:LYS:HD3	1.85	0.57
1:F:99:GLN:HG2	4:F:363:HOH:O	2.04	0.57
1:P:27:ARG:HB2	1:P:115:ILE:CD1	2.34	0.57
4:E:307:HOH:O	1:F:56:VAL:CG2	2.53	0.57
1:G:55:ASN:ND2	1:G:57:ARG:H	2.02	0.57
1:M:55:ASN:HD22	1:M:57:ARG:H	1.51	0.57
1:P:110:LEU:HD22	1:P:115:ILE:HG23	1.86	0.57
1:G:179:LYS:HD3	4:G:381:HOH:O	2.05	0.56
1:A:94:HIS:HD2	4:A:378:HOH:O	1.87	0.56
1:C:55:ASN:ND2	1:C:57:ARG:H	2.04	0.55
1:F:20:MET:O	1:F:24:GLU:HG3	2.06	0.55
1:E:42:ILE:CD1	1:E:52:LYS:HZ2	2.19	0.55
1:B:55:ASN:ND2	1:B:57:ARG:H	2.01	0.55
1:P:52:LYS:HE2	1:P:82:LEU:HD11	1.89	0.55
1:B:110:LEU:HD22	1:B:115:ILE:HG23	1.88	0.55
1:F:27:ARG:HB2	1:F:115:ILE:CD1	2.38	0.54
4:E:310:HOH:O	1:F:56:VAL:HG23	2.07	0.54
1:E:99:GLN:HG3	4:E:332:HOH:O	2.06	0.54
1:F:119:ASN:ND2	4:F:371:HOH:O	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:307:HOH:O	1:F:56:VAL:HG22	2.09	0.53
1:M:163:ARG:HE	1:M:163:ARG:HA	1.74	0.52
1:F:74:ILE:HD12	1:F:87:CYS:SG	2.50	0.52
1:K:52:LYS:HE2	1:K:82:LEU:HD11	1.90	0.52
1:B:57:ARG:HG3	4:B:394:HOH:O	2.08	0.52
1:E:27:ARG:HB2	1:E:115:ILE:HD12	1.91	0.51
1:J:55:ASN:HD22	1:J:57:ARG:H	1.58	0.51
1:G:68:SER:HB3	1:G:179:LYS:HD2	1.91	0.51
1:F:28:LEU:HD21	1:F:109:LEU:HD13	1.93	0.50
1:G:94:HIS:HD2	4:G:325:HOH:O	1.93	0.50
1:C:99:GLN:CG	4:C:359:HOH:O	2.47	0.49
1:N:55:ASN:ND2	1:N:57:ARG:H	2.07	0.49
1:E:42:ILE:HG12	1:F:56:VAL:CG1	2.43	0.48
1:C:8:LEU:O	1:C:14:PRO:HA	2.13	0.48
1:E:128:ILE:O	1:E:128:ILE:HG13	2.13	0.48
1:K:68:SER:HB3	1:K:179:LYS:HD3	1.95	0.48
1:O:55:ASN:HD22	1:O:57:ARG:H	1.62	0.48
1:P:55:ASN:ND2	1:P:57:ARG:H	2.09	0.47
1:J:55:ASN:ND2	1:J:57:ARG:H	2.10	0.47
1:I:63:ARG:HE	1:I:186:GLN:HE22	1.63	0.47
1:N:116:ALA:H	1:N:119:ASN:HD22	1.62	0.47
1:L:55:ASN:HD22	1:L:57:ARG:N	2.12	0.47
1:K:110:LEU:HD22	1:K:115:ILE:HG23	1.96	0.47
1:F:55:ASN:HD22	1:F:58:ASP:H	1.63	0.47
1:H:55:ASN:ND2	1:H:57:ARG:H	2.12	0.47
1:D:94:HIS:HD2	4:D:356:HOH:O	1.98	0.47
1:N:115:ILE:HG12	1:N:119:ASN:HB2	1.97	0.47
1:E:80:ALA:H	1:E:97:GLN:HE22	1.61	0.47
1:G:99:GLN:CG	4:G:327:HOH:O	2.59	0.47
1:B:27:ARG:HB2	1:B:115:ILE:HD12	1.97	0.47
1:E:76:THR:HG22	1:E:97:GLN:HA	1.96	0.46
1:G:99:GLN:NE2	4:G:327:HOH:O	2.14	0.46
1:P:27:ARG:HB2	1:P:115:ILE:HD12	1.97	0.46
1:E:28:LEU:HD21	1:E:109:LEU:HD13	1.98	0.46
1:E:42:ILE:HD11	1:E:52:LYS:HZ2	1.81	0.45
1:P:27:ARG:HB2	1:P:115:ILE:HD11	1.98	0.45
