WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:42 PM GMT

PDB ID	:	4U0T
Title	:	Crystal structure of ADC-7 beta-lactamase
Authors	:	Powers, R.A.; Wallar, B.J.
Deposited on	:	2014-07-14
Resolution	:	1.73 Å(reported)

The following versions of software and data (see references (i)) 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
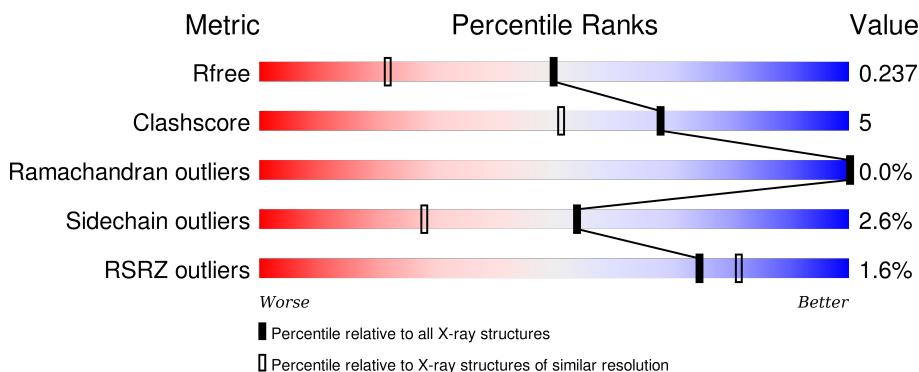
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	2417 (1.76-1.72)
Clashscore	102246	2570 (1.76-1.72)
Ramachandran outliers	100387	2544 (1.76-1.72)
Sidechain outliers	100360	2544 (1.76-1.72)
RSRZ outliers	91569	2420 (1.76-1.72)

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 <=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	360	92% ... 6% ••
1	B	360	89% ... 10% •
1	C	360	85% ... 12% ••
1	D	360	81% ... 14% • •
1	E	360	87% ... 11% •

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Mol	Chain	Length	Quality of chain
1	F	360	4% ▬ 83% ▬▬▬▬▬ 15% ··
1	G	360	% ▬ 86% ▬▬▬▬▬ 10% ··
1	H	360	5% ▬ 89% ▬▬▬▬▬ 7% ··

2 Entry composition (i)
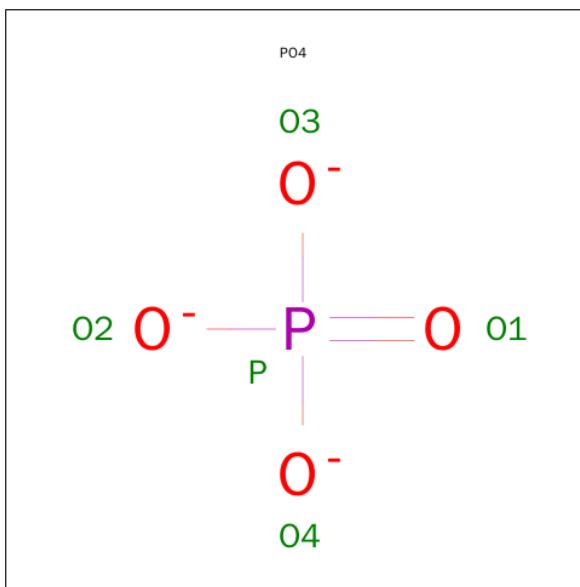
There are 3 unique types of molecules in this entry. The entry contains 23766 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ADC-7 beta-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	7	0
			2845	1833	467	534	11			
1	B	358	Total	C	N	O	S	0	8	0
			2857	1841	471	535	10			
1	C	352	Total	C	N	O	S	0	2	0
			2743	1767	452	515	9			
1	D	346	Total	C	N	O	S	0	3	0
			2684	1730	439	506	9			
1	E	354	Total	C	N	O	S	0	4	0
			2795	1801	465	520	9			
1	F	355	Total	C	N	O	S	0	1	0
			2768	1783	458	518	9			
1	G	348	Total	C	N	O	S	0	4	0
			2723	1757	446	511	9			
1	H	349	Total	C	N	O	S	0	1	0
			2711	1749	446	507	9			

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	P 1	0	0
2	B	1	Total 5	O 4	P 1	0	0
2	C	1	Total 5	O 4	P 1	0	0
2	D	1	Total 5	O 4	P 1	0	0
2	E	1	Total 5	O 4	P 1	0	0
2	F	1	Total 5	O 4	P 1	0	0
2	G	1	Total 5	O 4	P 1	0	0
2	H	1	Total 5	O 4	P 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	322	Total 331	O 331	0	9
3	B	335	Total 340	O 340	0	5
3	C	161	Total 163	O 163	0	2
3	D	163	Total 165	O 165	0	2

