



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:54 AM UTC

PDB ID : 3MBH / pdb_00003mbh
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

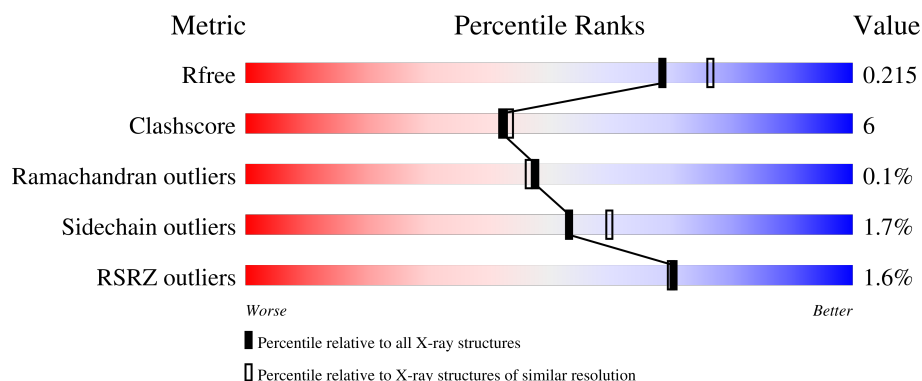
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

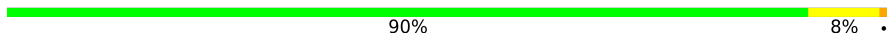
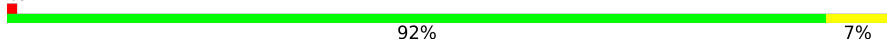
The reported resolution of this entry is 2.00 Å.

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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 $\leq 5\%$. 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	 90% 8% .
1	B	291	 89% 10% .
1	C	291	 92% 7% ..
1	D	291	 84% 14% .
1	E	291	 86% 13%

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Mol	Chain	Length	Quality of chain
1	F	291	 A horizontal bar chart showing the quality of chain F. The bar is divided into three segments: a red segment at the beginning labeled '5%', a large green segment in the middle labeled '88%', and a yellow segment at the end labeled '11%'. A small black dot is located at the far right end of the bar.

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.

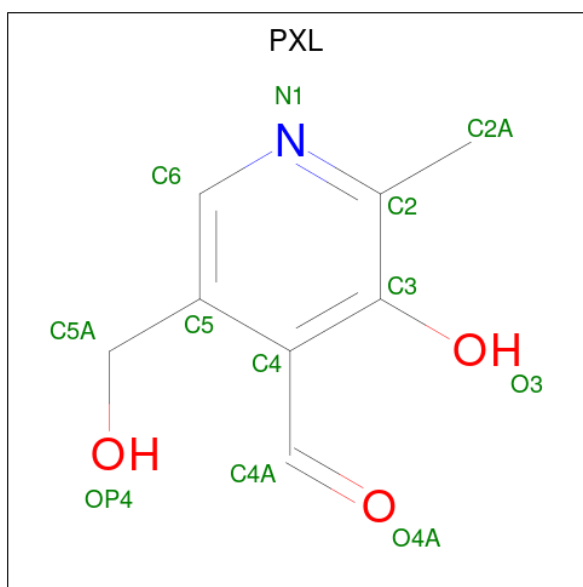
- Molecule 1 is a protein called Putative phosphomethylpyrimidine kinase.

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	-	expression tag	UNP Q89ZB9
B	0	GLY	-	expression tag	UNP Q89ZB9
C	0	GLY	-	expression tag	UNP Q89ZB9
D	0	GLY	-	expression tag	UNP Q89ZB9
E	0	GLY	-	expression tag	UNP Q89ZB9
F	0	GLY	-	expression tag	UNP Q89ZB9

- Molecule 2 is 3-HYDROXY-5-(HYDROXYMETHYL)-2-METHYLISONICOTINALDEHYDE (CCD ID: 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 (CCD ID: 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	E	1	Total	Cl	0	0
			1	1		
3	F	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

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.

