



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3MBH
Title : Crystal structure of a putative phosphomethylpyrimidine kinase (BT_4458) from BACTEROIDES THETA IOTAOMICRON VPI-5482 at 2.00 Å resolution (orthorhombic form with pyridoxal)
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2010-03-25
Resolution : 2.00 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

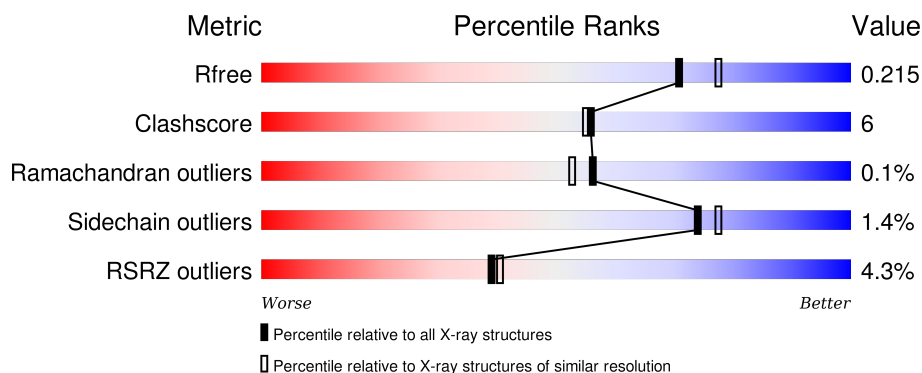
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	291	
1	B	291	
1	C	291	
1	D	291	
1	E	291	

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Mol	Chain	Length	Quality of chain
1	F	291	<div><div></div><div>7%</div><div>89%</div><div>10%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15283 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.

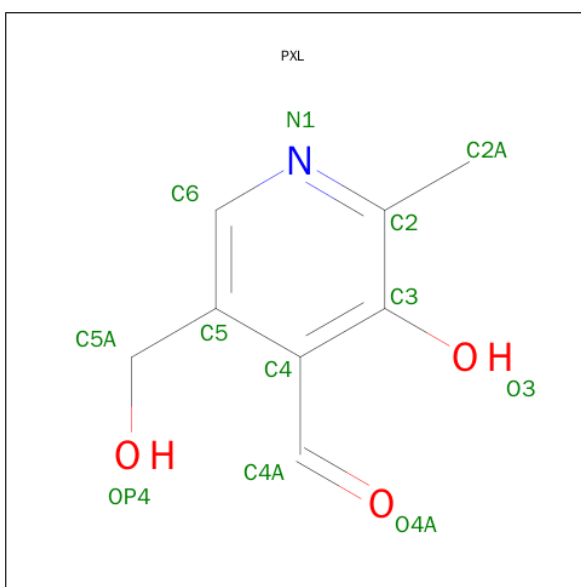
- Molecule 1 is a protein called Putative phosphomethylpyrimidine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	Se	0	14	0
			2409	1543	398	451	3	14			
1	B	287	Total	C	N	O	S	Se	0	11	0
			2350	1509	379	446	2	14			
1	C	289	Total	C	N	O	S	Se	0	7	0
			2329	1496	379	440	3	11			
1	D	286	Total	C	N	O	S	Se	0	9	0
			2344	1508	383	435	3	15			
1	E	290	Total	C	N	O	S	Se	0	17	0
			2411	1547	390	456	2	16			
1	F	290	Total	C	N	O	S	Se	0	9	0
			2341	1510	379	436	2	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	leader sequence	UNP Q89ZB9
B	0	GLY	-	leader sequence	UNP Q89ZB9
C	0	GLY	-	leader sequence	UNP Q89ZB9
D	0	GLY	-	leader sequence	UNP Q89ZB9
E	0	GLY	-	leader sequence	UNP Q89ZB9
F	0	GLY	-	leader sequence	UNP Q89ZB9

- Molecule 2 is 3-HYDROXY-5-(HYDROXYMETHYL)-2-METHYLISONICOTINALDEHYDE (three-letter code: PXL) (formula: C₈H₉NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			12	8	1	3		
2	B	1	Total	C	N	O	0	0
			12	8	1	3		
2	C	1	Total	C	N	O	0	0
			12	8	1	3		
2	D	1	Total	C	N	O	0	0
			12	8	1	3		
2	E	1	Total	C	N	O	0	0
			12	8	1	3		
2	F	1	Total	C	N	O	0	0
			12	8	1	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	F	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

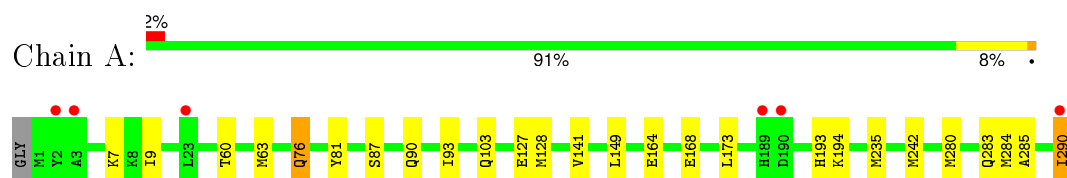
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total 206	O 206	0	0
4	B	160	Total 160	O 160	0	0
4	C	213	Total 214	O 214	0	1
4	D	145	Total 145	O 145	0	0
4	E	215	Total 215	O 215	0	0
4	F	83	Total 83	O 83	0	0