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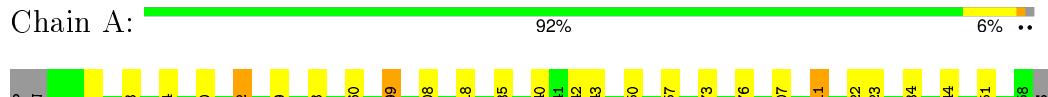
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	180	Total 180	O 180	0	0
3	F	157	Total 158	O 158	0	1
3	G	123	Total 124	O 124	0	1
3	H	139	Total 139	O 139	0	0
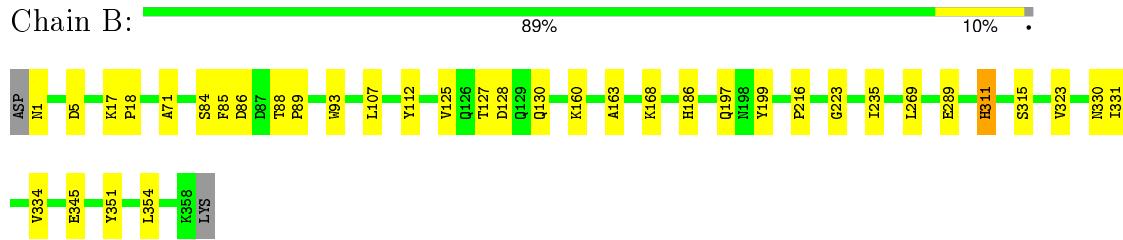
3 Residue-property plots ⓘ

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.
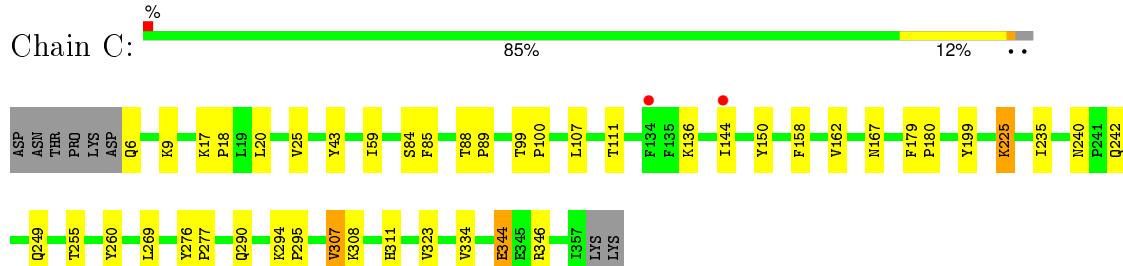
- Molecule 1: ADC-7 beta-lactamase
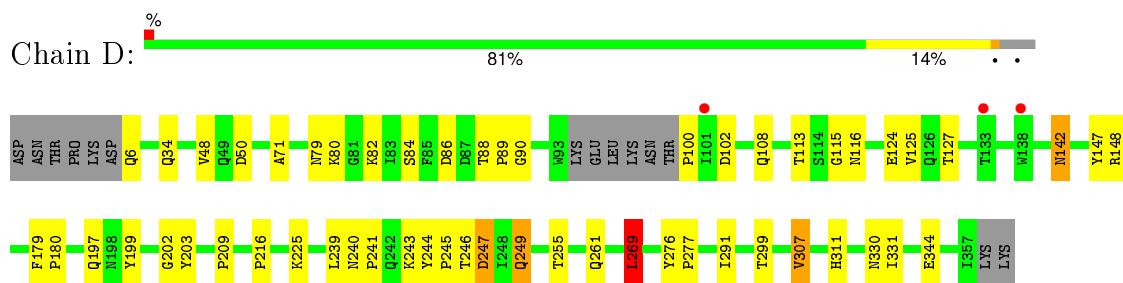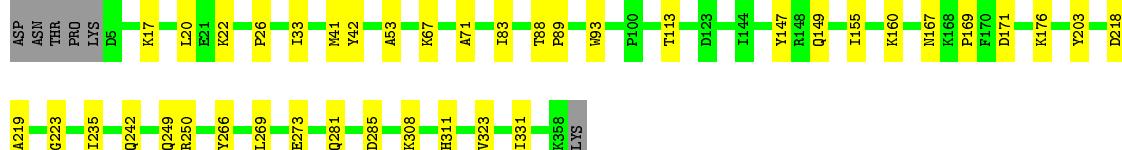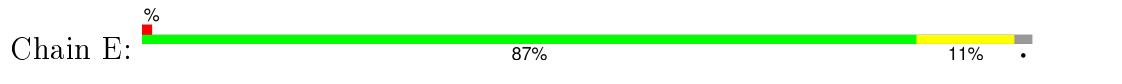
- Molecule 1: ADC-7 beta-lactamase

- Molecule 1: ADC-7 beta-lactamase

- Molecule 1: ADC-7 beta-lactamase

- Molecule 1: ADC-7 beta-lactamase

Chain E:

- Molecule 1: ADC-7 beta-lactamase

Chain F:

- Molecule 1: ADC-7 beta-lactamase

Chain G:

- Molecule 1: ADC-7 beta-lactamase

Chain H:
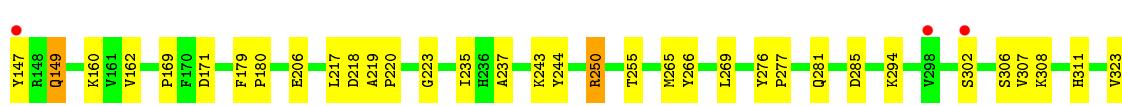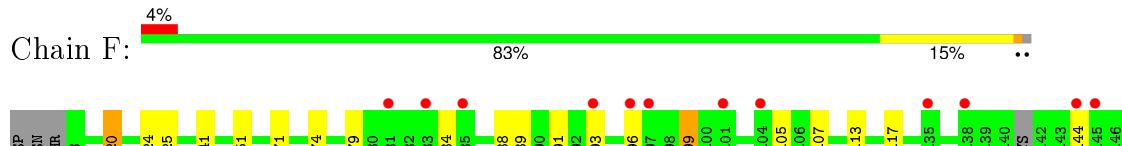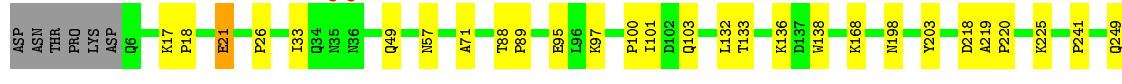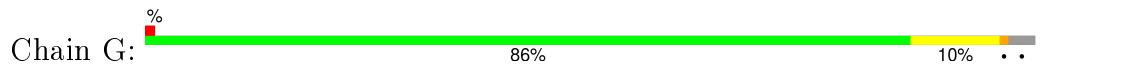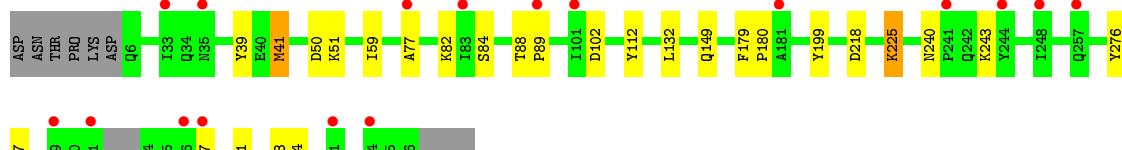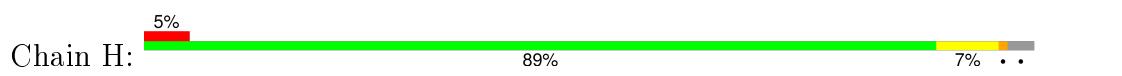
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	81.00Å 88.57Å 105.88Å 67.29° 89.84° 89.40°	Depositor
Resolution (Å)	40.00 – 1.73 39.79 – 1.73	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.00-1.73) 83.9 (39.79-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.57 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.194 , 0.239 0.195 , 0.237	Depositor DCC
R_{free} test set	13789 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 27.8	EDS
Estimated twinning fraction	0.387 for h,-k,-l 0.001 for -h,k,k-l 0.000 for -h,-k,-k+l	Xtriage
L-test for twinning[2]	$< |L| >$ = 0.50, $< L^2 >$ = 0.34	Xtriage
Outliers	0 of 273483 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	23766	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.86 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.0227e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: PO4

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	1.18	3/2935 (0.1%)	1.06	5/3988 (0.1%)
1	B	1.18	4/2951 (0.1%)	1.06	2/4012 (0.0%)
1	C	1.04	1/2816 (0.0%)	1.03	3/3835 (0.1%)
1	D	1.05	1/2759 (0.0%)	0.99	5/3763 (0.1%)
1	E	0.84	0/2871	0.92	5/3902 (0.1%)
1	F	0.83	0/2838	0.91	4/3859 (0.1%)
1	G	0.82	0/2801	0.89	3/3812 (0.1%)
1	H	0.86	0/2780	0.90	1/3785 (0.0%)
All	All	0.99	9/22751 (0.0%)	0.97	28/30956 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	F	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	344	GLU	CD-OE2	9.94	1.36	1.25
1	A	273	GLU	CD-OE1	-8.01	1.16	1.25
1	D	344	GLU	CD-OE2	7.93	1.34	1.25
1	A	344	GLU	CD-OE2	7.38	1.33	1.25
1	B	112	TYR	CG-CD1	6.22	1.47	1.39
1	A	351	TYR	CE1-CZ	-5.98	1.30	1.38
1	B	315[A]	SER	CB-OG	5.14	1.49	1.42
1	B	315[B]	SER	CB-OG	5.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	GLU	CD-OE2	5.11	1.31	1.25

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	40	GLU	OE1-CD-OE2	-8.09	113.59	123.30
1	F	218	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	148	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	218	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	G	218	ASP	CB-CG-OD1	6.42	124.07	118.30
1	E	250	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	F	41	MET	CG-SD-CE	6.10	109.96	100.20
1	E	42	TYR	CB-CG-CD1	-5.95	117.43	121.00
1	E	218	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	50	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	H	218	ASP	CB-CG-OD1	5.81	123.53	118.30
1	F	24	ASP	CB-CG-OD1	5.78	123.51	118.30
1	D	50	ASP	CB-CG-OD2	5.77	123.50	118.30
1	A	250	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	250	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	G	168	LYS	CB-CA-C	-5.39	99.62	110.40
1	E	41	MET	CG-SD-CE	5.37	108.78	100.20
1	C	323	VAL	CG1-CB-CG2	-5.34	102.35	110.90
1	C	240	ASN	CB-CA-C	-5.24	99.92	110.40
1	A	322	TYR	CB-CG-CD2	5.21	124.12	121.00
1	D	307	VAL	CB-CA-C	5.20	121.27	111.40
1	D	269	LEU	CA-CB-CG	5.15	127.14	115.30
1	E	53	ALA	CB-CA-C	-5.08	102.48	110.10
1	C	346	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	B	351	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	A	23	TYR	CB-CG-CD2	5.02	124.01	121.00
1	G	269	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	6	GLN	Peptide
1	F	357	ILE	Peptide

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	2845	0	2838	21	0
1	B	2857	0	2849	28	0
1	C	2743	0	2692	38	0
1	D	2684	0	2606	37	0
1	E	2795	0	2780	18	0
1	F	2768	0	2727	28	0
1	G	2723	0	2669	22	0
1	H	2711	0	2648	17	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	331	0	0	6	0
3	B	340	0	0	9	0
3	C	163	0	0	4	0
3	D	165	0	0	2	0
3	E	180	0	0	1	0
3	F	158	0	0	2	0
3	G	124	0	0	1	0
3	H	139	0	0	1	0
All	All	23766	0	21809	208	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 5.