1:F:27:ARG:HB2	1:F:115:ILE:HD11	1.98	0.45
1:O:101:ASN:HB3	1:O:104:ILE:HD12	1.98	0.45
1:B:71:GLU:HG3	4:B:397:HOH:O	2.17	0.44
1:H:27:ARG:HB2	1:H:115:ILE:CD1	2.47	0.44
1:M:55:ASN:ND2	1:M:57:ARG:H	2.13	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:89:THR:HG22	1:K:188:ILE:HD12	1.98	0.44
1:E:8:LEU:O	1:E:14:PRO:HA	2.18	0.44
1:J:74:ILE:HD12	1:J:87:CYS:SG	2.57	0.44
1:P:94:HIS:HD2	4:P:599:HOH:O	2.00	0.44
1:G:94:HIS:HE1	4:G:395:HOH:O	1.99	0.44
1:E:109:LEU:HD22	1:E:113:LEU:HD12	1.99	0.44
1:E:18:ASP:HB2	4:E:375:HOH:O	2.17	0.44
1:E:55:ASN:ND2	1:E:57:ARG:H	2.11	0.44
1:F:24:GLU:HG2	1:F:176:ALA:HB1	2.00	0.44
1:B:94:HIS:HE1	4:B:379:HOH:O	2.00	0.44
1:H:27:ARG:HB2	1:H:115:ILE:HD12	1.99	0.43
1:B:96:TYR:CE1	1:B:109:LEU:HG	2.54	0.43
1:K:130:TRP:HA	1:K:133:MET:HB2	2.01	0.43
1:A:55:ASN:ND2	1:A:57:ARG:H	2.12	0.43
4:E:307:HOH:O	1:F:56:VAL:HG23	2.16	0.43
1:B:45:GLY:HA2	1:C:50:GLU:O	2.19	0.43
1:H:94:HIS:HD2	4:H:363:HOH:O	2.01	0.43
1:D:55:ASN:ND2	1:D:57:ARG:H	2.12	0.42
1:P:64:CYS:HB3	1:P:174:LEU:HD11	2.00	0.42
1:A:99:GLN:OE1	4:A:391:HOH:O	2.22	0.42
1:K:64:CYS:HB3	1:K:174:LEU:HD11	2.01	0.42
1:B:163:ARG:HD3	4:B:407:HOH:O	2.18	0.42
1:G:55:ASN:HD22	1:G:55:ASN:C	2.23	0.42
1:E:76:THR:HG22	1:E:97:GLN:HG2	2.02	0.42
1:M:68:SER:HB3	1:M:179:LYS:HD3	2.02	0.42
1:K:73:ALA:CB	1:K:109:LEU:HD11	2.50	0.41
1:O:57:ARG:HB2	1:O:57:ARG:HE	1.56	0.41
1:B:96:TYR:HE1	1:B:109:LEU:HG	1.85	0.41
1:A:68:SER:HB3	1:A:179:LYS:HD3	2.02	0.41
1:A:74:ILE:HD12	1:A:87:CYS:SG	2.60	0.41
1:J:68:SER:HB3	1:J:179:LYS:HD3	2.01	0.41
1:G:27:ARG:HB2	1:G:115:ILE:HD12	2.02	0.41
1:E:80:ALA:H	1:E:97:GLN:NE2	2.18	0.41
1:P:57:ARG:HG2	1:P:167:ARG:HG2	2.01	0.41
1:G:68:SER:O	1:G:179:LYS:NZ	2.53	0.41
1:I:74:ILE:HD12	1:I:87:CYS:SG	2.61	0.41
1:G:73:ALA:CB	1:G:109:LEU:HD11	2.50	0.41
1:L:27:ARG:HB2	1:L:115:ILE:HD11	2.02	0.41
1:K:28:LEU:HD21	1:K:109:LEU:HD13	2.03	0.40
1:E:71:GLU:OE1	1:E:94:HIS:HE1	2.04	0.40
1:A:100:SER:HA	4:A:393:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:ARG:NH1	4:G:367:HOH:O	2.53	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	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	B	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	C	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	D	179/188 (95%)	175 (98%)	4 (2%)	0	100	100
