Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 12:05 pm GMT

PDB ID	:	7NMM
Title	:	Complex of rice blast (Magnaporthe oryzae) effector protein APikL2F with the host target sHMA94 from Setaria italica
Authors	:	Bentham, A.R.; Banfield, M.J.
Deposited on	:	2021-02-23
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

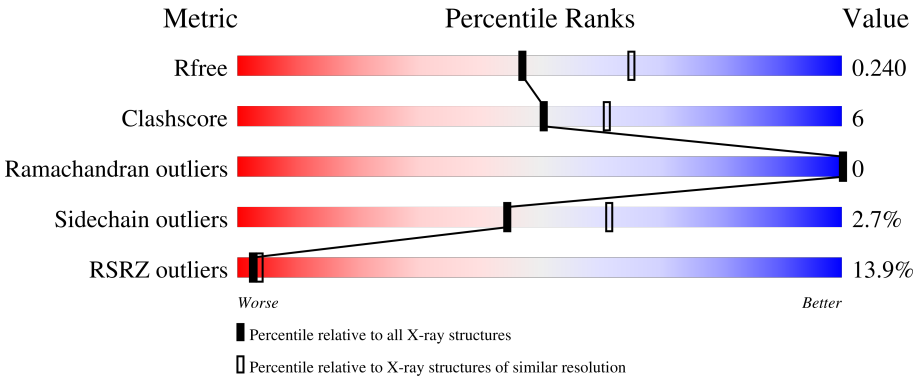
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	79	27% 73% 23%
1	B	79	33% 72% 23%
1	C	79	23% 76% 18%
1	D	79	20% 76% 22%
1	E	79	13% 76% 22%

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Mol	Chain	Length	Quality of chain
1	F	79	10% 75% 22%
1	G	79	10% 81% 18%
1	H	79	8% 76% 22%
2	I	95	12% 91% 5%
2	J	95	12% 92%
2	K	95	8% 91% 5%
2	L	95	9% 87% 7% 5%
2	M	95	13% 88% 7%
2	N	95	12% 91% 5%
2	O	95	9% 95%
2	P	95	4% 92%

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
3	EDO	C	101	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 10945 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 sHMAx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	78	Total	C	N	O	S	0	1	0
			592	373	103	109	7			
1	B	78	Total	C	N	O	S	0	2	0
			601	378	105	111	7			
1	C	77	Total	C	N	O	S	0	1	0
			587	370	103	107	7			
1	D	78	Total	C	N	O	S	0	1	0
			595	374	104	110	7			
1	E	78	Total	C	N	O	S	0	1	0
			595	374	104	110	7			
1	F	78	Total	C	N	O	S	0	1	0
			595	374	104	110	7			
1	G	78	Total	C	N	O	S	0	1	0
			595	374	104	110	7			
1	H	78	Total	C	N	O	S	0	1	0
			595	374	104	110	7			

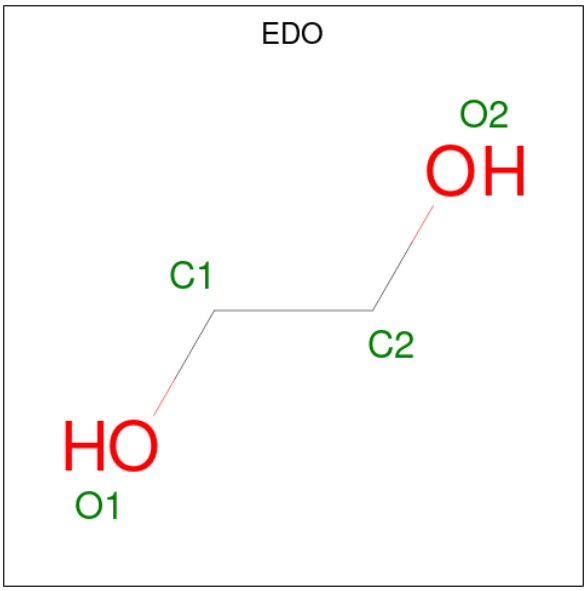
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP K3YDQ6
B	2	MET	-	initiating methionine	UNP K3YDQ6
C	2	MET	-	initiating methionine	UNP K3YDQ6
D	2	MET	-	initiating methionine	UNP K3YDQ6
E	2	MET	-	initiating methionine	UNP K3YDQ6
F	2	MET	-	initiating methionine	UNP K3YDQ6
G	2	MET	-	initiating methionine	UNP K3YDQ6
H	2	MET	-	initiating methionine	UNP K3YDQ6

- Molecule 2 is a protein called APikL2F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			
2	J	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			
2	K	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			
2	L	90	Total	C	N	O	S	0	0	0
			732	473	126	128	5			
2	M	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			
2	N	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			
2	O	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			
2	P	91	Total	C	N	O	S	0	0	0
			740	477	128	130	5			

