W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:34 am GMT

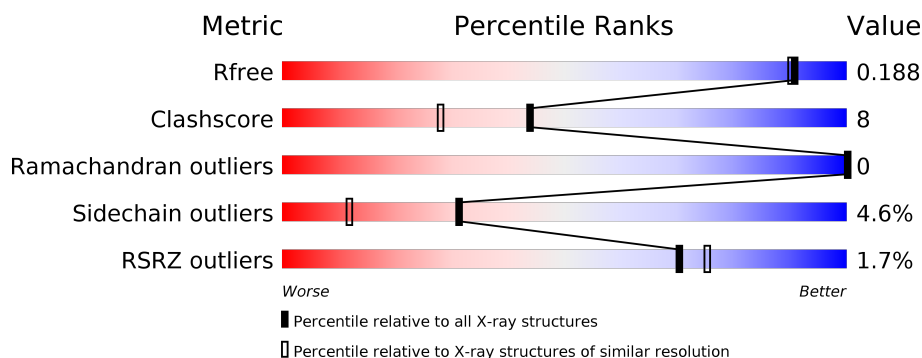|		
PDB ID	:	3OCC
Title	:	Crystal structure of PNP with DADMEimmH from Yersinia pseudotuberculosis
Authors	:	Kim, J.; Ramagopal, U.A.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2010-08-09
Resolution	:	1.70 Å(reported)

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 1.70 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	Percentile Ranks	Value
Rfree		0.188
Clashscore		8
Ramachandran outliers		0
Sidechain outliers		4.6%
RSRZ outliers		1.7%

Worse .... Better

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3453 (1.70-1.70)
Clashscore	112137	3876 (1.70-1.70)
Ramachandran outliers	110173	3815 (1.70-1.70)
Sidechain outliers	110143	3815 (1.70-1.70)
RSRZ outliers	101464	3491 (1.70-1.70)

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	239	90% ... 9%
1	B	239	87% ... 12%
1	C	239	90% ... 8%
1	D	239	88% ... 10%
1	E	239	89% ... 9%
1	F	239	86% ... 11%

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	DIH	A	500	X	-	-	-
2	DIH	B	500	X	-	-	-
2	DIH	C	500	X	-	-	-
2	DIH	D	500	X	-	-	-
2	DIH	E	500	X	-	-	-
2	DIH	F	500	X	-	-	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12217 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 Purine nucleoside phosphorylase deoD-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	2	0
			1812	1139	313	343	17			
1	B	237	Total	C	N	O	S	0	1	0
			1797	1130	308	342	17			
1	C	236	Total	C	N	O	S	0	3	0
			1831	1148	321	346	16			
1	D	238	Total	C	N	O	S	0	2	0
			1821	1144	314	346	17			
1	E	238	Total	C	N	O	S	0	3	0
			1830	1149	315	349	17			
1	F	238	Total	C	N	O	S	0	1	0
			1812	1138	312	345	17			

- Molecule 2 is 3-HYDROXY-4-HYDROXYMETHYL-1-(4-OXO-4,4A,5,7A-TETRAHYDRO -3H-PYRROLO[3,2-D]PYRIMIDIN-7-YLMETHYL)-PYRROLIDINIUM (three-letter code: DIH) (formula: $C_{12}H_{19}N_4O_3$).
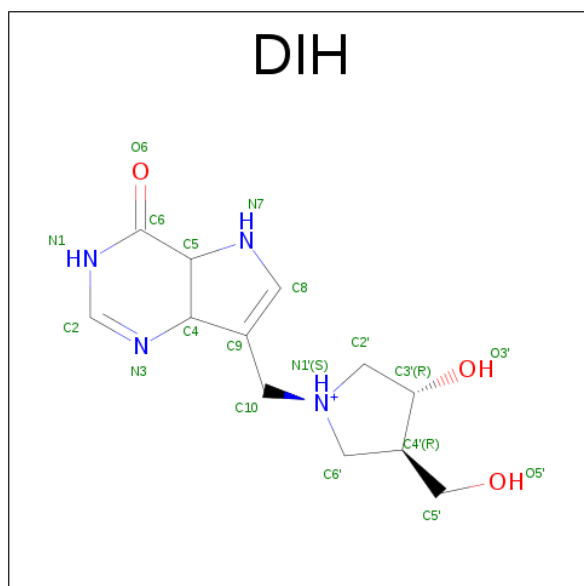
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	12	4	3		
2	B	1	Total	C	N	O	0	0
			19	12	4	3		
2	C	1	Total	C	N	O	0	0
			19	12	4	3		
2	D	1	Total	C	N	O	0	0
			19	12	4	3		
2	E	1	Total	C	N	O	0	0
			19	12	4	3		
2	F	1	Total	C	N	O	0	0
			19	12	4	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
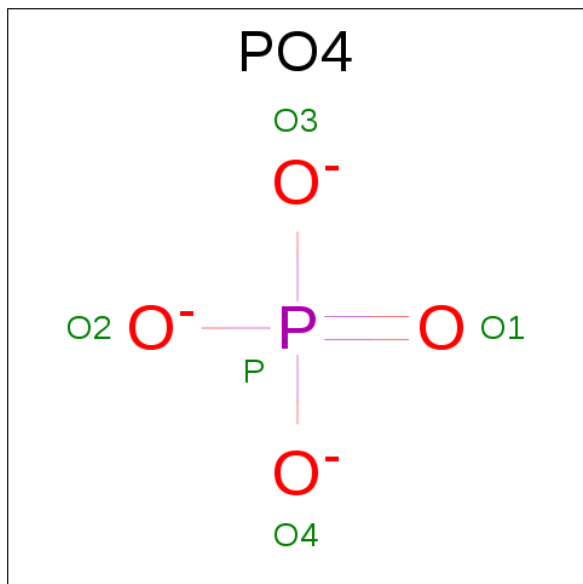
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total 195	O 195	0	0
4	B	182	Total 182	O 182	0	0
4	C	201	Total 201	O 201	0	0
4	D	213	Total 213	O 213	0	0
4	E	193	Total 193	O 193	0	0
4	F	186	Total 186	O 186	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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Purine nucleoside phosphorylase deoD-type
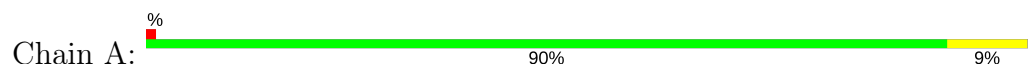
- Molecule 1: Purine nucleoside phosphorylase deoD-type