1	E	179/188 (95%)	176 (98%)	3 (2%)	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	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	I	179/188 (95%)	175 (98%)	4 (2%)	0	100	100
1	J	179/188 (95%)	175 (98%)	4 (2%)	0	100	100
1	K	179/188 (95%)	173 (97%)	6 (3%)	0	100	100
1	L	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	M	179/188 (95%)	176 (98%)	3 (2%)	0	100	100
1	N	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
1	O	179/188 (95%)	178 (99%)	1 (1%)	0	100	100
1	P	179/188 (95%)	177 (99%)	2 (1%)	0	100	100
All	All	2855/3008 (95%)	2807 (98%)	48 (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%)	139 (98%)	3 (2%)	61	45
1	B	141/147 (96%)	137 (97%)	4 (3%)	51	33
1	C	141/147 (96%)	138 (98%)	3 (2%)	61	45
1	D	141/147 (96%)	139 (99%)	2 (1%)	74	63
1	E	141/147 (96%)	135 (96%)	6 (4%)	35	16
1	F	134/147 (91%)	132 (98%)	2 (2%)	72	60
1	G	141/147 (96%)	139 (99%)	2 (1%)	74	63
1	H	141/147 (96%)	139 (99%)	2 (1%)	74	63
1	I	141/147 (96%)	139 (99%)	2 (1%)	74	63
1	J	141/147 (96%)	139 (99%)	2 (1%)	74	63
1	K	140/147 (95%)	138 (99%)	2 (1%)	74	63
1	L	140/147 (95%)	136 (97%)	4 (3%)	50	31
1	M	141/147 (96%)	138 (98%)	3 (2%)	61	45
1	N	141/147 (96%)	137 (97%)	4 (3%)	51	33
1	O	139/147 (95%)	137 (99%)	2 (1%)	74	63
1	P	141/147 (96%)	138 (98%)	3 (2%)	61	45
All	All	2246/2352 (96%)	2200 (98%)	46 (2%)	63	47

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	55	ASN
1	A	181	ASP
1	B	55	ASN
1	B	71	GLU
1	B	109	LEU
1	B	187	SER
1	C	55	ASN

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Mol	Chain	Res	Type
1	C	163	ARG
1	C	187	SER
1	D	55	ASN
1	D	57	ARG
1	E	25	ASN
1	E	52	LYS
1	E	55	ASN
1	E	100	SER
1	E	109	LEU
1	E	187	SER
1	F	109	LEU
1	F	125	ASP
1	G	55	ASN
1	G	71	GLU
1	H	25	ASN
1	H	55	ASN
1	I	55	ASN
1	I	186	GLN
1	J	55	ASN
1	J	100	SER
1	K	55	ASN
1	K	187	SER
1	L	55	ASN
1	L	57	ARG
1	L	181	ASP
1	L	187	SER
1	M	55	ASN
1	M	125	ASP
1	M	163	ARG
1	N	25	ASN
1	N	55	ASN
1	N	100	SER
1	N	187	SER
1	O	55	ASN
1	O	57	ARG
1	P	55	ASN
1	P	109	LEU
1	P	187	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	94	HIS
1	A	119	ASN
1	B	55	ASN
1	B	94	HIS
1	C	25	ASN
1	C	47	ASN
1	C	55	ASN
1	C	94	HIS
1	C	119	ASN
1	D	55	ASN
1	D	94	HIS
1	E	55	ASN
1	E	94	HIS
1	F	55	ASN
1	F	94	HIS
1	F	119	ASN
1	G	47	ASN
1	G	55	ASN
1	G	94	HIS
1	H	55	ASN
1	H	94	HIS
1	I	47	ASN
1	I	55	ASN
1	I	94	HIS
1	I	186	GLN
1	J	47	ASN