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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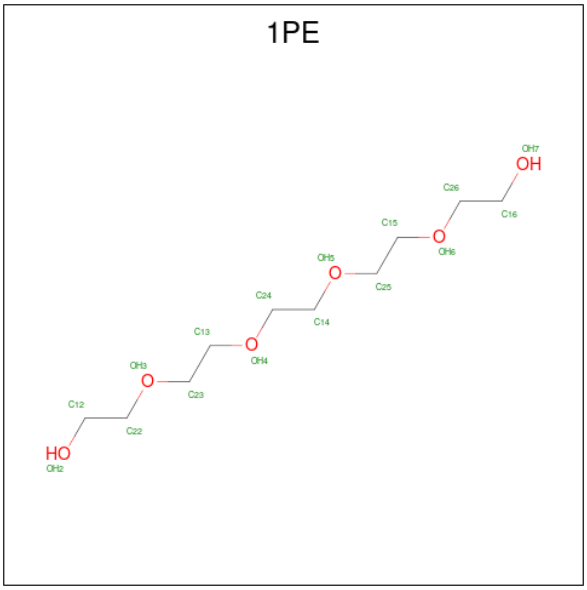
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total C O 4 2 2	0	0
3	I	1	Total C O 4 2 2	0	0
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	M	1	Total C O 4 2 2	0	0
3	N	1	Total C O 4 2 2	0	0
3	P	1	Total C O 4 2 2	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

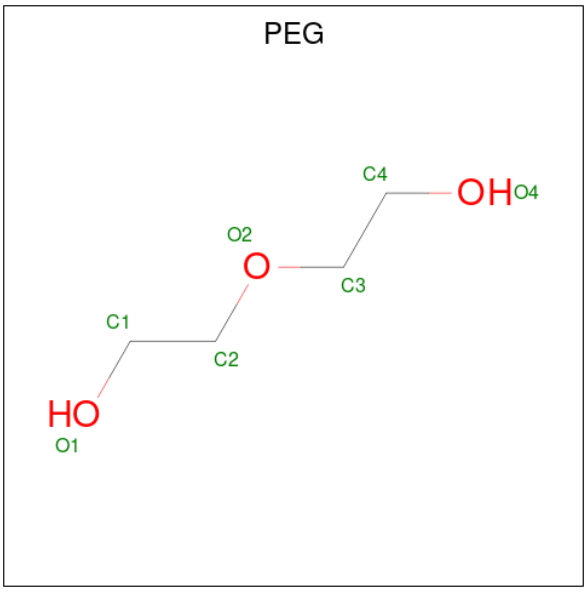


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 16 10 6	0	0
4	P	1	Total C O 16 10 6	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	1	Total Cl 1 1	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	2	Total O 2 2	0	0
7	C	5	Total O 5 5	0	0
7	D	1	Total O 1 1	0	0
7	E	9	Total O 9 9	0	0
7	F	10	Total O 10 10	0	0
7	G	8	Total O 8 8	0	0

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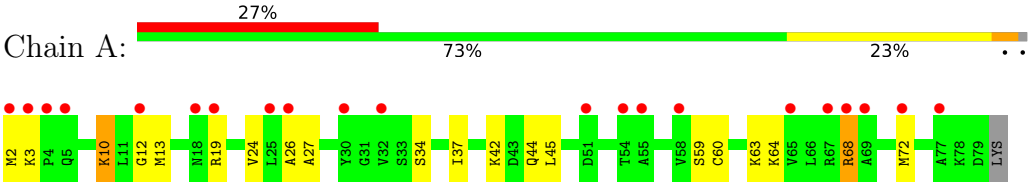
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	12	Total O 12 12	0	0
7	I	14	Total O 14 14	0	0
7	J	17	Total O 17 17	0	0
7	K	7	Total O 7 7	0	0
7	L	8	Total O 8 8	0	0
7	M	19	Total O 19 19	0	0
7	N	22	Total O 22 22	0	0
7	O	22	Total O 22 22	0	0
7	P	27	Total O 27 27	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

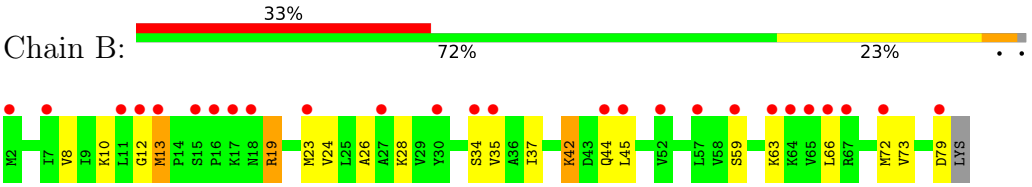
• Molecule 1: sHMAx

Chain A:



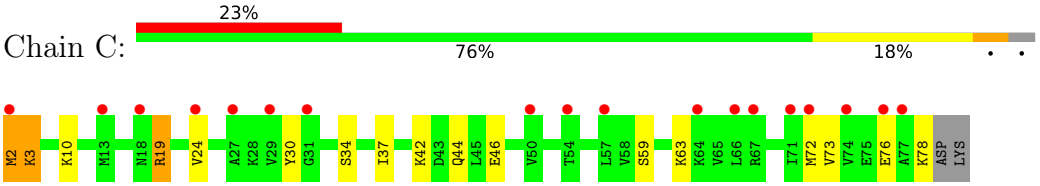
• Molecule 1: sHMAx

Chain B:



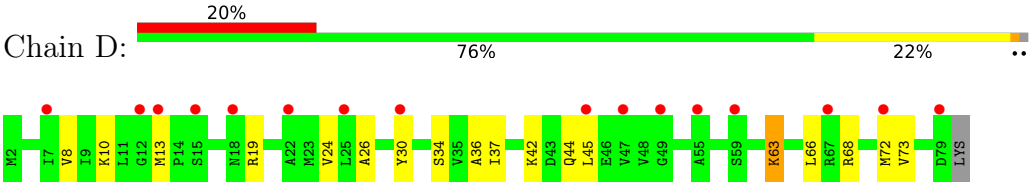
• Molecule 1: sHMAx

Chain C:



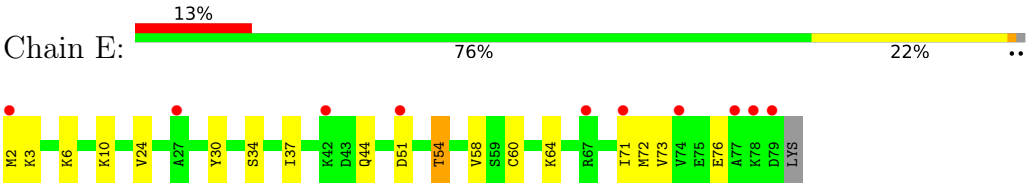
• Molecule 1: sHMAx

Chain D:



• Molecule 1: sHMAx

Chain E:

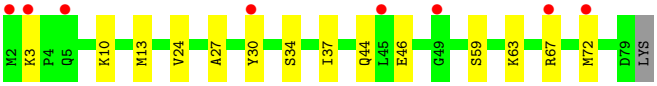


• Molecule 1: sHMAx

Chain F:

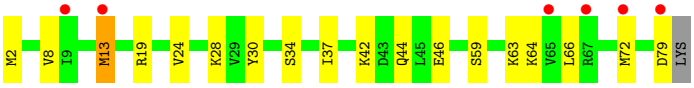
• Molecule 1: sHMAx

Chain G:



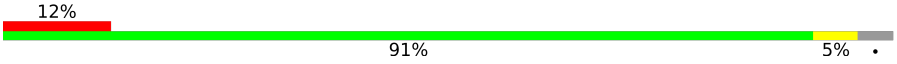
• Molecule 1: sHMAx

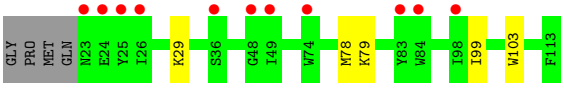
Chain H:



• Molecule 2: APikL2F

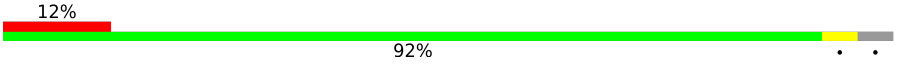
Chain I:

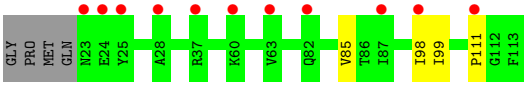




• Molecule 2: APikL2F

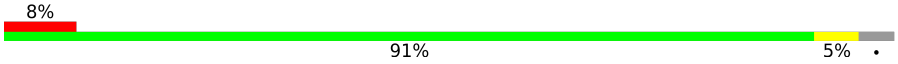
Chain J:

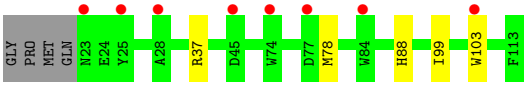




• Molecule 2: APikL2F

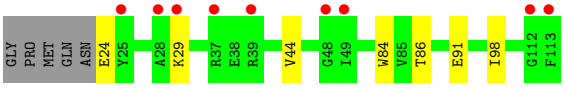
Chain K:





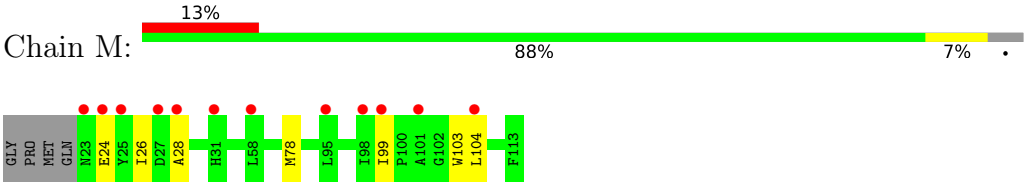
• Molecule 2: APikL2F

Chain L:



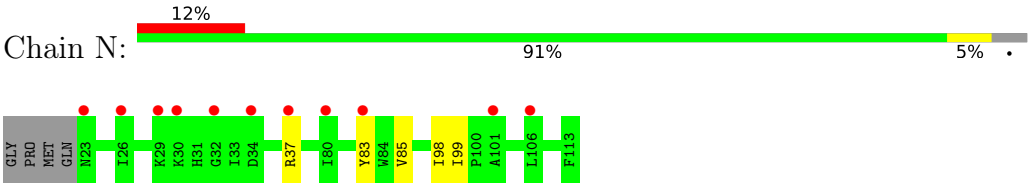
• Molecule 2: APikL2F

Chain M:



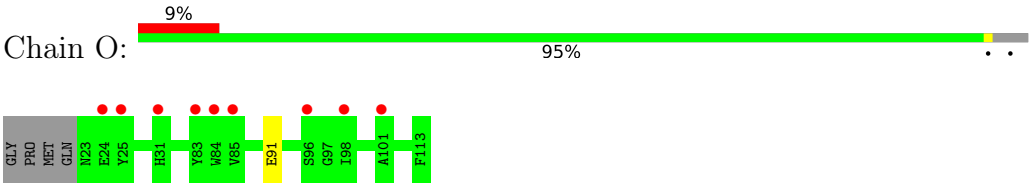
• Molecule 2: APikL2F

Chain N:



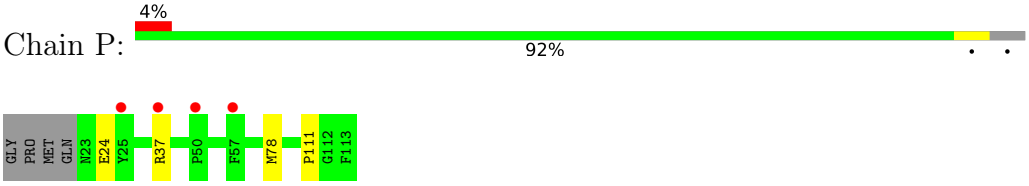
• Molecule 2: APikL2F

Chain O:



• Molecule 2: APikL2F

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.44Å 222.48Å 102.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	109.51 – 2.30 109.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (109.51-2.30) 99.9 (109.27-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.207 , 0.242 0.210 , 0.240	Depositor DCC
R_{free} test set	3170 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	50.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.000 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10945	wwPDB-VP
Average B, all atoms (Å^2)	61.0	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 36.58 % 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 4.8864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: PEG, EDO, 1PE, 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	0.77	0/598	0.88	0/802
1	B	0.76	0/607	0.88	1/814 (0.1%)
1	C	0.78	1/590 (0.2%)	0.95	2/791 (0.3%)
1	D	0.76	0/598	0.89	0/802
1	E	0.81	0/598	0.95	0/802
1	F	0.78	0/598	0.94	2/802 (0.2%)
1	G	0.82	1/598 (0.2%)	0.92	0/802
1	H	0.82	1/598 (0.2%)	0.92	0/802
2	I	0.72	0/765	0.90	0/1036
2	J	0.73	0/765	0.87	0/1036
2	K	0.71	0/765	0.88	1/1036 (0.1%)
2	L	0.72	0/757	0.84	0/1025
2	M	0.75	0/765	0.88	0/1036
2	N	0.75	0/765	0.87	0/1036
2	O	0.73	0/765	0.90	0/1036
2	P	0.75	0/765	0.87	0/1036
All	All	0.76	3/10897 (0.0%)	0.89	6/14694 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	GLU	CD-OE1	-6.38	1.18	1.25
1	G	46	GLU	CD-OE2	5.96	1.32	1.25
1	H	46	GLU	CD-OE2	5.28	1.31	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	19	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	C	19	ARG	NE-CZ-NH2	6.45	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	37	ARG	CB-CG-CD	6.23	127.79	111.60
1	F	13	MET	CG-SD-CE	5.82	109.51	100.20
1	F	19	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	19	ARG	NE-CZ-NH2	-5.13	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	592	0	648	14	0
1	B	601	0	655	17	0
1	C	587	0	643	14	0
1	D	595	0	647	13	0
1	E	595	0	647	16	0
1	F	595	0	647	20	0
1	G	595	0	647	13	0
1	H	595	0	647	19	0
2	I	740	0	703	3	0
2	J	740	0	703	4	0
2	K	740	0	703	5	0
2	L	732	0	697	5	0
2	M	740	0	703	3	0
2	N	740	0	703	5	0
2	O	740	0	703	0	0
2	P	740	0	703	2	0
3	C	8	0	12	0	0
3	E	8	0	12	0	0
3	I	8	0	12	0	0
3	J	4	0	6	0	0
3	K	4	0	6	0	0
3	L	8	0	12	0	0
3	M	4	0	6	0	0
3	N	4	0	6	0	0
3	P	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	L	16	0	22	2	0
4	P	16	0	22	1	0
5	M	1	0	0	0	0
6	O	7	0	10	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	5	0	0	0	0
7	D	1	0	0	0	0
7	E	9	0	0	3	0
7	F	10	0	0	1	0
7	G	8	0	0	0	0
7	H	12	0	0	0	0
7	I	14	0	0	0	0
7	J	17	0	0	2	0
7	K	7	0	0	1	0
7	L	8	0	0	0	0
7	M	19	0	0	0	0
7	N	22	0	0	0	0
7	O	22	0	0	1	0
7	P	27	0	0	0	0
All	All	10945	0	10931	124	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 6.