- Molecule 1: Purine nucleoside phosphorylase deoD-type

- Molecule 1: Purine nucleoside phosphorylase deoD-type

- Molecule 1: Purine nucleoside phosphorylase deoD-type

• Molecule 1: Purine nucleoside phosphorylase deoD-type

Chain F:
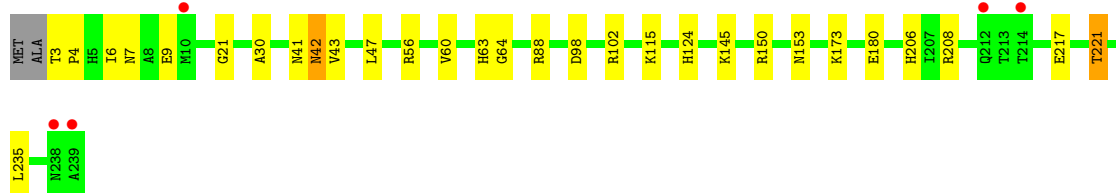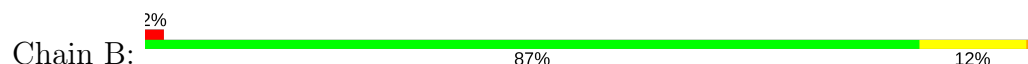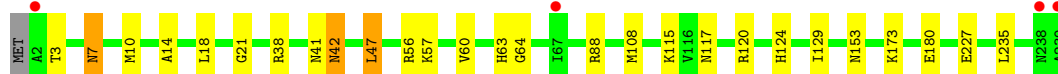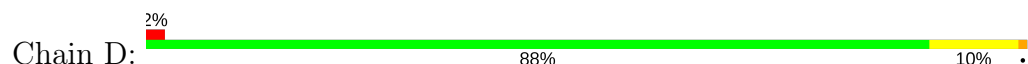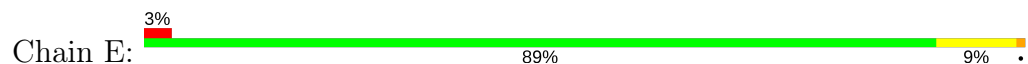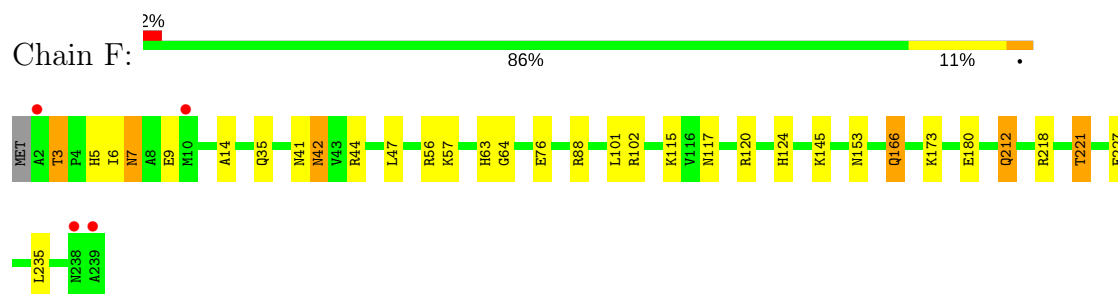
4 Data and refinement statistics (i)

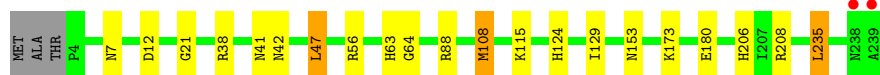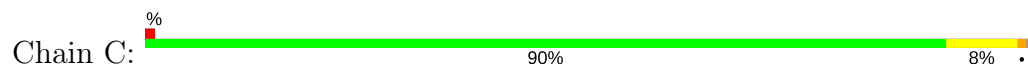| Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.65Å 109.83Å 154.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 45.06 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-1.70) 99.7 (45.06-1.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.149 , 0.181 0.156 , 0.188	Depositor DCC
R_{free} test set	8553 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	17.8	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 40.5	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12217	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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 23.33 % 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 4.7667e-03. 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PO4, DIH