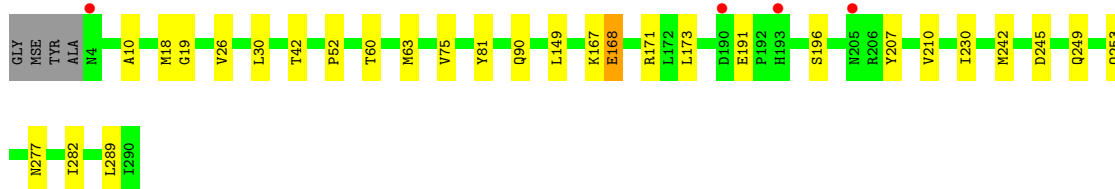
- Molecule 1: Putative phosphomethylpyrimidine kinase

Chain A: 



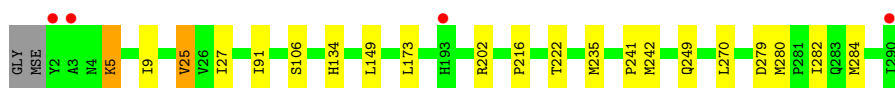
- Molecule 1: Putative phosphomethylpyrimidine kinase

Chain B: 



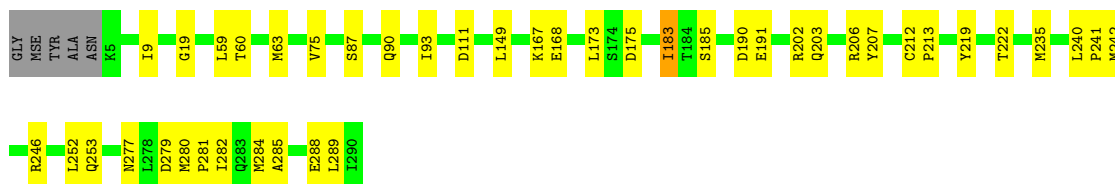
- Molecule 1: Putative phosphomethylpyrimidine kinase

Chain C: 



- Molecule 1: Putative phosphomethylpyrimidine kinase

Chain D: 

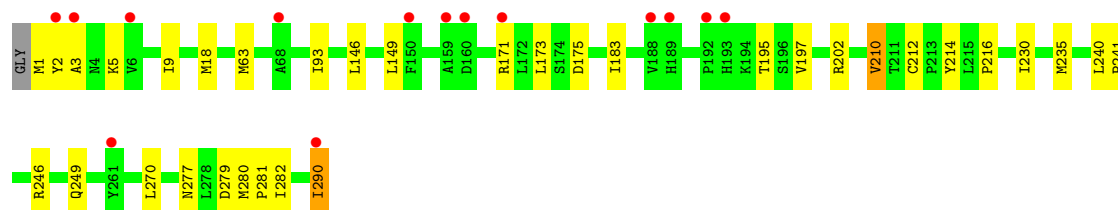
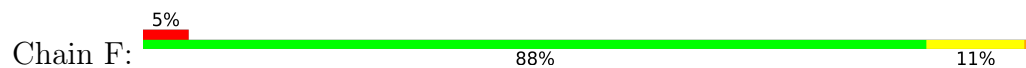


- Molecule 1: Putative phosphomethylpyrimidine kinase

Chain E: 