All (124) 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:H:13:MET:O	1:H:13:MET:HG3	1.46	1.13
1:E:60:CYS:SG	1:E:64:LYS:NZ	2.22	1.12
1:F:60:CYS:SG	1:F:64:LYS:NZ	2.27	1.06
1:A:60:CYS:SG	1:A:64:LYS:NZ	2.27	1.06
1:E:6:LYS:NZ	7:E:201:HOH:O	2.02	0.93
1:F:44:GLN:HG2	1:F:72[B]:MET:CE	2.02	0.89
1:B:23:MET:HE3	1:B:35:VAL:HG23	1.56	0.87
1:B:23:MET:CE	1:B:35:VAL:HG23	2.08	0.83
1:H:13:MET:O	1:H:13:MET:CG	2.27	0.83
2:L:98:ILE:HG22	2:N:98:ILE:HG22	1.65	0.79
1:F:28:LYS:HD3	1:G:30:TYR:CD1	2.17	0.79
2:J:98:ILE:HD12	7:J:314:HOH:O	1.85	0.76
1:E:54:THR:HG23	1:E:71:ILE:CD1	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:8:VAL:HG12	1:H:72[B]:MET:HE1	1.74	0.69
1:D:13:MET:O	1:D:13:MET:CG	2.41	0.69
2:K:88:HIS:ND1	7:K:301:HOH:O	2.26	0.68
1:E:34:SER:HA	1:F:24:VAL:HG21	1.76	0.67
1:G:10:LYS:HB2	1:G:72[A]:MET:HG3	1.75	0.67
1:C:24:VAL:HG21	1:D:34:SER:HA	1.77	0.66
1:C:34:SER:HA	1:D:24:VAL:HG21	1.76	0.66
1:E:54:THR:HG23	1:E:71:ILE:HD11	1.77	0.66
1:F:44:GLN:HG2	1:F:72[B]:MET:HE1	1.74	0.65
1:A:10:LYS:HB2	1:A:72[B]:MET:HG3	1.79	0.65
1:D:10:LYS:HB2	1:D:72[A]:MET:HG3	1.79	0.65
1:H:44:GLN:HG2	1:H:72[B]:MET:CE	2.26	0.64
1:E:24:VAL:HG21	1:F:34:SER:HA	1.78	0.64
1:F:44:GLN:HG2	1:F:72[B]:MET:HE3	1.79	0.64
1:D:13:MET:O	1:D:13:MET:HG3	1.99	0.63
1:E:3:LYS:HD3	1:E:76:GLU:OE2	1.97	0.63
1:G:34:SER:HA	1:H:24:VAL:HG21	1.80	0.62
1:E:10:LYS:HB2	1:E:72[A]:MET:HG3	1.82	0.62
1:C:10:LYS:HB2	1:C:72[B]:MET:HG3	1.81	0.61
1:F:19:ARG:HD2	1:F:37:ILE:HG21	1.84	0.59
1:B:19:ARG:HD2	1:B:37:ILE:HG21	1.84	0.59
1:H:44:GLN:HG2	1:H:72[B]:MET:HE2	1.83	0.59
1:G:24:VAL:HG21	1:H:34:SER:HA	1.85	0.58
1:H:8:VAL:CG1	1:H:72[B]:MET:HE1	2.33	0.58
2:J:98:ILE:CD1	7:J:314:HOH:O	2.49	0.58
1:H:8:VAL:HG12	1:H:72[B]:MET:CE	2.34	0.57
1:H:19:ARG:HD2	1:H:37:ILE:HG21	1.86	0.57
1:C:19:ARG:HD2	1:C:37:ILE:HG21	1.88	0.56
1:B:10:LYS:HB2	1:B:72[A]:MET:HG3	1.88	0.56
1:E:51:ASP:O	1:H:64:LYS:NZ	2.39	0.56
1:F:59:SER:O	1:F:63:LYS:HG3	2.07	0.56
1:E:58:VAL:HG21	1:E:71:ILE:HG13	1.87	0.55
1:A:27:ALA:O	1:B:28:LYS:NZ	2.29	0.55
1:A:64:LYS:HE2	1:D:30:TYR:CE2	2.41	0.55
1:E:73:VAL:HG22	2:M:78:MET:HG3	1.88	0.55
1:A:24:VAL:HG21	1:B:34:SER:HA	1.89	0.54
1:B:23:MET:HE2	1:B:35:VAL:HG23	1.89	0.54
1:B:79:ASP:C	1:G:13:MET:HG3	2.27	0.54
1:F:2:MET:N	7:F:101:HOH:O	2.40	0.54
1:H:59:SER:O	1:H:63:LYS:HG3	2.07	0.54
1:D:19:ARG:HD3	1:D:42:LYS:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:SER:HA	1:B:24:VAL:HG21	1.90	0.53
1:A:59:SER:O	1:A:63:LYS:HG3	2.09	0.53
1:A:19:ARG:HD3	1:A:42:LYS:O	2.09	0.53
2:N:85:VAL:HG11	2:N:99:ILE:HG22	1.91	0.53
1:F:44:GLN:CG	1:F:72[B]:MET:HE3	2.39	0.53
1:F:19:ARG:HD3	1:F:42:LYS:O	2.10	0.52
1:B:59:SER:O	1:B:63:LYS:HG3	2.10	0.52
1:A:19:ARG:HD2	1:A:37:ILE:HG21	1.92	0.51
1:G:72[A]:MET:HE1	7:O:312:HOH:O	2.12	0.50
1:B:28:LYS:HD3	1:C:30:TYR:CD1	2.47	0.50
1:C:59:SER:O	1:C:63:LYS:HG3	2.12	0.50
1:F:44:GLN:CD	1:F:72[B]:MET:HE3	2.32	0.50
1:B:72[B]:MET:HE2	1:B:73:VAL:HG23	1.92	0.49
2:J:111:PRO:HB3	2:P:111:PRO:HB3	1.93	0.49
1:D:19:ARG:HD2	1:D:37:ILE:HG21	1.95	0.49
1:A:13:MET:CE	1:H:79:ASP:O	2.61	0.49
1:B:19:ARG:HD3	1:B:42:LYS:O	2.12	0.49
1:G:59:SER:O	1:G:63:LYS:HG3	2.13	0.48
1:A:12:GLY:HA3	1:A:68:ARG:HB3	1.94	0.48
1:F:28:LYS:HE3	1:G:30:TYR:CE1	2.48	0.48
1:H:19:ARG:HD3	1:H:42:LYS:O	2.13	0.48
1:E:54:THR:HG23	1:E:71:ILE:HD13	1.94	0.48
2:L:98:ILE:HD11	2:N:83:TYR:CD2	2.49	0.48
1:F:28:LYS:CD	1:G:30:TYR:CD1	2.93	0.47
2:J:85:VAL:HG11	2:J:99:ILE:HG22	1.95	0.47
7:E:209:HOH:O	1:G:30:TYR:CE1	2.56	0.47
1:G:27:ALA:O	1:H:28:LYS:NZ	2.37	0.47