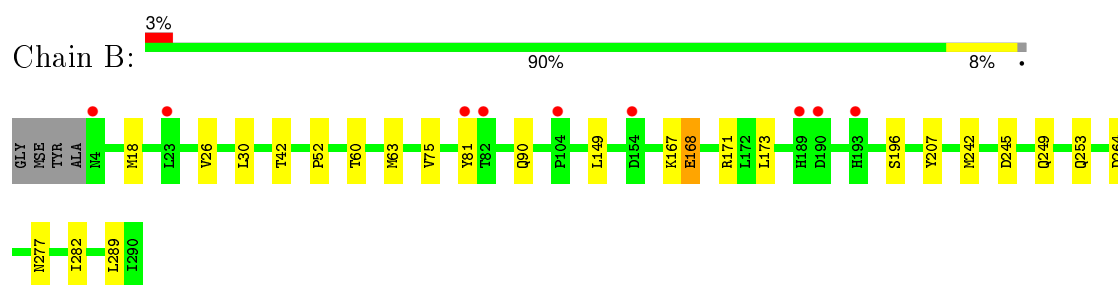
3 Residue-property plots [i](#)

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

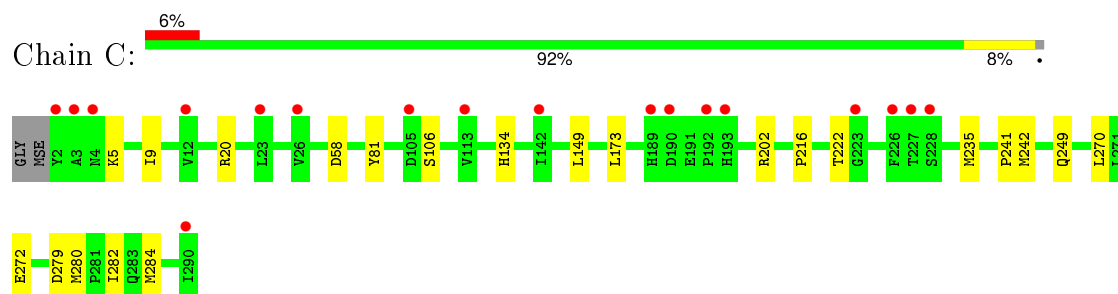
- Molecule 1: Putative phosphomethylpyrimidine kinase



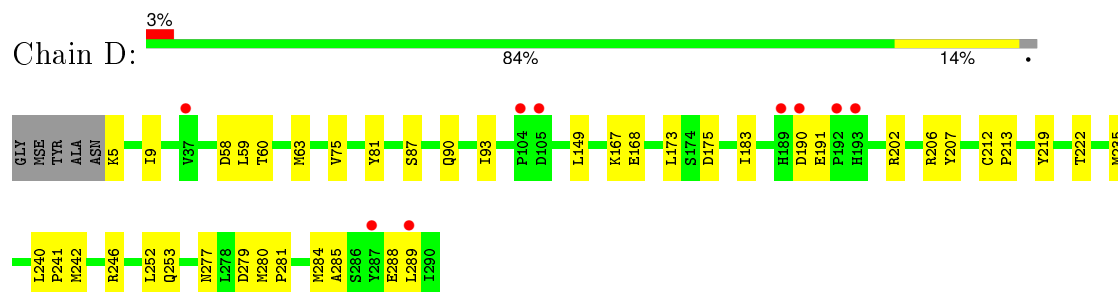
- Molecule 1: Putative phosphomethylpyrimidine kinase



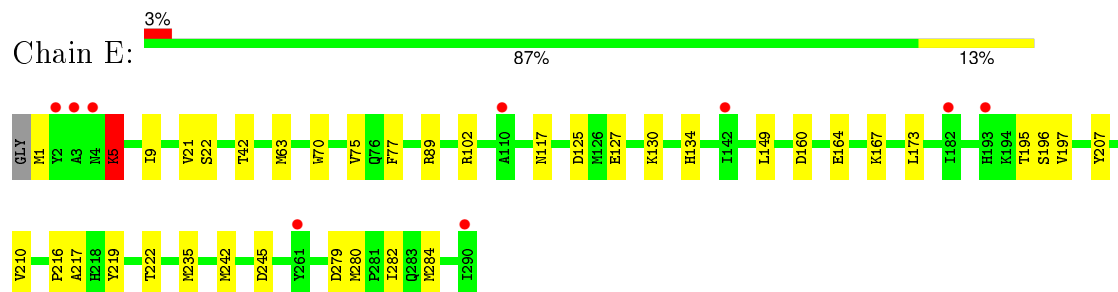
- Molecule 1: Putative phosphomethylpyrimidine kinase