All (208) 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:C:107:LEU:O	1:C:111[B]:THR:HG22	1.40	1.19
1:B:235[A]:ILE:HD11	1:B:323[A]:VAL:HG11	1.34	1.09
1:B:235[A]:ILE:HD11	1:B:323[A]:VAL:CG1	1.91	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240[B]:ASN:OD1	1:D:243:LYS:HE3	1.68	0.94
1:E:235:ILE:HD11	1:E:323[A]:VAL:CG2	2.05	0.86
1:C:235:ILE:CD1	1:C:334:VAL:HG23	2.07	0.85
1:C:235:ILE:HD11	1:C:334:VAL:CG2	2.07	0.85
1:G:132:LEU:C	1:G:132:LEU:HD23	1.99	0.82
1:B:186[A]:HIS:CD2	3:B:501:HOH:O	2.33	0.81
1:C:111[B]:THR:OG1	1:C:260:TYR:HE2	1.63	0.79
1:C:242:GLN:HA	1:C:249:GLN:NE2	1.98	0.79
1:F:235:ILE:HD11	1:F:323:VAL:CG1	2.14	0.78
1:F:79:ASN:OD1	1:F:250:ARG:NH1	2.15	0.78
1:D:115:GLY:O	1:D:142:ASN:HB2	1.83	0.77
1:D:261:GLN:HG2	1:D:299:THR:HG23	1.69	0.75
1:D:239:LEU:C	1:D:240[B]:ASN:HD22	1.89	0.75
1:B:1:ASN:HB3	3:B:506:HOH:O	1.86	0.73
1:C:235:ILE:HD11	1:C:334:VAL:HG23	1.66	0.73
1:D:240[B]:ASN:OD1	1:D:243:LYS:CE	2.37	0.73
1:E:235:ILE:HD11	1:E:323[A]:VAL:HG23	1.68	0.72
1:A:235[B]:ILE:CD1	1:A:334:VAL:HG23	2.20	0.72
1:F:20:LEU:HD22	1:F:25:VAL:HB	1.73	0.71
1:C:111[B]:THR:OG1	1:C:260:TYR:CE2	2.43	0.70
1:C:235:ILE:CD1	1:C:334:VAL:CG2	2.69	0.70
1:F:235:ILE:HD11	1:F:323:VAL:HG13	1.74	0.67
2:B:401:PO4:O4	3:B:776:HOH:O	2.13	0.66
1:C:290:GLN:NE2	1:H:50:ASP:OD1	2.29	0.66
1:B:186[A]:HIS:HD2	3:B:501:HOH:O	1.75	0.66
1:C:225:LYS:HD3	1:C:225:LYS:N	2.11	0.65
1:A:4:LYS:HE3	1:A:34:GLN:OE1	1.96	0.65
1:A:240:ASN:OD1	3:A:735:HOH:O	2.14	0.65
1:A:235[B]:ILE:HD11	1:A:334:VAL:HG23	1.78	0.64
1:E:235:ILE:HD11	1:E:323[A]:VAL:HG21	1.78	0.63
1:C:235:ILE:HD11	1:C:334:VAL:HG22	1.80	0.63
1:H:276:TYR:O	1:H:307:VAL:HG13	1.98	0.63
1:C:290:GLN:HB3	1:C:294:LYS:HE3	1.81	0.62
1:D:125:VAL:O	1:D:216:PRO:HG3	1.99	0.62
1:C:107:LEU:HD23	1:C:111[B]:THR:HG21	1.80	0.62
1:B:235[B]:ILE:CD1	1:B:334:VAL:HG23	2.30	0.61
1:H:132:LEU:C	1:H:132:LEU:HD23	2.21	0.61
1:B:323[B]:VAL:HG12	1:B:334:VAL:HG22	1.83	0.60
1:B:186[A]:HIS:HE1	3:B:505:HOH:O	1.83	0.60
1:D:261:GLN:HG2	1:D:299:THR:CG2	2.32	0.60
1:C:235:ILE:HD12	1:C:334:VAL:HG23	1.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:GLY:HA2	3:B:707:HOH:O	2.00	0.60
1:F:88:THR:HB	1:F:89:PRO:HD2	1.84	0.59
1:F:71:ALA:HB1	1:F:269:LEU:HB3	1.84	0.59
1:C:20:LEU:HD11	1:C:43:TYR:HB3	1.84	0.59
1:H:39:TYR:HB3	1:H:41:MET:HE1	1.84	0.59
1:D:90:GLY:N	1:D:102:ASP:OD2	2.35	0.59
1:C:107:LEU:O	1:C:111[B]:THR:CG2	2.33	0.58
1:C:242:GLN:HA	1:C:249:GLN:CD	2.24	0.58
1:E:242:GLN:HA	1:E:249:GLN:OE1	2.04	0.58
1:E:281:GLN:NE2	1:E:285:ASP:OD1	2.36	0.58
1:A:257:GLN:HG3	3:A:533[A]:HOH:O	2.03	0.57
1:A:235[B]:ILE:HD11	1:A:334:VAL:CG2	2.33	0.57
1:B:235[A]:ILE:CD1	1:B:323[A]:VAL:CG1	2.77	0.57
1:A:257:GLN:HG3	3:A:533[B]:HOH:O	2.04	0.57
1:C:107:LEU:HD23	1:C:111[B]:THR:CG2	2.35	0.57
1:C:167:ASN:ND2	3:C:501:HOH:O	2.37	0.57
1:E:93:TRP:CZ2	1:E:160:LYS:HE2	2.39	0.57
1:D:84:SER:OG	1:D:86:ASP:OD1	2.22	0.57
1:G:241:PRO:O	1:G:249:GLN:HG3	2.05	0.57
1:A:52:LYS:HD2	3:A:591:HOH:O	2.05	0.57
1:E:71:ALA:HB1	1:E:269:LEU:HB3	1.87	0.57
1:D:71:ALA:HB1	1:D:269:LEU:HB3	1.85	0.57
1:F:96:LEU:O	1:F:99:THR:HG22	2.05	0.56
1:A:235[B]:ILE:HD12	1:A:334:VAL:HG23	1.87	0.56
1:H:276:TYR:CD1	1:H:277:PRO:HA	2.41	0.56