1:B:12:GLY:C	1:B:13:MET:HG2	2.35	0.47
1:F:8:VAL:HB	1:F:73:VAL:HB	1.97	0.46
1:C:72[A]:MET:O	2:K:78:MET:HA	2.16	0.46
2:I:78:MET:HE2	2:I:78:MET:HB2	1.80	0.45
1:D:63:LYS:HB3	1:D:63:LYS:HE2	1.73	0.45
2:N:37:ARG:HB3	2:N:37:ARG:NH1	2.31	0.45
1:A:44:GLN:OE1	1:A:72[A]:MET:SD	2.75	0.44
1:E:64:LYS:HE2	1:H:30:TYR:CD2	2.53	0.44
1:C:37:ILE:HA	1:C:44:GLN:O	2.18	0.44
1:C:19:ARG:HD3	1:C:42:LYS:O	2.17	0.43
1:C:72[B]:MET:O	2:K:78:MET:HA	2.18	0.43
1:C:3:LYS:H	1:C:3:LYS:HD2	1.83	0.43
1:F:10:LYS:HB2	1:F:72[A]:MET:HG3	2.00	0.43
1:D:36:ALA:HB2	2:L:44:VAL:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:202:1PE:H232	4:P:202:1PE:H122	1.36	0.43
1:F:44:GLN:CG	1:F:72[B]:MET:CE	2.86	0.42
1:F:26:ALA:HB2	1:F:45:LEU:HD21	2.01	0.42
2:L:86:THR:OG1	4:L:202:1PE:H252	2.19	0.42
1:G:37:ILE:HA	1:G:44:GLN:O	2.19	0.42
1:H:37:ILE:HA	1:H:44:GLN:O	2.19	0.42
1:A:72[B]:MET:HE3	2:I:79:LYS:HB3	2.01	0.42
1:B:37:ILE:HA	1:B:44:GLN:O	2.20	0.42
7:E:209:HOH:O	1:G:30:TYR:HE1	1.95	0.41
1:F:37:ILE:HA	1:F:44:GLN:O	2.20	0.41
1:C:73:VAL:HG22	2:K:78:MET:HG3	2.03	0.41
1:E:54:THR:CG2	1:E:71:ILE:HD13	2.50	0.41
2:K:99:ILE:HD11	2:K:103:TRP:O	2.20	0.41
1:B:26:ALA:HB2	1:B:45:LEU:HD21	2.03	0.41
2:N:37:ARG:HH11	2:N:37:ARG:CB	2.34	0.41
1:D:37:ILE:HA	1:D:44:GLN:O	2.21	0.41
1:D:8:VAL:HB	1:D:73:VAL:HB	2.01	0.41
2:M:28:ALA:HB2	2:M:104:LEU:HD21	2.03	0.41
2:I:99:ILE:HD11	2:I:103:TRP:O	2.21	0.41
1:D:26:ALA:HB2	1:D:45:LEU:HD21	2.03	0.41
1:E:37:ILE:HA	1:E:44:GLN:O	2.20	0.41
2:L:84:TRP:HB3	4:L:202:1PE:H151	2.01	0.41
1:H:72[B]:MET:O	2:P:78:MET:HA	2.21	0.40
1:A:26:ALA:HB2	1:A:45:LEU:HD21	2.03	0.40
1:B:8:VAL:HB	1:B:73:VAL:HB	2.03	0.40
1:C:2:MET:CE	1:C:2:MET:HA	2.52	0.40
1:E:30:TYR:CG	1:H:28:LYS:HD3	2.57	0.40
2:M:99:ILE:HD11	2:M:103:TRP:O	2.22	0.40
1:C:44:GLN:OE1	1:C:72[A]:MET:SD	2.79	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	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
1	B	78/79 (99%)	77 (99%)	1 (1%)	0	100	100
1	C	76/79 (96%)	75 (99%)	1 (1%)	0	100	100
1	D	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
1	E	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
1	F	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
1	G	77/79 (98%)	76 (99%)	1 (1%)	0	100	100
1	H	77/79 (98%)	74 (96%)	3 (4%)	0	100	100
2	I	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
2	J	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
2	K	89/95 (94%)	89 (100%)	0	0	100	100
2	L	88/95 (93%)	87 (99%)	1 (1%)	0	100	100
2	M	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
2	N	89/95 (94%)	89 (100%)	0	0	100	100
2	O	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
2	P	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
All	All	1327/1392 (95%)	1311 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	68/68 (100%)	64 (94%)	4 (6%)	19	27
1	B	69/68 (102%)	66 (96%)	3 (4%)	29	40
1	C	67/68 (98%)	63 (94%)	4 (6%)	19	26
1	D	68/68 (100%)	65 (96%)	3 (4%)	28	39
1	E	68/68 (100%)	66 (97%)	2 (3%)	42	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	68/68 (100%)	67 (98%)	1 (2%)	65 79
1	G	68/68 (100%)	66 (97%)	2 (3%)	42 58
1	H	68/68 (100%)	65 (96%)	3 (4%)	28 39
2	I	78/81 (96%)	77 (99%)	1 (1%)	69 82
2	J	78/81 (96%)	78 (100%)	0	100 100
2	K	78/81 (96%)	78 (100%)	0	100 100
2	L	77/81 (95%)	74 (96%)	3 (4%)	32 46
2	M	78/81 (96%)	76 (97%)	2 (3%)	46 63
2	N	78/81 (96%)	78 (100%)	0	100 100
2	O	78/81 (96%)	77 (99%)	1 (1%)	69 82
2	P	78/81 (96%)	76 (97%)	2 (3%)	46 63
All	All	1167/1192 (98%)	1136 (97%)	31 (3%)	44 61