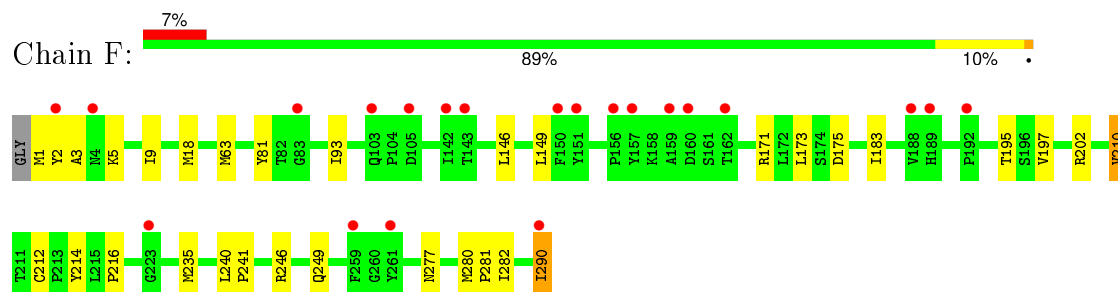
- Molecule 1: Putative phosphomethylpyrimidine kinase



- Molecule 1: Putative phosphomethylpyrimidine kinase



- Molecule 1: Putative phosphomethylpyrimidine kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	93.72Å 138.37Å 143.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 2.00 29.81 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (29.81-2.00) 99.6 (29.81-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.167 , 0.206 0.182 , 0.215	Depositor DCC
R_{free} test set	6306 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 125765 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15283	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PXL