1:H:333:LEU:HD23	1:H:333:LEU:C	2.27	0.56
1:B:235[B]:ILE:HD12	1:B:334:VAL:HG23	1.87	0.55
1:H:276:TYR:O	1:H:307:VAL:CG1	2.55	0.55
1:F:237:ALA:HA	1:F:244:TYR:CE1	2.41	0.55
1:G:299:THR:HG22	1:G:300:ALA:O	2.06	0.55
1:F:276:TYR:CD1	1:F:277:PRO:HA	2.41	0.55
1:B:127:THR:OG1	1:B:130:GLN:HG3	2.07	0.54
1:D:48[A]:VAL:HG22	1:D:203:TYR:OH	2.06	0.54
1:D:179:PHE:HB2	1:D:180:PRO:HD3	1.90	0.54
1:E:22[A]:LYS:NZ	3:E:630:HOH:O	2.39	0.54
1:G:33:ILE:O	1:G:331:ILE:HA	2.08	0.54
1:A:307[A]:VAL:HG12	3:A:514:HOH:O	2.07	0.54
1:F:235:ILE:HD11	1:F:323:VAL:HG11	1.88	0.53
1:G:276:TYR:CD1	1:G:277:PRO:HA	2.43	0.53
1:C:107:LEU:CD2	1:C:111[B]:THR:HG21	2.38	0.53
1:G:21:GLU:HG3	1:G:21:GLU:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:THR:HB	1:E:89:PRO:HD2	1.91	0.53
1:G:132:LEU:HD23	1:G:133:THR:N	2.23	0.53
1:D:255:THR:HA	1:D:269:LEU:HB2	1.91	0.53
1:D:276:TYR:CD1	1:D:277:PRO:HA	2.43	0.53
1:E:219:ALA:HA	1:E:223:GLY:HA3	1.90	0.53
1:H:59:ILE:CG2	1:H:225:LYS:HB2	2.39	0.53
1:C:111[B]:THR:HG1	1:C:260:TYR:HE2	1.53	0.52
1:D:88:THR:HB	1:D:89:PRO:HD2	1.92	0.52
1:B:93:TRP:CZ3	1:B:160:LYS:HD3	2.45	0.52
1:D:6:GLN:HA	3:D:589:HOH:O	2.09	0.52
1:A:242:GLN:HG2	1:A:243:LYS:HD3	1.90	0.52
1:C:290:GLN:O	1:C:294:LYS:HG2	2.11	0.51
1:E:93:TRP:CZ3	1:E:160:LYS:HD3	2.46	0.51
1:D:142:ASN:ND2	1:D:147:TYR:CD1	2.79	0.51
1:F:344:GLU:CD	1:F:344:GLU:H	2.14	0.51
1:H:51:LYS:NZ	3:H:501:HOH:O	2.41	0.51
1:A:4:LYS:CE	1:A:34:GLN:OE1	2.60	0.50
1:C:17:LYS:N	1:C:18:PRO:CD	2.73	0.50
1:C:276:TYR:HB3	1:C:307:VAL:HG22	1.94	0.50
1:F:96:LEU:O	1:F:99:THR:CG2	2.59	0.50
1:C:225:LYS:NZ	3:C:558:HOH:O	2.43	0.50
1:B:128:ASP:HB3	3:B:729:HOH:O	2.11	0.50
1:C:276:TYR:CD1	1:C:277:PRO:HA	2.46	0.50
1:C:107:LEU:HD23	1:C:107:LEU:O	2.12	0.49
1:D:102:ASP:O	1:D:102:ASP:OD1	2.30	0.49
1:E:169:PRO:HB2	1:E:171:ASP:OD1	2.12	0.49
1:B:163:ALA:HB1	1:B:168:LYS:O	2.13	0.49
1:C:20:LEU:HD23	1:C:25:VAL:HB	1.94	0.48
1:C:107:LEU:HD23	1:C:107:LEU:C	2.33	0.48
1:F:265:MET:HG2	1:F:266:TYR:N	2.28	0.48
1:B:235[B]:ILE:HD11	1:B:334:VAL:CG2	2.43	0.48
1:F:144:ILE:HD11	3:F:534:HOH:O	2.14	0.48
1:D:241:PRO:O	1:D:249:GLN:HG3	2.13	0.48
1:D:113:THR:HA	1:D:147:TYR:O	2.13	0.48
1:B:88:THR:HB	1:B:89:PRO:HD2	1.96	0.48
1:H:39:TYR:N	1:H:39:TYR:CD1	2.81	0.47
1:F:219:ALA:HA	1:F:223:GLY:HA3	1.95	0.47
1:H:88:THR:HG21	1:H:102:ASP:O	2.15	0.47
1:B:235[B]:ILE:HD11	1:B:334:VAL:HG23	1.95	0.47
1:D:88:THR:OG1	1:D:102:ASP:OD1	2.22	0.47
1:H:112:TYR:HB3	1:H:149:GLN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:ASN:CB	3:B:506:HOH:O	2.56	0.47
1:C:85:PHE:HB3	1:C:107:LEU:HB2	1.97	0.47
1:F:255:THR:HA	1:F:269:LEU:HB2	1.96	0.47
1:A:208:GLN:OE1	1:F:51:LYS:HA	2.15	0.47
1:A:235[B]:ILE:CD1	1:A:334:VAL:CG2	2.92	0.46
2:C:401:PO4:O4	3:C:521:HOH:O	2.20	0.46
1:E:17:LYS:O	1:E:20:LEU:HD12	2.15	0.46
1:F:79:ASN:OD1	1:F:250:ARG:HD3	2.16	0.46
1:G:100:PRO:HD2	3:G:594:HOH:O	2.15	0.46
1:D:80:LYS:HB3	1:D:82:LYS:HG3	1.98	0.46
1:C:294:LYS:HB2	1:C:295:PRO:HD2	1.98	0.46
1:C:59:ILE:CG2	1:C:225:LYS:HB3	2.45	0.46
1:H:77:ALA:HB1	1:H:82:LYS:HB2	1.97	0.46
1:D:48[A]:VAL:HG22	1:D:203:TYR:CZ	2.50	0.46
1:G:88:THR:HB	1:G:89:PRO:HD2	1.97	0.46
1:D:80:LYS:NZ	1:D:247:ASP:HB3	2.30	0.46
1:A:276:TYR:HB3	1:A:307[B]:VAL:HG12	1.99	0.45