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	0.72	0/1839	0.73	0/2476
1	B	0.72	0/1824	0.75	0/2458
1	C	0.75	0/1858	0.78	2/2499 (0.1%)
1	D	0.74	0/1848	0.76	1/2488 (0.0%)
1	E	0.74	0/1857	0.77	2/2500 (0.1%)
1	F	0.70	0/1839	0.74	0/2477
All	All	0.73	0/11065	0.75	5/14898 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	235	LEU	CB-CG-CD1	5.39	120.16	111.00
1	C	47	LEU	CB-CG-CD1	5.33	120.07	111.00
1	D	47	LEU	CB-CG-CD1	5.28	119.97	111.00
1	E	158	ASP	CB-CG-OD2	5.27	123.05	118.30
1	E	221	THR	OG1-CB-CG2	5.11	121.76	110.00

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.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1812	0	1812	25	1
1	B	1797	0	1789	42	0
1	C	1831	0	1832	26	0
1	D	1821	0	1821	36	1
1	E	1830	0	1826	30	0
1	F	1812	0	1809	37	0
2	A	19	0	16	0	0
2	B	19	0	16	0	0
2	C	19	0	16	0	0
2	D	19	0	16	0	0
2	E	19	0	16	0	0
2	F	19	0	16	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	195	0	0	6	0
4	B	182	0	0	4	0
4	C	201	0	0	3	0
4	D	213	0	0	3	0
4	E	193	0	0	3	0
4	F	186	0	0	3	0
All	All	12217	0	10985	168	1

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 8.