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	3	LYS
1	A	10	LYS
1	A	68	ARG
1	B	13	MET
1	B	42	LYS
1	B	66	LEU
1	C	2	MET
1	C	3	LYS
1	C	76	GLU
1	C	78	LYS
1	D	63	LYS
1	D	66	LEU
1	D	68	ARG
1	E	2	MET
1	E	54	THR
1	F	2	MET
1	G	3	LYS
1	G	67	ARG
1	H	2	MET
1	H	13	MET
1	H	66	LEU

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Mol	Chain	Res	Type
2	I	29	LYS
2	L	24	GLU
2	L	29	LYS
2	L	91	GLU
2	M	24	GLU
2	M	26	ILE
2	O	91	GLU
2	P	24	GLU
2	P	37	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	B	18	ASN
1	C	18	ASN
1	D	18	ASN
1	E	18	ASN
1	F	18	ASN
1	G	18	ASN
1	H	18	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	78/79 (98%)	1.58	21 (26%) 0 0	48, 68, 97, 112	0
1	B	78/79 (98%)	1.69	26 (33%) 0 0	52, 71, 98, 124	0
1	C	77/79 (97%)	1.44	18 (23%) 0 1	43, 65, 99, 127	0
1	D	78/79 (98%)	1.27	16 (20%) 1 1	48, 66, 98, 119	0
1	E	78/79 (98%)	0.96	10 (12%) 3 5	38, 50, 77, 106	0
1	F	78/79 (98%)	0.86	8 (10%) 6 9	41, 54, 85, 104	0
1	G	78/79 (98%)	0.88	8 (10%) 6 9	38, 55, 85, 112	0
1	H	78/79 (98%)	0.66	6 (7%) 13 17	37, 50, 82, 98	0
2	I	91/95 (95%)	0.94	11 (12%) 4 6	37, 54, 79, 115	0
2	J	91/95 (95%)	1.10	11 (12%) 4 6	46, 62, 84, 115	0
2	K	91/95 (95%)	1.28	8 (8%) 10 13	40, 66, 103, 130	0
2	L	90/95 (94%)	0.93	9 (10%) 7 10	45, 59, 93, 106	0
2	M	91/95 (95%)	1.04	12 (13%) 3 4	37, 51, 89, 114	0
2	N	91/95 (95%)	0.83	11 (12%) 4 6	40, 55, 90, 107	0
2	O	91/95 (95%)	0.78	9 (9%) 7 10	34, 54, 82, 103	0
2	P	91/95 (95%)	0.54	4 (4%) 34 41	32, 45, 75, 100	0
All	All	1350/1392 (96%)	1.04	188 (13%) 2 4	32, 58, 93, 130	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	23	ASN	30.8
1	A	2	MET	13.2
1	C	2	MET	12.6
2	M	25	TYR	8.6
2	J	37	ARG	8.0