- 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, PHENIX	Depositor
R, R_{free}	0.167 , 0.206 0.182 , 0.215	Depositor DCC
R_{free} test set	6306 reflections (4.99%)	wwPDB-VP
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 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	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, 0.333 respectively for untwinned datasets, and 0.375, 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: PXL, 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	1.04	2/2453 (0.1%)	0.94	0/3313
1	B	1.00	2/2392 (0.1%)	0.96	1/3231 (0.0%)
1	C	1.06	1/2372 (0.0%)	0.97	3/3209 (0.1%)
1	D	0.94	1/2388 (0.0%)	0.95	2/3227 (0.1%)
1	E	1.05	0/2453	0.94	1/3312 (0.0%)
1	F	0.93	1/2384 (0.0%)	0.90	1/3223 (0.0%)
All	All	1.01	7/14442 (0.0%)	0.94	8/19515 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	5	LYS	N-CA	7.39	1.55	1.45
1	D	183	ILE	CA-CB	5.93	1.61	1.54
1	A	240	LEU	C-O	-5.86	1.19	1.24
1	B	230	ILE	CA-CB	5.57	1.60	1.54
1	A	272	GLU	CA-C	-5.46	1.45	1.52
1	F	230	ILE	CA-CB	5.38	1.60	1.54
1	B	10	ALA	CA-CB	5.01	1.60	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	19	GLY	N-CA-C	-7.54	103.18	112.68
1	B	19	GLY	N-CA-C	-7.45	100.79	112.71
1	E	19	GLY	N-CA-C	-6.28	105.26	112.29
1	C	27	ILE	N-CA-CB	5.92	115.07	110.45
1	C	25	VAL	N-CA-CB	-5.54	107.09	111.64
1	C	91	ILE	N-CA-CB	5.51	117.00	110.55
1	D	111	ASP	N-CA-C	-5.10	102.15	109.24
1	F	279	ASP	N-CA-C	5.00	117.62	111.82

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	37	0
1	B	2350	0	2315	31	0
1	C	2329	0	2293	16	0
1	D	2344	0	2331	38	0
1	E	2411	0	2372	48	0
1	F	2341	0	2298	34	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	180	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 (180) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:242[B]:MSE:HG3	1:E:284[B]:MSE:HE1	1.46	0.97
1:A:290:ILE:HD12	1:A:290:ILE:O	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
1:A:284[B]:MSE:HE3	1:A:285:ALA:CA	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:613:HOH:O	1:E:284[B]:MSE:HE3	1.96	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
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:OXT	1:F:290:ILE:CG2	2.48	0.60
1:E:280[B]:MSE:HA	1:E:280[B]:MSE:CE	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:B:60:THR:HA	1:B:63[A]:MSE:HE2	1.85	0.59
1:C:216:PRO:CB	1:C:222[B]:THR:HG21	2.29	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:A:284[B]:MSE:HE3	1:A:284[B]:MSE:C	2.30	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:A:290:ILE:CD1	1:A:290:ILE:C	2.79	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:A:290:ILE:HD12	1:A:290:ILE:C	2.31	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76[B]:GLN:NE2	1:A:103:GLN:HE22	2.06	0.53
1:A:87:SER:C	1:A:128:MSE:HE1	2.33	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:279[B]:ASP:OD2	1:C:279[B]:ASP:C	2.52	0.52
1:C:9:ILE:HD11	1:C:235[A]:MSE:SE	2.60	0.52
1:E:21:VAL:HG23	1:E:22:SER:OG	2.09	0.52
1:F:1:MSE:HE3	4:F:957:HOH:O	2.09	0.52
1:C:241:PRO:HB2	1:C:284:MSE:HE1	1.91	0.51
1:D:63[B]:MSE:HE3	1:D:93:ILE:HD12	1.91	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:F:3:ALA:CB	1:F:5:LYS:NZ	2.76	0.49
1:D:240:LEU:N	1:D:241:PRO:HD2	2.27	0.49
1:E:127[A]:GLU:OE1	1:E:130:LYS:NZ	2.41	0.49
1:D:63[B]:MSE:HE3	1:D:93:ILE:CD1	2.43	0.49
1:A:283:GLN:NE2	1:D:284:MSE:HB3	2.27	0.49
1:B:18[B]:MSE:HE2	1:E:70:TRP:CD2	2.48	0.49
1:E:9:ILE:HD11	1:E:235[A]:MSE:SE	2.62	0.49
1:A:76[A]:GLN:HE21	1:A:76[A]:GLN:HA	1.78	0.48
1:C:249:GLN:OE1	1:C:282:ILE:HD12	2.13	0.48
1:A:9:ILE:HD11	1:A:235[A]:MSE:SE	2.64	0.48
1:A:280:MSE:HE1	1:E:282:ILE:C	2.38	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:E:127[A]:GLU:CD	1:E:130:LYS:HZ1	2.22	0.47
1:E:149:LEU:HD12	1:E:173:LEU:HD11	1.96	0.47
1:F:212:CYS:HB3	1:F:214:TYR:CE2	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:127[A]:GLU:CD	1:E:130:LYS:NZ	2.73	0.45
1:F:249:GLN:NE2	1:F:282:ILE:HD13	2.31	0.45
1:F:277:ASN:O	1:F:280[B]:MSE:HG2	2.15	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:C:9:ILE:CD1	1:C:235[A]:MSE:SE	3.15	0.44
1:F:195:THR:HG21	1:F:216:PRO:CD	2.44	0.44
1:A:76[B]:GLN:HE21	1:A:103:GLN:HE22	1.64	0.44
1:C:280:MSE:HE1	1:F:282:ILE:C	2.42	0.44
1:F:175:ASP:OD1	1:F:202[A]:ARG:NH2	2.37	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
2:E:400:PXL:H4A	2:E:400:PXL:H5A2	1.73	0.44
1:F:171[A]:ARG:NH1	1:F:202[A]:ARG:NH1	2.65	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: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:HE2	1:A:128:MSE:HB2	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:245:ASP:C	1:A:282:ILE:HD11	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:C:270:LEU:HA	1.84	0.41
1:E:5[B]:LYS:HD3	4:E:941:HOH:O	2.20	0.41
1:B:26:VAL:HG13	1:B:30:LEU:HD12	2.02	0.41
1:B:81:TYR:CD1	1:B:81:TYR:C	2.97	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:E:167:LYS:HE2	4:E:551:HOH:O	2.20	0.41
1:A:164:GLU:CG	4:A:913:HOH:O	2.68	0.41
1:B:167:LYS:HG2	1:B:207:TYR:CD2	2.56	0.41
1:E:197:VAL:HB	1:E:210:VAL:HG13	2.03	0.41
1:F:173:LEU:HD23	1:F:173:LEU:HA	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%)	18	14
1	F	297/291 (102%)	286 (96%)	11 (4%)	0	100	100
All	All	1788/1746 (102%)	1734 (97%)	52 (3%)	2 (0%)	48	46