All (168) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HH22	1:B:221:THR:HG21	0.99	1.09
1:C:108:MET:HG3	1:D:108[B]:MET:HE3	1.36	1.08
1:B:102:ARG:HH22	1:B:221:THR:CG2	1.72	1.02
1:D:38:ARG:HH11	1:D:38:ARG:HG2	1.30	0.95
1:F:3:THR:HG21	1:F:76:GLU:OE1	1.64	0.94
1:B:102:ARG:NH2	1:B:221:THR:HG21	1.84	0.91
1:B:173:LYS:HD3	4:B:577:HOH:O	1.71	0.90
1:E:7:ASN:HD22	1:E:41:ASN:ND2	1.69	0.90
1:F:7:ASN:HD22	1:F:41:ASN:HD22	1.17	0.89
1:F:7:ASN:HD22	1:F:41:ASN:ND2	1.70	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:MET:HG3	1:D:108[B]:MET:CE	2.07	0.84
1:D:7:ASN:HD22	1:D:41:ASN:HD22	1.26	0.82
1:F:102:ARG:HH22	1:F:221:THR:HG21	1.42	0.82
1:E:7:ASN:H	1:E:7:ASN:HD22	1.28	0.80
1:B:102:ARG:HH12	1:B:221:THR:HG23	1.47	0.80
1:F:7:ASN:ND2	1:F:41:ASN:ND2	2.30	0.80
4:C:994:HOH:O	1:D:173[A]:LYS:HD3	1.81	0.79
1:E:7:ASN:H	1:E:41:ASN:ND2	1.81	0.79
1:D:7:ASN:ND2	1:D:41:ASN:HD22	1.80	0.78
1:B:115:LYS:NZ	1:D:124:HIS:HD2	1.81	0.78
1:F:7:ASN:HD22	1:F:7:ASN:H	1.32	0.78
1:F:3:THR:HG23	1:F:5:HIS:H	1.49	0.76
4:E:1065:HOH:O	1:F:173:LYS:HD3	1.85	0.75
1:F:102:ARG:HH22	1:F:221:THR:CG2	1.99	0.75
1:E:7:ASN:ND2	1:E:41:ASN:ND2	2.34	0.75
4:A:953:HOH:O	1:B:173:LYS:CG	2.35	0.74
1:F:102:ARG:HH12	1:F:221:THR:HG23	1.51	0.74
1:A:7:ASN:HD22	1:A:41:ASN:HD22	1.36	0.74
4:A:953:HOH:O	1:B:173:LYS:HG2	1.88	0.74
1:F:7:ASN:ND2	1:F:41:ASN:HD22	1.83	0.73
1:B:7:ASN:H	1:B:41:ASN:ND2	1.86	0.73
1:E:7:ASN:HD22	1:E:41:ASN:HD22	1.34	0.73
1:A:7:ASN:H	1:A:41:ASN:ND2	1.87	0.72
1:A:115:LYS:NZ	1:E:124:HIS:HD2	1.88	0.71
4:A:953:HOH:O	1:B:173:LYS:HE3	1.92	0.70
1:E:7:ASN:HD21	1:E:42:ASN:H	1.40	0.70
1:C:63:HIS:HD2	1:C:64:GLY:O	1.75	0.70
1:E:63:HIS:HD2	1:E:64:GLY:O	1.75	0.69
1:B:124:HIS:HD2	1:F:115:LYS:NZ	1.89	0.69
1:F:3:THR:HB	4:F:697:HOH:O	1.93	0.68
1:B:102:ARG:NH2	1:B:221:THR:CG2	2.50	0.68
1:F:3:THR:CG2	1:F:5:HIS:H	2.06	0.67
1:B:63:HIS:HD2	1:B:64:GLY:O	1.76	0.67
1:F:7:ASN:HD21	1:F:42:ASN:H	1.42	0.66
1:B:102:ARG:HH12	1:B:221:THR:CG2	2.08	0.66
1:F:7:ASN:H	1:F:41:ASN:ND2	1.93	0.66
1:A:124:HIS:HD2	1:C:115:LYS:NZ	1.93	0.66
1:F:3:THR:HG22	1:F:6:ILE:H	1.60	0.66
1:A:63:HIS:HD2	1:A:64:GLY:O	1.79	0.65
1:C:7:ASN:H	1:C:41:ASN:ND2	1.94	0.65
1:F:63:HIS:HD2	1:F:64:GLY:O	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LYS:NZ	1:F:124:HIS:HD2	1.96	0.63
1:C:124:HIS:HD2	1:E:115:LYS:NZ	1.97	0.62
1:D:7:ASN:ND2	1:D:41:ASN:ND2	2.47	0.62
1:C:108:MET:CG	1:D:108[B]:MET:CE	2.78	0.61
1:D:38:ARG:NH1	1:D:38:ARG:HG2	2.02	0.61
1:B:115:LYS:HZ3	1:D:124:HIS:HD2	1.45	0.61
1:C:108:MET:CG	1:D:108[B]:MET:HE3	2.24	0.61
1:A:7:ASN:ND2	1:A:41:ASN:HD22	1.99	0.60
1:D:7:ASN:H	1:D:41:ASN:ND2	1.99	0.60
1:E:221:THR:HG23	4:E:250:HOH:O	2.01	0.60
1:E:63:HIS:HE1	1:E:88:ARG:HH11	1.49	0.60
1:D:63:HIS:HD2	1:D:64:GLY:O	1.85	0.60
1:D:63:HIS:HE1	1:D:88:ARG:HH11	1.50	0.59
1:C:63:HIS:HE1	1:C:88:ARG:HH11	1.50	0.59
1:F:63:HIS:HE1	1:F:88:ARG:HH11	1.51	0.59
1:D:63:HIS:CE1	1:D:88:ARG:HH11	2.21	0.57
1:E:63:HIS:CE1	1:E:88:ARG:HH11	2.22	0.57
1:B:217:GLU:O	1:B:221:THR:HB	2.05	0.56
1:A:208:ARG:HG2	4:A:1012:HOH:O	2.05	0.56
1:F:63:HIS:CE1	1:F:88:ARG:HH11	2.24	0.56
4:E:475:HOH:O	1:F:124:HIS:HE1	1.88	0.55
1:C:63:HIS:CE1	1:C:88:ARG:HH11	2.25	0.54
1:C:108:MET:HE3	1:D:129:ILE:HD12	1.90	0.54
1:B:98:ASP:O	1:B:150:ARG:NH1	2.41	0.54
1:E:217:GLU:O	1:E:221:THR:HB	2.08	0.54
1:E:63:HIS:CD2	1:E:64:GLY:O	2.58	0.54
1:A:7:ASN:ND2	1:A:41:ASN:ND2	2.55	0.54
1:B:3:THR:N	4:B:770:HOH:O	2.41	0.54
1:F:7:ASN:H	1:F:41:ASN:HD22	1.56	0.53
1:B:63:HIS:CD2	1:B:64:GLY:O	2.61	0.52
1:C:63:HIS:CD2	1:C:64:GLY:O	2.60	0.52
1:A:7:ASN:H	1:A:41:ASN:HD22	1.53	0.52
1:B:124:HIS:HD2	1:F:115:LYS:HZ3	1.56	0.52
1:E:7:ASN:N	1:E:7:ASN:HD22	2.01	0.52