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	0.87	2/2453 (0.1%)	0.80	0/3313
1	B	0.82	0/2392	0.80	2/3231 (0.1%)
1	C	0.87	1/2372 (0.0%)	0.82	2/3209 (0.1%)
1	D	0.76	0/2388	0.80	1/3227 (0.0%)
1	E	0.89	0/2453	0.82	3/3312 (0.1%)
1	F	0.72	0/2384	0.73	0/3223
All	All	0.82	3/14442 (0.0%)	0.80	8/19515 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	GLU	CB-CG	-5.87	1.41	1.52
1	A	141	VAL	CB-CG1	5.71	1.64	1.52
1	C	272	GLU	CD-OE1	5.36	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	102	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	264	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	58	ASP	CB-CG-OD1	6.07	123.76	118.30
1	C	20	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	264	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	E	102	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	D	58	ASP	CB-CG-OD1	5.55	123.29	118.30
1	E	125	ASP	CB-CG-OD1	5.07	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2409	0	2391	36	0
1	B	2350	0	2315	30	0
1	C	2329	0	2293	15	0
1	D	2344	0	2331	38	0
1	E	2411	0	2372	48	0
1	F	2341	0	2298	33	0
2	A	12	0	8	0	0
2	B	12	0	9	0	0
2	C	12	0	8	0	0
2	D	12	0	9	0	0
2	E	12	0	8	1	0
2	F	12	0	9	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	206	0	0	4	0
4	B	160	0	0	2	0
4	C	214	0	0	2	0
4	D	145	0	0	2	0
4	E	215	0	0	6	0
4	F	83	0	0	3	0
All	All	15283	0	14051	177	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 (177) 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:D:9:ILE:HD11	1:D:235[B]:MSE:CE	1.62	1.29
1:D:9:ILE:HD11	1:D:235[B]:MSE:HE1	1.31	1.09
1:A:60:THR:HA	1:A:63[A]:MSE:HE2	1.41	1.03
1:A:63[A]:MSE:HE1	1:A:90:GLN:HG2	1.45	0.99
1:B:18[B]:MSE:HE3	1:E:75:VAL:HG11	1.46	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242[B]:MSE:HG3	1:E:284[B]:MSE:HE1	1.46	0.97
1:A:290:ILE:O	1:A:290:ILE:HD12	1.66	0.95
1:E:242[B]:MSE:HG2	1:E:284[B]:MSE:CE	1.96	0.94
1:D:9:ILE:HD11	1:D:235[B]:MSE:HE2	1.48	0.94
1:B:18[B]:MSE:HE1	1:E:77:PHE:CZ	2.03	0.93
1:F:280[A]:MSE:HA	1:F:280[A]:MSE:HE2	1.49	0.93
1:E:242[B]:MSE:CG	1:E:284[B]:MSE:CE	2.48	0.92
1:B:18[B]:MSE:CE	1:E:75:VAL:HG11	1.99	0.91
1:C:216:PRO:HB2	1:C:222[B]:THR:HG21	1.49	0.91
1:B:18[B]:MSE:CE	1:E:75:VAL:HG21	2.01	0.89
1:D:9:ILE:CD1	1:D:235[B]:MSE:HE1	2.02	0.89
1:F:2:TYR:HB3	4:F:957:HOH:O	1.72	0.88
1:F:171[A]:ARG:NH1	1:F:202[A]:ARG:CZ	2.36	0.87
1:F:195:THR:HG22	1:F:214:TYR:O	1.75	0.87
1:D:9:ILE:CD1	1:D:235[B]:MSE:CE	2.50	0.86
1:B:149:LEU:HD12	1:B:173:LEU:HD11	1.59	0.85
1:E:242[B]:MSE:CG	1:E:284[B]:MSE:HE1	2.06	0.85
1:B:63[A]:MSE:HE1	1:B:90:GLN:HG2	1.58	0.84
1:E:280[B]:MSE:HA	1:E:280[B]:MSE:HE2	1.58	0.83
1:E:242[B]:MSE:HA	1:E:284[B]:MSE:HE2	1.58	0.83
1:F:149:LEU:HD22	1:F:183:ILE:HD13	1.63	0.81
1:F:171[A]:ARG:NH1	1:F:202[A]:ARG:NH2	2.29	0.80
1:D:63[A]:MSE:HE1	1:D:90:GLN:HG2	1.65	0.78
1:B:18[B]:MSE:HE3	1:E:75:VAL:HG21	1.65	0.78
1:E:242[B]:MSE:HG2	1:E:284[B]:MSE:HE3	1.68	0.76
1:D:60:THR:HA	1:D:63[A]:MSE:HE2	1.68	0.74
1:B:18[B]:MSE:HE3	1:E:75:VAL:CG1	2.18	0.74
1:F:171[A]:ARG:HH12	1:F:202[A]:ARG:CZ	2.00	0.73
1:B:242[B]:MSE:HE1	1:B:282:ILE:H	1.54	0.72
1:F:195:THR:HG21	1:F:216:PRO:HD3	1.72	0.71
1:B:18[B]:MSE:HE1	1:E:77:PHE:HZ	1.55	0.70
1:A:290:ILE:O	1:A:290:ILE:CD1	2.39	0.70
1:A:284[B]:MSE:SE	1:D:252:LEU:HD21	2.44	0.68
1:B:168:GLU:HG2	1:B:171[A]:ARG:HH11	1.58	0.68
