



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:31 PM UTC

PDB ID : 2X4Y / pdb_00002x4y
Title : Molecular basis of Histone H3K36me3 recognition by the PWWP domain of BRPF1.
Authors : Vezzoli, A.; Bonadies, N.; Allen, M.D.; Freund, S.M.V.; Santiveri, C.M.; Kvinaug, B.; Huntly, B.J.P.; Gottgens, B.; Bycroft, M.
Deposited on : 2010-02-02
Resolution : 1.70 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:

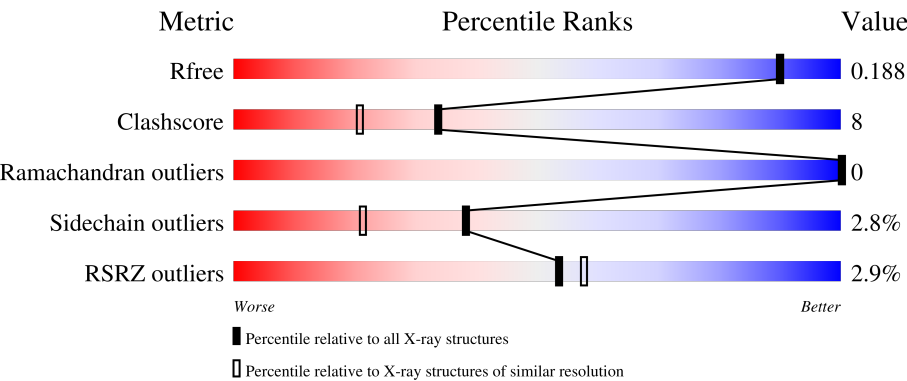
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	132	2% 80% 14% • •
1	C	132	2% 78% 15% • 5%
1	E	132	3% 85% 9% • 5%
1	G	132	84% 8% • 6%
1	I	132	2% 88% 5% • 5%

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Mol	Chain	Length	Quality of chain
1	K	132	2% 78% 16% • 5%
1	M	132	% 81% 12% • 5%
1	O	132	7% 73% 17% • 7%
2	B	21	5% 57% 29% 14%
2	D	21	5% 48% 19% 33%
2	F	21	5% 43% 29% 29%
2	H	21	38% 14% 48%
2	J	21	5% 48% 10% 43%
2	L	21	5% 29% 24% 48%
2	N	21	5% 52% 14% 33%
2	P	21	5% 43% 19% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10140 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 PEREGRIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	3	0
			1059	679	193	182	5			
1	C	125	Total	C	N	O	S	0	0	0
			1023	658	185	175	5			
1	E	126	Total	C	N	O	S	0	0	0
			1033	663	186	179	5			
1	G	124	Total	C	N	O	S	0	0	0
			1019	656	184	174	5			
1	I	125	Total	C	N	O	S	0	0	0
			1023	658	185	175	5			
1	K	126	Total	C	N	O	S	0	3	0
			1050	674	188	183	5			
1	M	126	Total	C	N	O	S	0	0	0
			1033	663	186	179	5			
1	O	123	Total	C	N	O	S	0	0	0
			1010	651	182	172	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1074	GLY	-	expression tag	UNP P55201
A	1075	GLY	-	expression tag	UNP P55201
C	1074	GLY	-	expression tag	UNP P55201
C	1075	GLY	-	expression tag	UNP P55201
E	1074	GLY	-	expression tag	UNP P55201
E	1075	GLY	-	expression tag	UNP P55201
G	1074	GLY	-	expression tag	UNP P55201
G	1075	GLY	-	expression tag	UNP P55201
I	1074	GLY	-	expression tag	UNP P55201
I	1075	GLY	-	expression tag	UNP P55201
K	1074	GLY	-	expression tag	UNP P55201
K	1075	GLY	-	expression tag	UNP P55201
M	1074	GLY	-	expression tag	UNP P55201