1:G:17:LYS:N	1:G:18:PRO:HD2	2.32	0.45
1:G:71:ALA:HB1	1:G:269:LEU:HB3	1.99	0.45
1:B:85:PHE:HB3	1:B:107:LEU:HB2	1.98	0.45
1:H:240:ASN:HB3	1:H:243:LYS:HG3	1.98	0.45
1:B:331:ILE:HG12	1:B:354:LEU:HD22	1.99	0.45
1:B:235[B]:ILE:CD1	1:B:334:VAL:CG2	2.95	0.45
1:D:239:LEU:O	1:D:240[B]:ASN:ND2	2.47	0.44
1:A:307[A]:VAL:CG1	3:A:507:HOH:O	2.66	0.44
1:F:169:PRO:HB2	1:F:171:ASP:OD1	2.18	0.44
1:A:93:TRP:CZ3	1:A:160:LYS:HD3	2.53	0.44
1:C:99:THR:HB	1:C:100:PRO:CD	2.48	0.44
1:F:74:GLY:HA2	1:F:162:VAL:HG21	2.00	0.44
1:B:71:ALA:HB1	1:B:269:LEU:HB3	2.00	0.43
1:A:323:VAL:HG12	1:A:334:VAL:HG22	2.00	0.43
1:G:225:LYS:CD	1:G:225:LYS:N	2.81	0.43
1:A:59:ILE:HB	1:A:199:TYR:HA	2.00	0.43
1:G:219:ALA:N	1:G:220:PRO:HD2	2.34	0.43
1:D:291:ILE:CG1	1:G:49[A]:GLN:NE2	2.81	0.43
1:D:241:PRO:HB2	1:D:249:GLN:HG2	1.99	0.43
1:B:186[B]:HIS:CE1	3:B:501:HOH:O	2.70	0.43
1:D:100:PRO:C	1:D:102:ASP:N	2.69	0.43
1:H:333:LEU:HD23	1:H:334:VAL:N	2.33	0.43
1:D:124:GLU:CD	1:D:124:GLU:H	2.20	0.43
1:C:255:THR:HA	1:C:269:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:LEU:HD21	1:G:136:LYS:HE3	2.00	0.43
1:F:113:THR:HA	1:F:147:TYR:O	2.19	0.43
1:D:244:TYR:O	1:D:245:PRO:C	2.55	0.43
1:D:34:GLN:HG3	1:D:331:ILE:HG22	2.02	0.42
1:F:144:ILE:CD1	3:F:534:HOH:O	2.67	0.42
1:F:179:PHE:HB2	1:F:180:PRO:HD3	2.01	0.42
1:E:33:ILE:O	1:E:331:ILE:HA	2.20	0.42
1:F:117:LEU:O	1:F:149:GLN:HG2	2.19	0.42
1:F:276:TYR:O	1:F:307:VAL:HG13	2.19	0.42
1:G:26:PRO:HG2	1:G:203:TYR:CD2	2.54	0.42
1:G:333:LEU:HD23	1:G:333:LEU:C	2.39	0.42
1:G:101:ILE:HD13	1:G:138:TRP:CD2	2.55	0.42
1:F:217:LEU:O	1:F:220:PRO:HD2	2.20	0.42
1:C:158:PHE:O	1:C:162:VAL:HG23	2.20	0.42
1:C:150:TYR:N	3:C:608:HOH:O	2.31	0.41
1:E:67:LYS:HE3	1:E:155:ILE:HG21	2.03	0.41
1:H:88:THR:HB	1:H:89:PRO:HD2	2.03	0.41
1:D:108:GLN:HA	3:D:503:HOH:O	2.19	0.41
1:H:179:PHE:HB2	1:H:180:PRO:HD3	2.02	0.41
1:G:57:ASN:O	1:G:198:ASN:HB3	2.21	0.41
1:E:266:TYR:HB2	1:E:273:GLU:HB3	2.02	0.41
1:B:17:LYS:N	1:B:18:PRO:CD	2.84	0.41
1:E:26:PRO:HG2	1:E:203:TYR:CD1	2.56	0.41
1:D:100:PRO:C	1:D:102:ASP:H	2.24	0.41
1:A:311:HIS:CD2	1:A:311:HIS:C	2.94	0.41
1:B:311:HIS:C	1:B:311:HIS:CD2	2.95	0.41
1:G:95[B]:GLU:H	1:G:95[B]:GLU:CD	2.25	0.41
1:G:219:ALA:HB3	1:G:220:PRO:HD3	2.03	0.41
1:F:93:TRP:CZ2	1:F:160:LYS:HE2	2.56	0.41
1:D:202:GLY:O	1:D:209:PRO:HA	2.21	0.41
1:C:88:THR:HB	1:C:89:PRO:HD2	2.03	0.41
1:C:179:PHE:HB2	1:C:180:PRO:HD3	2.03	0.40
1:F:281:GLN:NE2	1:F:285:ASP:OD1	2.53	0.40
1:E:113:THR:HA	1:E:147:TYR:O	2.21	0.40
1:D:246:THR:HG23	1:D:247:ASP:N	2.36	0.40
1:B:125:VAL:O	1:B:216:PRO:HG3	2.21	0.40
1:D:225:LYS:N	1:D:225:LYS:HD2	2.36	0.40
1:B:84:SER:OG	1:B:86[B]:ASP:OD1	2.34	0.40
1:A:52:LYS:HD2	1:A:52:LYS:HA	1.92	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	362/360 (101%)	350 (97%)	12 (3%)	0	100	100
1	B	364/360 (101%)	354 (97%)	10 (3%)	0	100	100
1	C	352/360 (98%)	338 (96%)	14 (4%)	0	100	100
1	D	345/360 (96%)	336 (97%)	8 (2%)	1 (0%)	46	26
1	E	356/360 (99%)	348 (98%)	8 (2%)	0	100	100
1	F	352/360 (98%)	341 (97%)	11 (3%)	0	100	100
1	G	348/360 (97%)	341 (98%)	7 (2%)	0	100	100
1	H	346/360 (96%)	334 (96%)	12 (4%)	0	100	100
All	All	2825/2880 (98%)	2742 (97%)	82 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	116	ASN