1:D:9:ILE:CG1	1:D:235[B]:MSE:HE1	2.24	0.68
1:D:63[A]:MSE:HE1	1:D:90:GLN:CG	2.25	0.67
4:A:613:HOH:O	1:E:284[B]:MSE:HE3	1.96	0.66
1:A:284[B]:MSE:HE3	1:A:285:ALA:CA	2.26	0.66
4:A:907:HOH:O	1:C:5:LYS:HA	1.94	0.66
1:E:219:TYR:O	1:E:222[B]:THR:HG23	1.96	0.65
1:A:76[A]:GLN:NE2	4:A:1021:HOH:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63[A]:MSE:HE1	1:A:90:GLN:CG	2.23	0.65
1:A:149:LEU:HD12	1:A:173:LEU:HD11	1.80	0.64
1:B:18[B]:MSE:HE1	1:E:75:VAL:HG21	1.81	0.63
1:A:60:THR:HA	1:A:63[A]:MSE:CE	2.25	0.61
1:B:42:THR:HG22	1:B:63[B]:MSE:CE	2.30	0.61
1:B:18[B]:MSE:HE3	1:E:75:VAL:CG2	2.30	0.61
1:A:284[B]:MSE:SE	1:D:252:LEU:CD2	2.99	0.60
1:F:290:ILE:CG2	1:F:290:ILE:OXT	2.48	0.60
1:E:280[B]:MSE:CE	1:E:280[B]:MSE:HA	2.31	0.60
1:C:202:ARG:HD3	4:C:457:HOH:O	2.02	0.60
1:D:9:ILE:CD1	1:D:235[B]:MSE:HE2	2.23	0.60
1:E:279:ASP:HB2	4:E:1022:HOH:O	2.01	0.59
1:B:63[A]:MSE:HE1	1:B:90:GLN:CG	2.32	0.59
1:C:216:PRO:CB	1:C:222[B]:THR:HG21	2.29	0.59
1:B:60:THR:HA	1:B:63[A]:MSE:HE2	1.85	0.59
1:D:284:MSE:HE2	1:D:285:ALA:O	2.02	0.59
1:C:149:LEU:HD12	1:C:173:LEU:HD11	1.86	0.58
1:B:18[B]:MSE:HE3	1:E:75:VAL:CB	2.33	0.58
1:B:63[A]:MSE:CE	1:B:90:GLN:HG2	2.33	0.58
1:D:242[C]:MSE:SE	4:D:412:HOH:O	2.72	0.58
1:A:284[B]:MSE:HE3	1:A:285:ALA:HA	1.87	0.57
1:F:290:ILE:OXT	1:F:290:ILE:HG22	2.04	0.57
1:E:42:THR:HG22	1:E:63[B]:MSE:CE	2.35	0.57
1:D:219:TYR:O	1:D:222:THR:HG23	2.04	0.56
1:E:117:ASN:HD21	1:E:217:ALA:HB1	1.71	0.56
1:E:160:ASP:CB	4:E:1002:HOH:O	2.53	0.56
1:E:242[B]:MSE:CA	1:E:284[B]:MSE:HE2	2.33	0.56
1:C:242:MSE:HA	1:C:284:MSE:HE3	1.88	0.56
1:F:280[A]:MSE:HA	1:F:280[A]:MSE:CE	2.30	0.55
1:A:63[B]:MSE:HE3	1:A:93:ILE:HB	1.88	0.55
1:E:134:HIS:HB2	4:E:1017:HOH:O	2.07	0.55
1:B:253:GLN:OE1	1:B:277:ASN:ND2	2.40	0.55
1:D:206:ARG:NH1	1:D:289:LEU:HD11	2.22	0.54
1:D:75:VAL:HG11	1:F:18:MSE:HG3	1.90	0.54
1:A:76[B]:GLN:NE2	1:A:103:GLN:HE22	2.06	0.53
1:B:18[B]:MSE:HE2	1:E:70:TRP:CG	2.43	0.53
1:A:60:THR:CA	1:A:63[A]:MSE:HE2	2.27	0.53
1:B:52:PRO:HD2	4:B:381:HOH:O	2.10	0.52
1:C:9:ILE:HD11	1:C:235[A]:MSE:SE	2.60	0.52
1:F:1:MSE:HE3	4:F:957:HOH:O	2.09	0.52
1:E:21:VAL:HG23	1:E:22:SER:OG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284[B]:MSE:HE3	1:A:284[B]:MSE:C	2.30	0.52
1:D:63[B]:MSE:HE3	1:D:93:ILE:HD12	1.91	0.51
1:C:241:PRO:HB2	1:C:284:MSE:HE1	1.91	0.51
1:A:290:ILE:C	1:A:290:ILE:CD1	2.79	0.51
1:B:18[B]:MSE:HE2	1:E:70:TRP:CD1	2.45	0.51
1:F:9:ILE:HD11	1:F:235[A]:MSE:SE	2.61	0.51
1:D:63[A]:MSE:CE	1:D:90:GLN:HG2	2.39	0.50
1:F:197:VAL:HB	1:F:210:VAL:HG13	1.92	0.50
1:F:3:ALA:HB1	1:F:5:LYS:NZ	2.26	0.50
1:F:146:LEU:HD12	1:F:149:LEU:HD23	1.92	0.50
1:A:193[B]:HIS:CE1	1:A:194:LYS:HE3	2.47	0.50
1:E:167:LYS:HG2	1:E:207:TYR:CD2	2.46	0.50
1:D:284:MSE:HE3	1:D:285:ALA:H	1.76	0.50
1:A:290:ILE:C	1:A:290:ILE:HD12	2.31	0.49
1:F:3:ALA:CB	1:F:5:LYS:NZ	2.76	0.49
1:E:127[A]:GLU:OE1	1:E:130:LYS:NZ	2.41	0.49
1:D:240:LEU:N	1:D:241:PRO:HD2	2.27	0.49
1:D:63[B]:MSE:HE3	1:D:93:ILE:CD1	2.43	0.49
1:B:18[B]:MSE:HE2	1:E:70:TRP:CD2	2.48	0.49
1:A:283:GLN:NE2	1:D:284:MSE:HB3	2.27	0.49
1:E:9:ILE:HD11	1:E:235[A]:MSE:SE	2.62	0.49
1:A:76[A]:GLN:HA	1:A:76[A]:GLN:HE21	1.78	0.48
1:C:249:GLN:OE1	1:C:282:ILE:HD12	2.13	0.48
1:A:87:SER:C	1:A:128:MSE:HE1	2.33	0.48
1:C:279[B]:ASP:C	1:C:279[B]:ASP:OD2	2.52	0.48
1:A:9:ILE:HD11	1:A:235[A]:MSE:SE	2.64	0.48