1:A:63:HIS:CE1	1:A:88:ARG:HH11	2.28	0.51
1:A:124:HIS:HD2	1:C:115:LYS:HZ1	1.59	0.51
1:B:102:ARG:NH1	1:B:221:THR:HG23	2.21	0.51
1:B:63:HIS:CE1	1:B:88:ARG:HH11	2.29	0.51
1:C:7:ASN:H	1:C:41:ASN:HD22	1.57	0.51
1:B:124:HIS:HD2	1:F:115:LYS:HZ1	1.58	0.51
1:E:124:HIS:HE1	4:F:303:HOH:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:ASN:HD21	1:D:42:ASN:H	1.60	0.50
1:F:35:GLN:NE2	4:F:588:HOH:O	2.42	0.50
1:D:7:ASN:H	1:D:7:ASN:HD22	1.59	0.50
1:F:63:HIS:CD2	1:F:64:GLY:O	2.64	0.50
1:C:173[A]:LYS:HE2	4:C:331:HOH:O	2.11	0.50
1:F:7:ASN:HD22	1:F:7:ASN:N	2.06	0.49
1:A:115:LYS:HZ1	1:E:124:HIS:HD2	1.58	0.49
1:D:10:MET:HE1	4:D:748:HOH:O	2.11	0.49
1:D:117:ASN:ND2	1:D:120:ARG:HH11	2.09	0.49
1:F:14:ALA:HB2	1:F:57:LYS:HG2	1.94	0.49
1:A:7:ASN:H	1:A:7:ASN:HD22	1.61	0.49
1:B:63:HIS:HE1	1:B:88:ARG:HH11	1.61	0.49
1:E:14:ALA:HB2	1:E:57:LYS:HG2	1.95	0.49
1:D:115:LYS:HZ3	1:F:124:HIS:HD2	1.59	0.48
1:E:6:ILE:HA	1:E:41:ASN:ND2	2.27	0.48
1:B:3:THR:N	4:B:314:HOH:O	2.45	0.48
1:C:124:HIS:HE1	4:D:392:HOH:O	1.97	0.48
1:E:21:GLY:HA2	1:E:63:HIS:CD2	2.49	0.48
1:B:7:ASN:H	1:B:41:ASN:HD21	1.60	0.48
1:C:21:GLY:HA2	1:C:63:HIS:CD2	2.49	0.48
1:A:63:HIS:HE1	1:A:88:ARG:HH11	1.59	0.48
1:A:115:LYS:HZ3	1:E:124:HIS:HD2	1.57	0.47
1:B:102:ARG:NH1	1:B:221:THR:CG2	2.76	0.47
1:B:7:ASN:HD21	1:B:42:ASN:ND2	2.12	0.47
1:D:7:ASN:H	1:D:41:ASN:HD22	1.63	0.47
1:F:212:GLN:HG2	1:F:218:ARG:NH2	2.29	0.47
4:C:383:HOH:O	1:D:124:HIS:HE1	1.98	0.47
4:A:953:HOH:O	1:B:173:LYS:CE	2.55	0.47
1:E:7:ASN:H	1:E:41:ASN:HD21	1.56	0.47
1:B:7:ASN:OD1	1:B:41:ASN:ND2	2.48	0.46
1:A:117:ASN:ND2	1:A:120:ARG:HH11	2.14	0.46
1:E:6:ILE:HA	1:E:41:ASN:HD21	1.80	0.46
1:D:173[A]:LYS:HE2	4:D:285:HOH:O	2.15	0.46
1:A:21:GLY:HA2	1:A:63:HIS:CD2	2.50	0.46
1:A:14:ALA:HB2	1:A:57:LYS:HG2	1.98	0.46
1:B:30:ALA:HB2	1:B:60:VAL:CG1	2.46	0.46
1:B:21:GLY:HA2	1:B:63:HIS:CD2	2.51	0.46
1:F:102:ARG:NH1	1:F:221:THR:HG23	2.26	0.46
1:D:14:ALA:HB2	1:D:57:LYS:HG2	1.98	0.45
1:A:124:HIS:HE1	4:B:315:HOH:O	1.99	0.45
1:B:115:LYS:HZ1	1:D:124:HIS:HD2	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:357:HOH:O	1:B:124:HIS:HE1	1.97	0.45
1:A:7:ASN:CG	1:A:43:VAL:HG23	2.37	0.45
1:B:7:ASN:CG	1:B:43:VAL:HG23	2.38	0.44
1:E:42:ASN:HD22	1:E:42:ASN:C	2.20	0.44
1:B:206:HIS:CE1	1:B:208:ARG:HB2	2.52	0.44
1:C:124:HIS:HD2	1:E:115:LYS:HZ1	1.65	0.44
1:E:117:ASN:ND2	1:E:120:ARG:HH11	2.16	0.43
1:B:6:ILE:HA	1:B:41:ASN:HD21	1.84	0.43
1:A:63:HIS:CD2	1:A:64:GLY:O	2.65	0.43
1:B:7:ASN:H	1:B:41:ASN:HD22	1.62	0.43
1:D:63:HIS:CD2	1:D:64:GLY:O	2.69	0.43
1:E:7:ASN:H	1:E:41:ASN:HD22	1.58	0.43
1:A:7:ASN:HD22	1:A:41:ASN:ND2	2.08	0.43
1:B:3:THR:HB	1:B:4:PRO:HD2	2.01	0.43
1:C:206:HIS:CE1	1:C:208:ARG:HB2	2.54	0.42
1:D:18:LEU:O	1:D:60:VAL:HA	2.19	0.42
1:B:6:ILE:HA	1:B:41:ASN:ND2	2.34	0.42
1:C:7:ASN:OD1	1:C:41:ASN:ND2	2.52	0.42
1:E:7:ASN:CG	1:E:43:VAL:HG23	2.39	0.42
1:A:124:HIS:HD2	1:C:115:LYS:HZ3	1.68	0.42
1:B:4:PRO:O	1:B:43:VAL:HG11	2.20	0.42
1:B:115:LYS:NZ	1:D:124:HIS:CD2	2.73	0.42
1:F:117:ASN:ND2	1:F:120:ARG:HH11	2.17	0.42
1:E:122:LYS:NZ	1:F:166:GLN:HE21	2.18	0.42
1:C:108:MET:CG	1:D:108[B]:MET:HE2	2.48	0.41
1:C:12:ASP:OD1	1:C:38:ARG:NH1	2.54	0.41
1:A:22:ASP:OD1	1:F:44:ARG:HA	2.20	0.41
1:C:129:ILE:HB	1:D:108[A]:MET:HE2	2.02	0.41
1:D:21:GLY:HA2	1:D:63:HIS:CD2	2.55	0.41
1:D:42:ASN:HD22	1:D:42:ASN:C	2.24	0.41
1:F:145:LYS:HE2	1:F:227:GLU:OE2	2.21	0.41
1:F:212:GLN:HG2	1:F:218:ARG:HH21	1.86	0.41
1:E:209:THR:OG1	1:E:211[B]:GLU:HG3	2.20	0.41
1:C:108:MET:HG2	1:D:108[B]:MET:HE2	2.03	0.40
1:A:124:HIS:CD2	1:C:115:LYS:HZ1	2.39	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLU:OE2	1:D:227:GLU:OE2[1_455]	2.17	0.03