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%)	50	56
1	B	260/247 (105%)	253 (97%)	7 (3%)	39	42
1	C	256/247 (104%)	255 (100%)	1 (0%)	84	89
1	D	260/247 (105%)	253 (97%)	7 (3%)	39	42
1	E	266/247 (108%)	259 (97%)	7 (3%)	40	44
1	F	253/247 (102%)	250 (99%)	3 (1%)	63	70
All	All	1563/1482 (106%)	1533 (98%)	30 (2%)	53	56

All (30) 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	168	GLU
1	A	282	ILE
1	A	290	ILE
1	B	75	VAL
1	B	168	GLU
1	B	191	GLU
1	B	196[A]	SER
1	B	196[B]	SER
1	B	210	VAL
1	B	245	ASP
1	C	25	VAL
1	D	87	SER
1	D	168	GLU
1	D	185	SER
1	D	203	GLN

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Mol	Chain	Res	Type
1	D	279	ASP
1	D	282	ILE
1	D	288	GLU
1	E	5[A]	LYS
1	E	5[B]	LYS
1	E	25	VAL
1	E	196[A]	SER
1	E	196[B]	SER
1	E	212	CYS
1	E	282	ILE
1	F	210	VAL
1	F	270	LEU
1	F	290	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	103	GLN
1	A	134	HIS
1	A	179	GLN
1	A	205	ASN
1	B	92	GLN
1	C	92	GLN
1	C	117	ASN
1	C	134	HIS
1	C	179	GLN
1	C	253	GLN
1	C	277	ASN
1	D	92	GLN
1	D	218	HIS
1	E	4	ASN
1	E	92	GLN
1	E	117	ASN
1	E	193	HIS
1	E	205	ASN
1	E	253	GLN
1	F	92	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 oligosaccharides 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	C	400	-	12,12,12	3.00	3 (25%)	15,16,16	2.41	6 (40%)
2	PXL	F	400	-	12,12,12	3.13	4 (33%)	15,16,16	2.38	8 (53%)
2	PXL	D	400	-	12,12,12	3.08	4 (33%)	15,16,16	2.51	9 (60%)
2	PXL	A	400	-	12,12,12	2.35	2 (16%)	15,16,16	3.20	9 (60%)
2	PXL	E	400	-	12,12,12	2.33	3 (25%)	15,16,16	3.06	5 (33%)
2	PXL	B	400	-	12,12,12	2.89	2 (16%)	15,16,16	3.04	5 (33%)