1:A:284[B]:MSE:CE	1:A:284[B]:MSE:O	2.61	0.48
1:E:164[B]:GLU:OE1	1:E:167:LYS:NZ	2.47	0.48
1:F:5:LYS:HA	4:F:920:HOH:O	2.14	0.47
1:F:212:CYS:HB3	1:F:214:TYR:CE2	2.49	0.47
1:E:149:LEU:HD12	1:E:173:LEU:HD11	1.96	0.47
1:F:195:THR:CG2	1:F:214:TYR:O	2.56	0.47
1:C:134:HIS:HD2	4:C:304:HOH:O	1.97	0.47
1:D:212[A]:CYS:SG	1:D:213:PRO:HD2	2.56	0.46
1:E:89[B]:ARG:NH1	4:E:754:HOH:O	2.48	0.46
1:D:277:ASN:O	1:D:280[A]:MSE:HG2	2.14	0.46
1:A:63[B]:MSE:HE3	1:A:93:ILE:CB	2.45	0.46
1:E:127[A]:GLU:OE2	1:E:130:LYS:NZ	2.49	0.46
1:B:242[B]:MSE:HE3	4:B:740:HOH:O	2.15	0.46
1:D:280[B]:MSE:CG	1:D:281:PRO:HD2	2.46	0.46
1:F:277:ASN:O	1:F:280[B]:MSE:HG2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:GLN:NE2	1:F:282:ILE:HD13	2.31	0.45
1:A:63[B]:MSE:HE3	1:A:93:ILE:CG2	2.47	0.45
1:D:149:LEU:HD22	1:D:183:ILE:HD13	1.99	0.45
1:D:284:MSE:HE3	1:D:285:ALA:N	2.31	0.45
1:A:63[B]:MSE:HE3	1:A:93:ILE:HG21	1.99	0.44
1:B:207:TYR:O	1:B:289:LEU:HD12	2.17	0.44
1:B:18[B]:MSE:CE	1:E:75:VAL:CG2	2.85	0.44
1:F:195:THR:HG21	1:F:216:PRO:CD	2.44	0.44
1:C:9:ILE:CD1	1:C:235[A]:MSE:SE	3.15	0.44
1:F:175:ASP:OD1	1:F:202[A]:ARG:NH2	2.37	0.44
1:A:76[B]:GLN:HE21	1:A:103:GLN:HE22	1.64	0.44
1:C:106:SER:O	1:E:1:MSE:HA	2.18	0.44
1:B:168:GLU:HG2	1:B:171[A]:ARG:NH1	2.28	0.44
1:E:127[A]:GLU:CD	1:E:130:LYS:HZ1	2.21	0.44
1:F:171[A]:ARG:NH1	1:F:202[A]:ARG:NH1	2.65	0.44
2:E:400:PXL:H5A2	2:E:400:PXL:H4A	1.73	0.44
1:D:289:LEU:HD21	4:D:341:HOH:O	2.18	0.43
1:E:245:ASP:OD2	1:E:284[B]:MSE:HA	2.17	0.43
1:E:195:THR:HG21	1:E:216:PRO:HD3	1.99	0.43
1:A:280:MSE:HE1	1:E:282:ILE:C	2.38	0.43
1:E:245:ASP:OD2	1:E:284[B]:MSE:HG2	2.19	0.43
1:D:149:LEU:CD1	1:D:173:LEU:HD11	2.48	0.43
1:A:7[B]:LYS:NZ	1:F:2:TYR:OH	2.33	0.43
1:A:128:MSE:HB2	1:A:128:MSE:HE2	1.88	0.43
1:B:249:GLN:HG3	1:B:282:ILE:HD12	2.01	0.43
1:D:190:ASP:O	1:D:191:GLU:HG2	2.19	0.43
1:D:242[B]:MSE:HE3	1:D:246:ARG:HD2	2.01	0.42
1:D:167:LYS:HG2	1:D:207:TYR:CD2	2.54	0.42
1:F:240:LEU:N	1:F:241:PRO:HD2	2.34	0.42
1:F:246:ARG:HG2	1:F:282:ILE:HG13	2.01	0.42
1:F:149:LEU:CD2	1:F:183:ILE:HD13	2.41	0.42
1:D:280[B]:MSE:HG2	1:D:281:PRO:HD2	2.01	0.42
1:A:63[B]:MSE:HE1	1:A:90:GLN:CB	2.50	0.42
1:A:284[A]:MSE:HG3	1:D:253:GLN:HE21	1.85	0.42
1:A:242:MSE:HA	1:A:284[A]:MSE:HE3	2.02	0.41
1:A:283:GLN:HE22	1:D:284:MSE:HB3	1.85	0.41
1:C:270:LEU:HA	1:C:270:LEU:HD23	1.84	0.41
1:E:5[B]:LYS:HD3	4:E:941:HOH:O	2.20	0.41
1:C:280:MSE:HE3	1:F:281:PRO:HB2	2.02	0.41
1:D:175:ASP:OD1	1:D:202[B]:ARG:NH1	2.53	0.41
1:B:26:VAL:HG13	1:B:30:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:LYS:HE2	4:E:551:HOH:O	2.20	0.41
1:E:127[A]:GLU:CD	1:E:130:LYS:NZ	2.73	0.41
1:B:167:LYS:HG2	1:B:207:TYR:CD2	2.56	0.41
1:A:164:GLU:CG	4:A:913:HOH:O	2.68	0.41
1:E:197:VAL:HB	1:E:210:VAL:HG13	2.03	0.41
1:F:173:LEU:HA	1:F:173:LEU:HD23	1.98	0.40
1:D:59:LEU:O	1:D:63[A]:MSE:HG3	2.22	0.40
1:F:63:MSE:HE2	1:F:93:ILE:HG21	2.02	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	302/291 (104%)	293 (97%)	9 (3%)	0	100	100
1	B	296/291 (102%)	289 (98%)	7 (2%)	0	100	100
1	C	294/291 (101%)	287 (98%)	7 (2%)	0	100	100
1	D	294/291 (101%)	286 (97%)	8 (3%)	0	100	100
1	E	305/291 (105%)	293 (96%)	10 (3%)	2 (1%)	26	19
1	F	297/291 (102%)	286 (96%)	11 (4%)	0	100	100
All	All	1788/1746 (102%)	1734 (97%)	52 (3%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5[A]	LYS
1	E	5[B]	LYS