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	237/239 (99%)	229 (97%)	8 (3%)	0	100	100
1	B	236/239 (99%)	229 (97%)	7 (3%)	0	100	100
1	C	238/239 (100%)	231 (97%)	7 (3%)	0	100	100
1	D	238/239 (100%)	230 (97%)	8 (3%)	0	100	100
1	E	239/239 (100%)	232 (97%)	7 (3%)	0	100	100
1	F	237/239 (99%)	231 (98%)	6 (2%)	0	100	100
All	All	1425/1434 (99%)	1382 (97%)	43 (3%)	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	190/190 (100%)	182 (96%)	8 (4%)	34	14
1	B	188/190 (99%)	179 (95%)	9 (5%)	30	11
1	C	192/190 (101%)	185 (96%)	7 (4%)	40	18
1	D	191/190 (100%)	183 (96%)	8 (4%)	34	14
1	E	192/190 (101%)	185 (96%)	7 (4%)	40	18
1	F	190/190 (100%)	177 (93%)	13 (7%)	18	4
All	All	1143/1140 (100%)	1091 (96%)	52 (4%)	31	12

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	42	ASN
1	A	47	LEU
1	A	56	ARG
1	A	121	PHE
1	A	153	ASN
1	A	180	GLU
1	A	235	LEU
1	B	9	GLU
1	B	42	ASN
1	B	47	LEU
1	B	56	ARG
1	B	145	LYS
1	B	153	ASN
1	B	180	GLU
1	B	221	THR
1	B	235	LEU
1	C	42	ASN
1	C	47	LEU
1	C	56	ARG
1	C	108	MET
1	C	153	ASN
1	C	180	GLU
1	C	235	LEU
1	D	3	THR
1	D	7	ASN
1	D	42	ASN
1	D	47	LEU
1	D	56	ARG
1	D	153	ASN
1	D	180	GLU
1	D	235	LEU
1	E	7	ASN
1	E	42	ASN
1	E	56	ARG
1	E	153	ASN
1	E	180	GLU
1	E	221	THR
1	E	235	LEU
1	F	3	THR
1	F	7	ASN
1	F	9	GLU

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Mol	Chain	Res	Type
1	F	42	ASN
1	F	47	LEU
1	F	56	ARG
1	F	101	LEU
1	F	153	ASN
1	F	166	GLN
1	F	180	GLU
1	F	212	GLN
1	F	221	THR
1	F	235	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	41	ASN
1	A	42	ASN
1	A	63	HIS
1	A	117	ASN
1	A	124	HIS
1	A	153	ASN
1	B	41	ASN
1	B	42	ASN
1	B	63	HIS
1	B	117	ASN
1	B	124	HIS
1	B	153	ASN
1	B	212	GLN
1	C	41	ASN
1	C	42	ASN
1	C	63	HIS
1	C	117	ASN
1	C	124	HIS
1	C	153	ASN
1	D	7	ASN
1	D	35	GLN
1	D	41	ASN
1	D	42	ASN
1	D	63	HIS
1	D	117	ASN
1	D	124	HIS
1	D	153	ASN

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Mol	Chain	Res	Type
1	E	7	ASN
1	E	41	ASN
1	E	42	ASN
1	E	63	HIS
1	E	117	ASN
1	E	124	HIS
1	E	153	ASN
1	F	7	ASN
1	F	35	GLN
1	F	41	ASN
1	F	42	ASN
1	F	63	HIS
1	F	117	ASN
1	F	124	HIS
1	F	153	ASN
1	F	166	GLN
1	F	212	GLN

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 ⓘ

12 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	DIH	A	500	-	16,21,21	2.69	6 (37%)	15,30,30	3.70	7 (46%)
3	PO4	A	501	-	4,4,4	1.33	1 (25%)	6,6,6	1.03	0
2	DIH	B	500	-	16,21,21	2.74	5 (31%)	15,30,30	3.68	7 (46%)
3	PO4	B	501	-	4,4,4	1.03	0	6,6,6	1.08	0
2	DIH	C	500	-	16,21,21	2.61	5 (31%)	15,30,30	3.52	6 (40%)
3	PO4	C	501	-	4,4,4	0.75	0	6,6,6	0.68	0
2	DIH	D	500	-	16,21,21	2.95	5 (31%)	15,30,30	3.51	7 (46%)
3	PO4	D	501	-	4,4,4	0.94	0	6,6,6	0.94	0
2	DIH	E	500	-	16,21,21	2.94	6 (37%)	15,30,30	3.60	6 (40%)
3	PO4	E	501	-	4,4,4	0.69	0	6,6,6	0.51	0
2	DIH	F	500	-	16,21,21	2.75	7 (43%)	15,30,30	3.88	7 (46%)
3	PO4	F	501	-	4,4,4	0.89	0	6,6,6	1.14	1 (16%)