1	J	55	ASN
1	K	47	ASN
1	K	55	ASN
1	K	119	ASN
1	L	47	ASN
1	L	55	ASN
1	L	119	ASN
1	M	25	ASN
1	M	55	ASN
1	M	119	ASN
1	N	25	ASN
1	N	55	ASN
1	N	94	HIS
1	N	119	ASN
1	O	55	ASN
1	P	47	ASN

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Mol	Chain	Res	Type
1	P	55	ASN
1	P	94	HIS
1	P	119	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](#)

Of 32 ligands modelled in this entry, 32 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 [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	181/188 (96%)	-0.24	0 100 100	13, 19, 30, 39	0
1	B	181/188 (96%)	-0.33	0 100 100	12, 18, 25, 30	0
1	C	181/188 (96%)	-0.26	0 100 100	12, 18, 26, 33	0
1	D	181/188 (96%)	-0.06	3 (1%) 73 72	14, 22, 35, 38	0
1	E	181/188 (96%)	-0.08	4 (2%) 65 63	14, 20, 29, 38	0
1	F	172/188 (91%)	-0.21	1 (0%) 90 90	12, 19, 29, 44	0
1	G	181/188 (96%)	-0.23	0 100 100	11, 18, 25, 34	0
1	H	181/188 (96%)	-0.14	1 (0%) 90 90	13, 21, 31, 37	0
1	I	181/188 (96%)	0.31	8 (4%) 38 36	25, 34, 47, 51	0
1	J	181/188 (96%)	0.62	14 (7%) 16 15	24, 34, 51, 54	0
1	K	181/188 (96%)	0.64	14 (7%) 16 15	28, 40, 53, 56	0
1	L	181/188 (96%)	0.70	16 (8%) 12 12	27, 41, 57, 59	0
1	M	181/188 (96%)	0.24	4 (2%) 65 63	24, 33, 46, 49	0
1	N	181/188 (96%)	0.07	4 (2%) 65 63	21, 29, 38, 43	0
1	O	181/188 (96%)	0.62	14 (7%) 16 15	25, 34, 48, 50	0
1	P	181/188 (96%)	0.18	6 (3%) 50 47	23, 31, 38, 46	0
All	All	2887/3008 (95%)	0.12	89 (3%) 52 49	11, 27, 46, 59	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	114	ALA	7.9
1	O	115	ILE	6.3
1	L	100	SER	5.9
1	O	114	ALA	5.2
1	J	115	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	J	100	SER	4.6
1	O	110	LEU	4.6
1	E	100	SER	4.5
1	L	115	ILE	4.5
1	I	182	GLU	4.5
1	O	116	ALA	4.4
1	L	113	LEU	4.4
1	M	114	ALA	4.2
1	J	182	GLU	3.8
1	J	110	LEU	3.7
1	J	116	ALA	3.7
1	P	181	ASP	3.7
1	L	114	ALA	3.6
1	K	101	ASN	3.5
1	D	100	SER	3.5
1	D	115	ILE	3.5
1	P	182	GLU	3.4
1	L	47	ASN	3.4
1	I	100	SER	3.3
1	O	69	ASP	3.3
1	L	116	ALA	3.3
1	P	9	ALA	3.2
1	P	100	SER	3.2
1	I	181	ASP	3.2
1	L	104	ILE	3.2
1	K	184	LYS	3.1
1	L	183	ALA	3.1
1	I	104	ILE	3.1
1	M	9	ALA	3.0
1	K	100	SER	3.0
1	I	47	ASN	2.8
1	O	28	LEU	2.8
1	O	109	LEU	2.8
1	E	115	ILE	2.8
1	L	109	LEU	2.7
1	K	8	LEU	2.7
1	F	9	ALA	2.6
1	M	148	LEU	2.6
1	J	113	LEU	2.6
1	J	47	ASN	2.6
1	J	181	ASP	2.6