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	268/247 (108%)	263 (98%)	5 (2%)	65	67
1	B	260/247 (105%)	254 (98%)	6 (2%)	58	60
1	C	256/247 (104%)	255 (100%)	1 (0%)	93	95
1	D	260/247 (105%)	254 (98%)	6 (2%)	58	60
1	E	266/247 (108%)	262 (98%)	4 (2%)	72	75
1	F	253/247 (102%)	250 (99%)	3 (1%)	78	81
All	All	1563/1482 (106%)	1538 (98%)	25 (2%)	74	73

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

Mol	Chain	Res	Type
1	A	76[A]	GLN
1	A	76[B]	GLN
1	A	81	TYR
1	A	168	GLU
1	A	290	ILE
1	B	75	VAL
1	B	81	TYR
1	B	168	GLU
1	B	196[A]	SER
1	B	196[B]	SER
1	B	245	ASP
1	C	81	TYR
1	D	5	LYS
1	D	81	TYR
1	D	87	SER
1	D	168	GLU
1	D	279	ASP
1	D	288	GLU
1	E	5[A]	LYS
1	E	5[B]	LYS
1	E	196[A]	SER
1	E	196[B]	SER

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Mol	Chain	Res	Type
1	F	81	TYR
1	F	210	VAL
1	F	290	ILE

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

Mol	Chain	Res	Type
1	A	117	ASN
1	C	92	GLN
1	C	134	HIS
1	D	92	GLN
1	E	4	ASN
1	E	117	ASN
1	E	253	GLN
1	F	117	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	PXL	A	400	-	12,12,12	3.38	2 (16%)	15,16,16	2.99	9 (60%)
2	PXL	B	400	-	12,12,12	4.22	3 (25%)	15,16,16	2.51	5 (33%)
2	PXL	C	400	-	12,12,12	4.21	3 (25%)	15,16,16	2.00	5 (33%)
2	PXL	D	400	-	12,12,12	4.31	4 (33%)	15,16,16	2.31	9 (60%)
2	PXL	E	400	-	12,12,12	3.24	2 (16%)	15,16,16	2.84	6 (40%)
2	PXL	F	400	-	12,12,12	4.29	3 (25%)	15,16,16	2.14	6 (40%)

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	PXL	A	400	-	-	0/4/4/4	0/1/1/1
2	PXL	B	400	-	-	0/4/4/4	0/1/1/1
2	PXL	C	400	-	-	0/4/4/4	0/1/1/1
2	PXL	D	400	-	-	0/4/4/4	0/1/1/1
2	PXL	E	400	-	-	0/4/4/4	0/1/1/1
2	PXL	F	400	-	-	0/4/4/4	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PXL	C4-C5	2.05	1.44	1.42
2	D	400	PXL	C2-N1	2.25	1.38	1.34
2	D	400	PXL	C4-C5	2.55	1.45	1.42
2	F	400	PXL	C4-C5	4.22	1.47	1.42
2	C	400	PXL	C4-C5	4.76	1.48	1.42
2	B	400	PXL	C4-C3	4.82	1.46	1.40
2	C	400	PXL	C4-C3	5.19	1.47	1.40
2	A	400	PXL	C4-C3	6.28	1.48	1.40
2	E	400	PXL	C4-C3	6.61	1.49	1.40
2	D	400	PXL	C4-C3	7.71	1.50	1.40
2	F	400	PXL	C4-C3	7.74	1.50	1.40
2	E	400	PXL	C3-C2	8.54	1.46	1.40
2	A	400	PXL	C3-C2	9.60	1.47	1.40
2	F	400	PXL	C3-C2	11.61	1.48	1.40
2	D	400	PXL	C3-C2	12.16	1.49	1.40
2	C	400	PXL	C3-C2	12.63	1.49	1.40
2	B	400	PXL	C3-C2	13.43	1.50	1.40

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	PXL	O4A-C4A-C4	-6.17	112.65	125.11
2	E	400	PXL	C5A-C5-C4	-5.57	112.84	122.34
2	E	400	PXL	O4A-C4A-C4	-5.31	114.37	125.11
2	B	400	PXL	C5A-C5-C4	-4.96	113.89	122.34
2	B	400	PXL	O4A-C4A-C4	-4.35	116.31	125.11
2	C	400	PXL	O4A-C4A-C4	-4.15	116.73	125.11
2	F	400	PXL	O4A-C4A-C4	-3.45	118.14	125.11
2	F	400	PXL	C5A-C5-C4	-3.41	116.52	122.34
2	C	400	PXL	C5A-C5-C4	-3.38	116.59	122.34
2	A	400	PXL	C5A-C5-C4	-3.33	116.66	122.34
2	D	400	PXL	C5A-C5-C4	-3.29	116.73	122.34
2	D	400	PXL	C5-C4-C4A	-3.13	115.20	122.35
2	D	400	PXL	O4A-C4A-C4	-2.94	119.16	125.11
2	E	400	PXL	C5-C4-C4A	-2.92	115.66	122.35
2	B	400	PXL	C5-C4-C4A	-2.80	115.94	122.35
2	A	400	PXL	C3-C2-N1	-2.77	116.79	120.61
2	A	400	PXL	C5-C4-C4A	-2.69	116.19	122.35
2	D	400	PXL	C3-C2-N1	-2.13	117.66	120.61
2	D	400	PXL	C2A-C2-C3	2.09	123.56	121.04
2	D	400	PXL	C6-N1-C2	2.14	123.65	119.28
2	C	400	PXL	C5A-C5-C6	2.16	123.39	119.31
2	C	400	PXL	C6-N1-C2	2.25	123.87	119.28
2	E	400	PXL	O3-C3-C2	2.28	121.62	117.66
2	F	400	PXL	C2A-C2-N1	2.37	123.19	117.95
2	F	400	PXL	C6-N1-C2	2.72	124.83	119.28
2	D	400	PXL	C5A-C5-C6	2.73	124.45	119.31
2	D	400	PXL	O3-C3-C2	2.82	122.56	117.66
2	A	400	PXL	C3-C4-C4A	2.86	124.16	119.84
2	C	400	PXL	C3-C4-C4A	2.87	124.18	119.84
2	F	400	PXL	C5A-C5-C6	3.01	124.98	119.31
2	F	400	PXL	C3-C4-C4A	3.02	124.41	119.84
2	A	400	PXL	C5A-C5-C6	3.22	125.39	119.31
2	B	400	PXL	C5A-C5-C6	3.38	125.69	119.31
2	A	400	PXL	C6-N1-C2	3.43	126.28	119.28
2	A	400	PXL	O3-C3-C2	3.78	124.23	117.66
2	A	400	PXL	C2A-C2-C3	4.41	126.36	121.04
2	D	400	PXL	C3-C4-C4A	4.54	126.70	119.84
2	E	400	PXL	C3-C4-C4A	4.54	126.71	119.84
2	E	400	PXL	C5A-C5-C6	4.54	127.88	119.31
2	B	400	PXL	C3-C4-C4A	4.56	126.73	119.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	400	PXL	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 ⓘ