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	DIH	A	500	-	2/2/7/11	0/6/41/41	0/3/3/3
3	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	DIH	B	500	-	2/2/7/11	0/6/41/41	0/3/3/3
3	PO4	B	501	-	-	0/0/0/0	0/0/0/0
2	DIH	C	500	-	2/2/7/11	0/6/41/41	0/3/3/3
3	PO4	C	501	-	-	0/0/0/0	0/0/0/0
2	DIH	D	500	-	2/2/7/11	0/6/41/41	0/3/3/3
3	PO4	D	501	-	-	0/0/0/0	0/0/0/0
2	DIH	E	500	-	2/2/7/11	0/6/41/41	0/3/3/3
3	PO4	E	501	-	-	0/0/0/0	0/0/0/0
2	DIH	F	500	-	2/2/7/11	0/6/41/41	0/3/3/3
3	PO4	F	501	-	-	0/0/0/0	0/0/0/0

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	DIH	C5-N7	-9.44	1.35	1.46
2	E	500	DIH	C5-N7	-9.41	1.35	1.46
2	B	500	DIH	C5-N7	-8.68	1.36	1.46
2	A	500	DIH	C5-N7	-8.38	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	DIH	C5-N7	-8.26	1.36	1.46
2	C	500	DIH	C5-N7	-7.81	1.37	1.46
2	D	500	DIH	C5-C6	-3.62	1.46	1.53
2	D	500	DIH	C4-N3	-3.44	1.36	1.46
2	C	500	DIH	C5-C6	-3.39	1.46	1.53
2	E	500	DIH	C5-C6	-3.33	1.47	1.53
2	B	500	DIH	C5-C6	-3.25	1.47	1.53
2	E	500	DIH	C4-N3	-3.15	1.37	1.46
2	A	500	DIH	C5-C6	-3.09	1.47	1.53
2	A	500	DIH	C4-N3	-2.92	1.37	1.46
2	B	500	DIH	C4-N3	-2.79	1.38	1.46
2	F	500	DIH	C4-N3	-2.76	1.38	1.46
2	F	500	DIH	C5-C6	-2.63	1.48	1.53
2	D	500	DIH	C6-N1	-2.37	1.33	1.37
2	C	500	DIH	C4-N3	-2.31	1.39	1.46
2	F	500	DIH	C6-N1	-2.28	1.33	1.37
2	E	500	DIH	C8-N7	2.18	1.36	1.33
2	A	500	DIH	C8-N7	2.26	1.36	1.33
2	A	500	DIH	O6-C6	2.30	1.27	1.23
3	A	501	PO4	P-O1	2.35	1.55	1.50
2	F	500	DIH	O6-C6	2.46	1.28	1.23
2	E	500	DIH	O6-C6	2.59	1.28	1.23
2	A	500	DIH	C2-N3	2.64	1.34	1.29
2	B	500	DIH	O6-C6	2.77	1.28	1.23
2	F	500	DIH	C8-N7	2.87	1.37	1.33
2	E	500	DIH	C2-N3	2.97	1.35	1.29
2	B	500	DIH	C2-N3	2.99	1.35	1.29
2	D	500	DIH	C2-N3	3.14	1.35	1.29
2	C	500	DIH	C2-N3	3.14	1.35	1.29
2	C	500	DIH	O6-C6	3.23	1.29	1.23
2	F	500	DIH	C2-N3	3.67	1.37	1.29