1	N	181	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	99	GLN	2.5
1	J	184	LYS	2.5
1	K	181	ASP	2.5
1	N	47	ASN	2.5
1	O	119	ASN	2.5
1	L	136	VAL	2.5
1	K	128	ILE	2.5
1	K	103	LEU	2.5
1	L	25	ASN	2.5
1	E	76	THR	2.5
1	L	182	GLU	2.4
1	L	9	ALA	2.4
1	P	47	ASN	2.4
1	K	115	ILE	2.4
1	N	100	SER	2.4
1	O	27	ARG	2.4
1	M	100	SER	2.4
1	I	115	ILE	2.4
1	O	183	ALA	2.4
1	H	115	ILE	2.3
1	L	128	ILE	2.3
1	J	25	ASN	2.3
1	O	8	LEU	2.3
1	E	42	ILE	2.2
1	K	47	ASN	2.2
1	J	185	GLY	2.2
1	O	25	ASN	2.2
1	K	9	ALA	2.2
1	L	119	ASN	2.2
1	I	110	LEU	2.1
1	P	175	LEU	2.1
1	D	101	ASN	2.1
1	O	112	LYS	2.1
1	K	182	GLU	2.1
1	J	109	LEU	2.1
1	L	118	GLU	2.1
1	K	131	PRO	2.1
1	I	9	ALA	2.0
1	N	128	ILE	2.0
1	K	66	LEU	2.0
1	K	96	TYR	2.0
1	O	117	PRO	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
3	CL	E	305	1/1	0.63	0.17	0.61	84,84,84,84	0
3	CL	L	312	1/1	0.94	0.15	-0.21	54,54,54,54	0
3	CL	N	314	1/1	0.99	0.09	-1.05	39,39,39,39	0
3	CL	K	311	1/1	0.97	0.07	-1.79	45,45,45,45	0
3	CL	C	303	1/1	0.99	0.03	-1.88	24,24,24,24	0
3	CL	M	313	1/1	0.95	0.07	-1.92	37,37,37,37	0
3	CL	F	306	1/1	0.99	0.05	-2.05	21,21,21,21	0
3	CL	P	316	1/1	0.97	0.07	-2.21	42,42,42,42	0
3	CL	O	315	1/1	0.98	0.05	-2.33	32,32,32,32	0
3	CL	G	307	1/1	0.99	0.05	-2.39	20,20,20,20	0
2	CA	A	201	1/1	1.00	0.05	-2.40	19,19,19,19	0
2	CA	M	213	1/1	0.96	0.05	-2.43	33,33,33,33	0
2	CA	G	207	1/1	1.00	0.05	-2.69	19,19,19,19	0
2	CA	E	205	1/1	0.97	0.04	-2.77	26,26,26,26	0
2	CA	I	209	1/1	0.99	0.02	-2.86	36,36,36,36	0
2	CA	K	211	1/1	0.94	0.06	-2.92	38,38,38,38	0
3	CL	I	309	1/1	0.97	0.04	-2.95	48,48,48,48	0
2	CA	N	214	1/1	0.97	0.06	-2.95	34,34,34,34	0
2	CA	L	212	1/1	0.91	0.06	-3.10	43,43,43,43	0
3	CL	H	308	1/1	0.99	0.04	-3.12	24,24,24,24	0
2	CA	C	203	1/1	0.99	0.02	-3.42	21,21,21,21	0
2	CA	D	204	1/1	1.00	0.03	-3.50	23,23,23,23	0
2	CA	J	210	1/1	0.99	0.03	-3.55	34,34,34,34	0
3	CL	A	301	1/1	0.99	0.04	-3.55	22,22,22,22	0
3	CL	B	302	1/1	1.00	0.05	-3.70	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	H	208	1/1	1.00	0.02	-4.23	19,19,19,19	0
2	CA	P	216	1/1	0.97	0.04	-4.26	37,37,37,37	0
3	CL	D	304	1/1	0.99	0.03	-5.48	27,27,27,27	0
2	CA	O	215	1/1	0.99	0.03	-5.77	34,34,34,34	0
2	CA	B	202	1/1	0.99	0.03	-5.94	20,20,20,20	0
2	CA	F	206	1/1	0.99	0.03	-6.30	19,19,19,19	0
3	CL	J	310	1/1	0.97	0.07	-10.70	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.