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	279/291 (95%)	0.02	6 (2%) 65 66	14, 19, 34, 52	0
1	B	277/291 (95%)	0.06	9 (3%) 51 52	14, 19, 33, 42	0
1	C	279/291 (95%)	0.14	18 (6%) 22 23	14, 19, 33, 52	0
1	D	276/291 (94%)	0.07	9 (3%) 50 51	14, 19, 32, 47	0
1	E	279/291 (95%)	0.05	9 (3%) 51 52	14, 19, 34, 58	0
1	F	279/291 (95%)	0.44	21 (7%) 17 18	14, 19, 32, 57	0
All	All	1669/1746 (95%)	0.13	72 (4%) 39 40	14, 19, 33, 58	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	TYR	9.2
1	A	2	TYR	7.1
1	F	189	HIS	6.8
1	F	290	ILE	6.3
1	F	2	TYR	5.6
1	C	2	TYR	5.1
1	D	189	HIS	5.0
1	F	188	VAL	4.8
1	F	261	TYR	4.8
1	B	190	ASP	4.6
1	E	3	ALA	4.5
1	C	290	ILE	4.5
1	A	189	HIS	4.4
1	F	4	ASN	4.3
1	E	4	ASN	4.2
1	D	190	ASP	4.1
1	F	159	ALA	3.9
1	C	189	HIS	3.8
1	F	157	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	192	PRO	3.8
1	C	4	ASN	3.7
1	B	4	ASN	3.6
1	D	104	PRO	3.5
1	A	190	ASP	3.5
1	C	190	ASP	3.5
1	F	259[A]	PHE	3.5
1	B	189	HIS	3.3
1	C	3	ALA	3.2
1	C	12	VAL	3.2
1	C	193	HIS	3.1
1	E	261	TYR	3.1
1	F	160	ASP	2.9
1	E	290	ILE	2.9
1	F	162	THR	2.8
1	A	3	ALA	2.8
1	B	23	LEU	2.8
1	F	156	PRO	2.8
1	F	142	ILE	2.7
1	E	142	ILE	2.6
1	E	110	ALA	2.6
1	C	228	SER	2.5
1	C	227	THR	2.5
1	C	23	LEU	2.5
1	C	26	VAL	2.4
1	D	193[A]	HIS	2.4
1	F	143	THR	2.4
1	F	103	GLN	2.4
1	C	226	PHE	2.4
1	D	287	TYR	2.4
1	C	223	GLY	2.3
1	F	151	TYR	2.3
1	A	23	LEU	2.3
1	B	193	HIS	2.3
1	E	182	ILE	2.3
1	B	81	TYR	2.2
1	F	223	GLY	2.2
1	C	142	ILE	2.2
1	F	150	PHE	2.2
1	D	192	PRO	2.2
1	E	193	HIS	2.1
1	D	105	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	83	GLY	2.1
1	C	113	VAL	2.1
1	D	289	LEU	2.1
1	B	154	ASP	2.1
1	D	37	VAL	2.1
1	F	105	ASP	2.1
1	B	82	THR	2.0
1	B	104	PRO	2.0
1	C	192	PRO	2.0
1	C	105	ASP	2.0
1	A	290	ILE	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	PXL	E	400	12/12	0.92	0.15	1.36	23,27,37,40	0
2	PXL	B	400	12/12	0.94	0.18	1.12	21,26,34,40	0
2	PXL	A	400	12/12	0.94	0.17	1.02	21,24,34,36	0
2	PXL	D	400	12/12	0.96	0.16	0.99	24,30,42,44	0
2	PXL	F	400	12/12	0.92	0.13	0.07	32,42,48,49	0
2	PXL	C	400	12/12	0.95	0.13	0.04	23,29,37,43	0
3	CL	C	291	1/1	0.99	0.09	-0.43	27,27,27,27	0
3	CL	F	291	1/1	0.98	0.07	-1.36	36,36,36,36	0
3	CL	A	291	1/1	0.99	0.07	-1.53	26,26,26,26	0
3	CL	E	291	1/1	0.99	0.08	-1.56	21,21,21,21	0

6.5 Other polymers

There are no such residues in this entry.