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	500	DIH	C4-C9-C8	-5.71	103.96	110.68
2	B	500	DIH	C4-C9-C8	-5.63	104.05	110.68
2	D	500	DIH	C4-C9-C8	-5.56	104.14	110.68
2	A	500	DIH	C4-C9-C8	-5.43	104.29	110.68
2	E	500	DIH	C4-C9-C8	-5.08	104.70	110.68
2	C	500	DIH	C4-C9-C8	-4.21	105.72	110.68
2	A	500	DIH	C3'-C2'-N1'	-3.08	99.53	104.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	DIH	C3'-C2'-N1'	-2.97	99.72	104.71
2	F	500	DIH	C3'-C2'-N1'	-2.85	99.93	104.71
2	E	500	DIH	C3'-C2'-N1'	-2.71	100.15	104.71
2	B	500	DIH	C3'-C2'-N1'	-2.64	100.28	104.71
2	C	500	DIH	C3'-C2'-N1'	-2.62	100.31	104.71
2	F	500	DIH	O3'-C3'-C2'	-2.45	104.98	110.90
2	D	500	DIH	O3'-C3'-C2'	-2.30	105.34	110.90
2	E	500	DIH	O5'-C5'-C4'	-2.23	106.31	111.35
2	B	500	DIH	O3'-C3'-C2'	-2.22	105.52	110.90
2	A	500	DIH	C4'-C6'-N1'	-2.03	99.89	103.92
2	D	500	DIH	C10-N1'-C2'	2.19	117.01	113.18
3	F	501	PO4	O3-P-O2	2.24	116.14	107.90
2	F	500	DIH	C10-N1'-C2'	2.51	117.56	113.18
2	A	500	DIH	C10-N1'-C2'	3.24	118.85	113.18
2	B	500	DIH	C10-N1'-C2'	3.62	119.50	113.18
2	B	500	DIH	C10-N1'-C6'	3.66	119.57	113.18
2	C	500	DIH	C10-N1'-C6'	3.78	119.79	113.18
2	A	500	DIH	C10-N1'-C6'	3.92	120.04	113.18
2	C	500	DIH	C10-N1'-C2'	4.06	120.28	113.18
2	E	500	DIH	C10-N1'-C6'	4.30	120.69	113.18
2	F	500	DIH	C10-N1'-C6'	4.37	120.82	113.18
2	D	500	DIH	C10-N1'-C6'	4.49	121.03	113.18
2	B	500	DIH	C10-C9-C4	5.30	129.84	122.87
2	D	500	DIH	C10-C9-C4	5.77	130.45	122.87
2	E	500	DIH	C10-C9-C4	5.82	130.53	122.87
2	A	500	DIH	C10-C9-C4	5.95	130.69	122.87
2	C	500	DIH	C10-C9-C4	6.32	131.18	122.87
2	F	500	DIH	C10-C9-C4	7.58	132.84	122.87
2	D	500	DIH	C2'-N1'-C6'	8.81	116.63	104.09
2	C	500	DIH	C2'-N1'-C6'	8.99	116.89	104.09
2	F	500	DIH	C2'-N1'-C6'	9.23	117.23	104.09
2	E	500	DIH	C2'-N1'-C6'	9.36	117.41	104.09
2	A	500	DIH	C2'-N1'-C6'	9.72	117.92	104.09
2	B	500	DIH	C2'-N1'-C6'	9.82	118.07	104.09

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	500	DIH	C4
2	D	500	DIH	C5
2	B	500	DIH	C4
2	B	500	DIH	C5

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Mol	Chain	Res	Type	Atom
2	C	500	DIH	C4
2	C	500	DIH	C5
2	E	500	DIH	C4
2	E	500	DIH	C5
2	A	500	DIH	C4
2	A	500	DIH	C5
2	F	500	DIH	C4
2	F	500	DIH	C5

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	237/239 (99%)	-0.22	3 (1%)	77	82	12, 18, 29, 50	0
1	B	237/239 (99%)	-0.24	5 (2%)	64	69	11, 18, 33, 49	0
1	C	236/239 (98%)	-0.36	2 (0%)	86	88	11, 16, 27, 46	0
1	D	238/239 (99%)	-0.23	4 (1%)	70	75	11, 17, 28, 46	0
1	E	238/239 (99%)	-0.27	6 (2%)	58	63	12, 17, 28, 51	0
1	F	238/239 (99%)	-0.25	4 (1%)	70	75	12, 18, 32, 47	0
All	All	1424/1434 (99%)	-0.26	24 (1%)	70	75	11, 17, 31, 51	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	239	ALA	8.0
1	D	239	ALA	7.2
1	A	239	ALA	6.6
1	B	239	ALA	5.9
1	D	2	ALA	4.7
1	C	239	ALA	4.5
1	F	239	ALA	4.2
1	E	2	ALA	3.9
1	F	2	ALA	3.8
1	F	238	ASN	3.7
1	F	10	MET	3.6
1	D	238	ASN	3.2
1	A	238	ASN	2.8
1	B	10	MET	2.8
1	B	212	GLN	2.6
1	E	238	ASN	2.6
1	E	10	MET	2.6
1	C	238	ASN	2.5
1	E	97	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	238	ASN	2.4
1	D	67	ILE	2.4
1	E	67	ILE	2.1
1	A	116	VAL	2.0
1	B	214	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	DIH	B	500	19/19	0.97	0.08	0.52	10,13,16,18	0
2	DIH	C	500	19/19	0.96	0.06	-0.53	9,11,14,16	0
2	DIH	F	500	19/19	0.96	0.06	-0.86	9,12,16,16	0
2	DIH	E	500	19/19	0.98	0.05	-1.07	8,11,13,15	0
2	DIH	A	500	19/19	0.97	0.06	-1.20	8,11,15,18	0
2	DIH	D	500	19/19	0.97	0.06	-1.38	8,10,14,16	0
3	PO4	D	501	5/5	0.99	0.05	-1.53	11,11,12,13	0
3	PO4	F	501	5/5	0.99	0.04	-1.85	10,12,12,12	0
3	PO4	A	501	5/5	0.99	0.05	-2.27	12,12,13,14	0
3	PO4	E	501	5/5	1.00	0.03	-2.42	9,10,10,12	0
3	PO4	B	501	5/5	0.99	0.04	-2.53	10,12,12,12	0
3	PO4	C	501	5/5	1.00	0.03	-3.16	9,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.