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	315/318 (99%)	312 (99%)	3 (1%)	82	69
1	B	316/318 (99%)	311 (98%)	5 (2%)	70	51
1	C	295/318 (93%)	285 (97%)	10 (3%)	44	18
1	D	287/318 (90%)	276 (96%)	11 (4%)	40	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	304/318 (96%)	298 (98%)	6 (2%)	63	39
1	F	298/318 (94%)	283 (95%)	15 (5%)	30	8
1	G	292/318 (92%)	286 (98%)	6 (2%)	61	36
1	H	288/318 (91%)	283 (98%)	5 (2%)	68	48
All	All	2395/2544 (94%)	2334 (98%)	61 (2%)	54	29

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LYS
1	A	199	TYR
1	A	311	HIS
1	B	197	GLN
1	B	199	TYR
1	B	289	GLU
1	B	311	HIS
1	B	330	ASN
1	C	9	LYS
1	C	84	SER
1	C	136	LYS
1	C	144	ILE
1	C	199	TYR
1	C	225	LYS
1	C	307	VAL
1	C	308	LYS
1	C	311	HIS
1	C	344	GLU
1	D	79	ASN
1	D	127	THR
1	D	142	ASN
1	D	197	GLN
1	D	199	TYR
1	D	247	ASP
1	D	249	GLN
1	D	269	LEU
1	D	307	VAL
1	D	311	HIS
1	D	330	ASN
1	E	83	ILE
1	E	149	GLN
1	E	167	ASN