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	C	400	-	-	0/4/4/4	0/1/1/1
2	PXL	F	400	-	-	0/4/4/4	0/1/1/1
2	PXL	D	400	-	-	0/4/4/4	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PXL	A	400	-	-	0/4/4/4	0/1/1/1
2	PXL	E	400	-	-	0/4/4/4	0/1/1/1
2	PXL	B	400	-	-	0/4/4/4	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PXL	C3-C2	8.75	1.50	1.41
2	C	400	PXL	C3-C2	8.22	1.49	1.41
2	D	400	PXL	C3-C2	7.91	1.49	1.41
2	F	400	PXL	C3-C2	7.55	1.48	1.41
2	A	400	PXL	C3-C2	6.21	1.47	1.41
2	F	400	PXL	C4-C3	5.70	1.50	1.41
2	D	400	PXL	C4-C3	5.68	1.50	1.41
2	E	400	PXL	C3-C2	5.50	1.46	1.41
2	E	400	PXL	C4-C3	4.84	1.49	1.41
2	C	400	PXL	C4-C5	4.63	1.48	1.42
2	A	400	PXL	C4-C3	4.59	1.48	1.41
2	F	400	PXL	C4-C5	4.10	1.47	1.42
2	C	400	PXL	C4-C3	3.75	1.47	1.41
2	B	400	PXL	C4-C3	3.46	1.46	1.41
2	D	400	PXL	C2-N1	2.80	1.38	1.33
2	D	400	PXL	C4-C5	2.47	1.45	1.42
2	E	400	PXL	C2-N1	2.14	1.37	1.33
2	F	400	PXL	C2A-C2	2.02	1.53	1.50

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	400	PXL	C5A-C5-C4	-6.73	112.84	122.34
2	B	400	PXL	C4-C3-C2	-6.21	116.65	120.14
2	B	400	PXL	C5A-C5-C4	-5.99	113.89	122.34
2	E	400	PXL	C5A-C5-C6	5.27	127.88	119.36
2	A	400	PXL	O4A-C4A-C4	-5.13	112.65	124.80
2	B	400	PXL	C3-C4-C4A	5.01	126.73	119.84
2	E	400	PXL	C3-C4-C4A	4.99	126.71	119.84
2	D	400	PXL	C3-C4-C4A	4.98	126.70	119.84
2	C	400	PXL	C4-C3-C2	-4.97	117.35	120.14
2	A	400	PXL	C4-C3-C2	-4.83	117.42	120.14
2	A	400	PXL	C2A-C2-C3	4.75	126.36	120.80
2	E	400	PXL	O4A-C4A-C4	-4.40	114.37	124.80
2	F	400	PXL	C5A-C5-C4	-4.13	116.52	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	PXL	C5A-C5-C4	-4.08	116.59	122.34
2	A	400	PXL	C5A-C5-C4	-4.03	116.66	122.34
2	D	400	PXL	C5A-C5-C4	-3.98	116.73	122.34
2	B	400	PXL	C5A-C5-C6	3.91	125.69	119.36
2	A	400	PXL	C6-N1-C2	3.90	126.28	119.20
2	A	400	PXL	C5A-C5-C6	3.72	125.39	119.36
2	B	400	PXL	O4A-C4A-C4	-3.58	116.31	124.80
2	D	400	PXL	C4-C3-C2	-3.49	118.18	120.14
2	F	400	PXL	C5A-C5-C6	3.48	124.98	119.36
2	C	400	PXL	O4A-C4A-C4	-3.40	116.73	124.80
2	F	400	PXL	C3-C4-C4A	3.32	124.41	119.84
2	A	400	PXL	C3-C2-N1	-3.31	116.79	120.96
2	A	400	PXL	O3-C3-C2	3.21	124.23	117.58
2	C	400	PXL	C3-C4-C4A	3.16	124.18	119.84
2	D	400	PXL	C5A-C5-C6	3.14	124.45	119.36
2	A	400	PXL	C3-C4-C4A	3.14	124.16	119.84
2	E	400	PXL	C4-C3-C2	-3.14	118.38	120.14
2	F	400	PXL	C6-N1-C2	3.11	124.83	119.20
2	F	400	PXL	C2A-C2-N1	2.95	123.19	117.64
2	F	400	PXL	O4A-C4A-C4	-2.81	118.14	124.80
2	D	400	PXL	C3-C2-N1	-2.61	117.66	120.96
2	C	400	PXL	C6-N1-C2	2.57	123.87	119.20
2	F	400	PXL	C4-C3-C2	-2.56	118.70	120.14
2	C	400	PXL	C5A-C5-C6	2.49	123.39	119.36
2	F	400	PXL	C3-C2-N1	-2.46	117.86	120.96
2	D	400	PXL	C6-N1-C2	2.46	123.65	119.20
2	D	400	PXL	O3-C3-C2	2.40	122.56	117.58
2	D	400	PXL	O4A-C4A-C4	-2.38	119.16	124.80
2	D	400	PXL	C2A-C2-C3	2.36	123.56	120.80