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Mol	Chain	Res	Type	RSRZ
2	M	28	ALA	7.9
1	B	27	ALA	7.2
2	K	25	TYR	6.9
1	H	13	MET	6.4
1	B	67	ARG	6.3
1	C	66	LEU	6.2
2	J	24	GLU	6.1
2	L	49	ILE	5.8
1	E	2	MET	5.6
1	D	67	ARG	5.6
1	A	30	TYR	5.4
1	F	18	ASN	5.4
1	D	13	MET	5.3
1	B	52	VAL	5.2
1	B	12	GLY	5.0
1	B	45	LEU	5.0
1	A	65	VAL	4.9
1	B	65	VAL	4.9
2	J	25	TYR	4.8
2	M	24	GLU	4.8
1	D	30	TYR	4.7
1	D	12	GLY	4.7
2	J	98	ILE	4.7
1	D	59	SER	4.6
2	I	23	ASN	4.6
1	D	45	LEU	4.6
1	A	12	GLY	4.5
2	I	25	TYR	4.5
2	L	48	GLY	4.4
1	B	13	MET	4.3
2	J	28	ALA	4.3
1	A	3	LYS	4.2
1	B	64	LYS	4.2
1	A	18	ASN	4.1
1	A	26	ALA	4.1
1	B	35	VAL	4.0
1	C	31	GLY	4.0
2	M	98	ILE	4.0
1	C	67	ARG	4.0
1	C	27	ALA	3.9
1	C	77	ALA	3.8
1	B	16	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	30	TYR	3.7
1	F	13	MET	3.7
2	N	26	ILE	3.7
1	E	79	ASP	3.7
2	N	83	TYR	3.7
1	D	47	VAL	3.7
1	D	49	GLY	3.6
2	N	101	ALA	3.6
2	M	27	ASP	3.6
2	J	82	GLN	3.6
1	C	54	THR	3.6
1	B	72[A]	MET	3.5
1	E	51	ASP	3.5
1	B	30	TYR	3.5
2	N	32	GLY	3.4
1	B	11	LEU	3.4
2	N	37	ARG	3.4
2	L	25	TYR	3.3
1	B	34	SER	3.3
1	F	72[A]	MET	3.3
2	N	23	ASN	3.3
1	A	58	VAL	3.3
2	K	45	ASP	3.3
1	H	67	ARG	3.3
1	D	22	ALA	3.3
1	A	25	LEU	3.3
1	G	2	MET	3.3
1	A	54	THR	3.2
1	D	7	ILE	3.2
1	C	50	VAL	3.2
2	K	103	TRP	3.2
2	O	101	ALA	3.1
1	D	18	ASN	3.1
2	I	24	GLU	3.1
1	A	32	VAL	3.1
1	B	79	ASP	3.1
2	I	98	ILE	3.1
1	G	67	ARG	3.1
2	I	48	GLY	3.0
2	I	36	SER	3.0
1	C	74	VAL	3.0
1	C	71	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	76	GLU	3.0
2	N	80	ILE	3.0
2	J	111	PRO	3.0
2	O	98	ILE	2.9
2	M	23	ASN	2.9
2	K	74	TRP	2.9
1	B	2	MET	2.9
2	I	83	TYR	2.9
2	O	25	TYR	2.9
1	F	55	ALA	2.9
1	D	55	ALA	2.9
1	B	23	MET	2.9
2	K	28	ALA	2.9
2	L	29	LYS	2.8
1	A	67	ARG	2.8
1	F	30	TYR	2.8
2	I	84	TRP	2.8
1	C	76	GLU	2.8
2	L	28	ALA	2.7
1	G	5	GLN	2.7
2	N	34	ASP	2.7
1	G	72[A]	MET	2.7
2	L	39	ARG	2.7
1	D	15	SER	2.6
2	P	50	PRO	2.6
1	E	74	VAL	2.6
1	E	42	LYS	2.6
1	E	77	ALA	2.6
2	P	37	ARG	2.5
1	C	57	LEU	2.5
2	N	29	LYS	2.5
2	N	30	LYS	2.5
2	J	63	VAL	2.5
2	M	31	HIS	2.5
1	D	25	LEU	2.5
1	D	72[A]	MET	2.5
2	O	24	GLU	2.5
1	F	77	ALA	2.5
1	B	7	ILE	2.5
1	H	72[A]	MET	2.4
2	O	85	VAL	2.4
2	O	84	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	17	LYS	2.4
2	P	25	TYR	2.4
2	L	113	PHE	2.4
1	B	66	LEU	2.4
2	O	31	HIS	2.4
1	G	3	LYS	2.4
2	L	112	GLY	2.4
1	A	72[A]	MET	2.3
1	C	18	ASN	2.3
2	J	87	ILE	2.3
1	A	68	ARG	2.3
2	I	74	TRP	2.3
2	K	84	TRP	2.3
2	M	101	ALA	2.3
2	M	58	LEU	2.3
1	B	15	SER	2.3
1	E	78	LYS	2.3
1	C	24	VAL	2.3
2	I	26	ILE	2.3
1	A	77	ALA	2.3
1	E	27	ALA	2.3
2	O	83	TYR	2.3
1	B	63	LYS	2.3
1	A	55	ALA	2.3
2	M	99	ILE	2.3
2	O	96	SER	2.3
1	G	49	GLY	2.2
1	C	13	MET	2.2
1	D	79	ASP	2.2
1	C	29	VAL	2.2
2	J	60	LYS	2.2
1	C	64	LYS	2.2
1	C	72[A]	MET	2.2
1	A	51	ASP	2.2
1	E	71	ILE	2.2
2	L	37	ARG	2.2
2	M	104	LEU	2.2
1	H	65	VAL	2.2
1	A	4	PRO	2.2
1	B	18	ASN	2.1
2	I	49	ILE	2.1
1	F	3	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	J	23	ASN	2.1
1	G	45	LEU	2.1
1	B	44	GLN	2.1
2	K	77	ASP	2.1
1	B	57	LEU	2.1
2	N	106	LEU	2.1
1	E	67	ARG	2.1
1	A	69	ALA	2.1
1	B	59	SER	2.1
2	M	95	LEU	2.1
1	A	19	ARG	2.0
1	H	9	ILE	2.0
1	H	79	ASP	2.0
2	P	57	PHE	2.0
1	A	5	GLN	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	C	101	4/4	0.31	0.68	80,85,92,93	0
3	EDO	K	201	4/4	0.51	0.26	67,68,75,78	0
6	PEG	O	201	7/7	0.58	0.28	82,84,90,91	0
3	EDO	I	202	4/4	0.71	0.34	83,86,87,91	0
3	EDO	E	102	4/4	0.72	0.24	73,76,78,79	0
3	EDO	C	102	4/4	0.72	0.22	70,74,77,82	0
3	EDO	L	201	4/4	0.76	0.18	81,81,82,84	0
3	EDO	P	201	4/4	0.77	0.25	55,62,66,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	N	201	4/4	0.78	0.28	71,75,79,81	0
3	EDO	I	201	4/4	0.80	0.19	61,66,66,72	0
3	EDO	L	203	4/4	0.81	0.18	71,74,74,78	0
3	EDO	J	201	4/4	0.81	0.19	65,69,75,78	0
3	EDO	E	101	4/4	0.82	0.19	73,76,81,82	0
4	1PE	P	202	16/16	0.85	0.22	30,44,48,50	16
4	1PE	L	202	16/16	0.85	0.26	50,74,92,92	0
3	EDO	M	201	4/4	0.87	0.23	75,76,78,79	0
5	CL	M	202	1/1	0.94	0.16	62,62,62,62	1

6.5 Other polymers (i)

There are no such residues in this entry.