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Mol	Chain	Res	Type
1	E	176	LYS
1	E	308	LYS
1	E	311	HIS
1	F	20	LEU
1	F	84	SER
1	F	91	LYS
1	F	99	THR
1	F	105	ASN
1	F	107	LEU
1	F	149	GLN
1	F	206	GLU
1	F	243	LYS
1	F	294	LYS
1	F	302	SER
1	F	306	SER
1	F	308	LYS
1	F	311	HIS
1	F	358	LYS
1	G	21	GLU
1	G	97	LYS
1	G	103	GLN
1	G	261	GLN
1	G	308	LYS
1	G	311	HIS
1	H	41	MET
1	H	84	SER
1	H	199	TYR
1	H	225	LYS
1	H	311	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	B	35	ASN
1	B	197	GLN
1	B	205	GLN
1	C	35	ASN
1	D	142	ASN
1	D	249	GLN
1	D	287	ASN
1	F	36	ASN

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Mol	Chain	Res	Type
1	F	98	ASN
1	F	263	ASN
1	F	281	GLN
1	G	172	GLN
1	H	35	ASN
1	H	172	GLN

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)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	401	-	4,4,4	0.46	0	6,6,6	0.35	0
2	PO4	B	401	-	4,4,4	0.87	0	6,6,6	0.47	0
2	PO4	C	401	-	4,4,4	0.80	0	6,6,6	0.52	0
2	PO4	D	401	-	4,4,4	0.93	0	6,6,6	0.28	0
2	PO4	E	401	-	4,4,4	0.38	0	6,6,6	0.32	0
2	PO4	F	401	-	4,4,4	0.31	0	6,6,6	0.34	0
2	PO4	G	401	-	4,4,4	0.37	0	6,6,6	0.36	0
2	PO4	H	401	-	4,4,4	0.45	0	6,6,6	0.33	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	401	-	-	0/0/0/0	0/0/0/0
2	PO4	B	401	-	-	0/0/0/0	0/0/0/0
2	PO4	C	401	-	-	0/0/0/0	0/0/0/0
2	PO4	D	401	-	-	0/0/0/0	0/0/0/0
2	PO4	E	401	-	-	0/0/0/0	0/0/0/0
2	PO4	F	401	-	-	0/0/0/0	0/0/0/0
2	PO4	G	401	-	-	0/0/0/0	0/0/0/0
2	PO4	H	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PO4	1	0
2	C	401	PO4	1	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	357/360 (99%)	-0.34	0	100	100	13, 21, 36, 45	0
1	B	358/360 (99%)	-0.39	0	100	100	13, 21, 35, 51	0
1	C	352/360 (97%)	-0.02	2 (0%)	90	93	16, 33, 63, 73	0
1	D	346/360 (96%)	-0.08	3 (0%)	85	90	16, 32, 60, 75	0
1	E	354/360 (98%)	-0.15	3 (0%)	87	91	17, 34, 56, 70	0
1	F	355/360 (98%)	0.14	15 (4%)	40	45	16, 38, 63, 80	0
1	G	348/360 (96%)	0.01	5 (1%)	78	84	19, 39, 56, 69	0
1	H	349/360 (96%)	0.28	17 (4%)	33	38	18, 38, 55, 71	0
All	All	2819/2880 (97%)	-0.07	45 (1%)	74	81	13, 31, 58, 80	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	301	ILE	5.9
1	F	85	PHE	4.6
1	H	35	ASN	4.2
1	G	35	ASN	3.9
1	H	257	GLN	3.8
1	F	298	VAL	3.5
1	F	97	LYS	3.4
1	F	145	GLY	3.3
1	G	301	ILE	3.2
1	F	104	VAL	3.1
1	F	83	ILE	2.9
1	F	101	ILE	2.9
1	H	181	ALA	2.8
1	H	307	VAL	2.8
1	G	36	ASN	2.8
1	F	93	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	135	PHE	2.8
1	H	83	ILE	2.7
1	C	134	PHE	2.6
1	E	123	ASP	2.6
1	H	77	ALA	2.6
1	H	354	LEU	2.6
1	H	248	ILE	2.5
1	F	147	TYR	2.5
1	H	299	THR	2.5
1	H	241	PRO	2.4
1	D	101	ILE	2.4
1	F	302	SER	2.4
1	H	33	ILE	2.3
1	G	351	TYR	2.3
1	F	138	TRP	2.3
1	F	96	LEU	2.3
1	H	351	TYR	2.3
1	E	100	PRO	2.3
1	D	133	THR	2.3
1	F	144	ILE	2.3
1	H	306	SER	2.2
1	F	81	GLY	2.2
1	H	89	PRO	2.2
1	H	244	TYR	2.1
1	C	144	ILE	2.1
1	D	138	TRP	2.1
1	E	144	ILE	2.1
1	H	101	ILE	2.1
1	G	354	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	C	401	5/5	0.93	0.10	0.84	35,36,38,39	0
2	PO4	D	401	5/5	0.96	0.09	-0.01	34,34,35,36	0
2	PO4	A	401	5/5	0.98	0.07	-0.10	23,24,25,26	0
2	PO4	B	401	5/5	0.97	0.07	-0.76	23,23,25,26	0
2	PO4	F	401	5/5	0.97	0.06	-1.33	41,42,45,49	0
2	PO4	E	401	5/5	0.98	0.05	-1.76	39,41,42,46	0
2	PO4	H	401	5/5	0.98	0.05	-2.87	31,32,34,34	0
2	PO4	G	401	5/5	0.99	0.05	-3.21	34,34,35,36	0

6.5 Other polymers (i)

There are no such residues in this entry.