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 ⓘ

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	279/291 (95%)	-0.43	1 (0%) 88 88	7, 18, 34, 52	11 (3%)
1	B	277/291 (95%)	0.01	4 (1%) 73 73	7, 19, 33, 42	6 (2%)
1	C	279/291 (95%)	-0.26	4 (1%) 73 73	8, 19, 33, 52	6 (2%)
1	D	276/291 (94%)	-0.34	0 100 100	9, 19, 32, 47	5 (1%)
1	E	279/291 (95%)	-0.44	4 (1%) 73 73	8, 18, 33, 58	12 (4%)
1	F	279/291 (95%)	0.42	14 (5%) 34 33	8, 19, 32, 57	6 (2%)
All	All	1669/1746 (95%)	-0.17	27 (1%) 70 70	7, 19, 33, 58	46 (2%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	2	TYR	6.5
1	A	2	TYR	4.9
1	F	171[A]	ARG	3.9
1	F	189	HIS	3.6
1	F	2	TYR	3.5
1	C	2	TYR	3.4
1	F	261	TYR	3.4
1	F	290	ILE	3.3
1	C	3	ALA	3.0
1	F	188	VAL	3.0
1	E	5[A]	LYS	2.8
1	B	190	ASP	2.7
1	F	6	VAL	2.7
1	F	3	ALA	2.7
1	F	150	PHE	2.6
1	B	4	ASN	2.5
1	F	192	PRO	2.5
1	F	68	ALA	2.5
1	E	3	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	4	ASN	2.3
1	F	159	ALA	2.3
1	B	193	HIS	2.2
1	B	205	ASN	2.2
1	C	193	HIS	2.2
1	C	290	ILE	2.1
1	F	160	ASP	2.1
1	F	193	HIS	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 oligosaccharides 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, 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	B-factors(Å ²)	Q<0.9
2	PXL	F	400	12/12	0.86	0.10	32,42,48,49	0
2	PXL	E	400	12/12	0.92	0.08	23,27,37,40	0
2	PXL	B	400	12/12	0.92	0.07	21,26,34,40	0
2	PXL	A	400	12/12	0.93	0.07	21,24,34,36	0
2	PXL	D	400	12/12	0.93	0.08	24,30,42,44	0
2	PXL	C	400	12/12	0.94	0.07	23,29,37,43	0
3	CL	F	291	1/1	0.97	0.05	36,36,36,36	0
3	CL	C	291	1/1	0.99	0.03	27,27,27,27	0
3	CL	E	291	1/1	0.99	0.03	21,21,21,21	0
3	CL	A	291	1/1	0.99	0.06	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.