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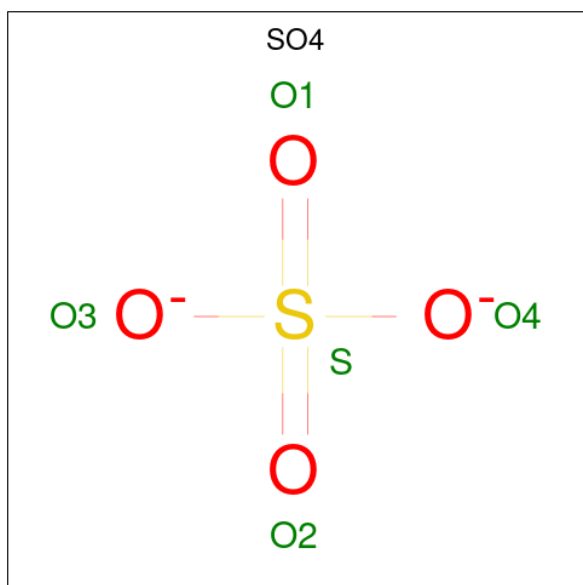
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Chain	Residue	Modelled	Actual	Comment	Reference
M	1075	GLY	-	expression tag	UNP P55201
O	1074	GLY	-	expression tag	UNP P55201
O	1075	GLY	-	expression tag	UNP P55201

- Molecule 2 is a protein called HISTONE H3.2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	18	Total	C	N	O	0	0	0
			136	86	29	21			
2	D	14	Total	C	N	O	0	0	0
			103	65	22	16			
2	F	15	Total	C	N	O	0	0	0
			108	68	23	17			
2	H	11	Total	C	N	O	0	0	0
			73	47	13	13			
2	J	12	Total	C	N	O	0	0	0
			83	53	16	14			
2	L	11	Total	C	N	O	0	0	0
			77	50	15	12			
2	N	14	Total	C	N	O	0	0	0
			106	68	21	17			
2	P	13	Total	C	N	O	0	0	0
			91	57	19	15			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	G	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	154	Total O 154 154	0	0
4	B	24	Total O 24 24	0	0
4	C	113	Total O 113 113	0	0
4	D	14	Total O 14 14	0	0
4	E	166	Total O 166 166	0	0
4	F	19	Total O 19 19	0	0
4	G	140	Total O 140 140	0	0
4	H	9	Total O 9 9	0	0
4	I	119	Total O 119 119	0	0
4	J	12	Total O 12 12	0	0
4	K	123	Total O 123 123	0	0
4	L	6	Total O 6 6	0	0
4	M	108	Total O 108 108	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	6	Total 6	O 6	0	0
4	O	62	Total 62	O 62	0	0
4	P	3	Total 3	O 3	0	0

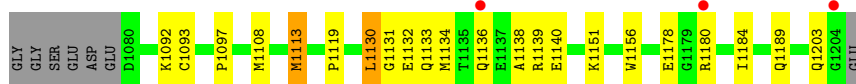
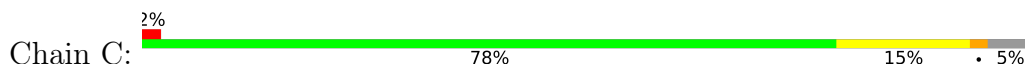
3 Residue-property plots [i](#)

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.

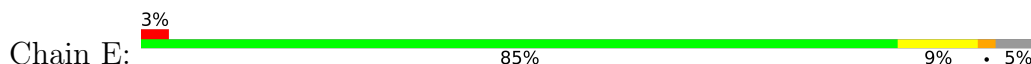
- Molecule 1: PEREGRIN



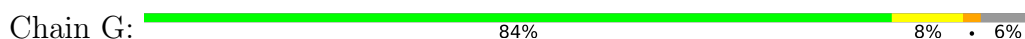
- Molecule 1: PEREGRIN



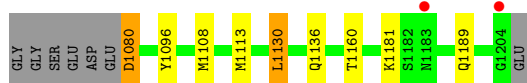
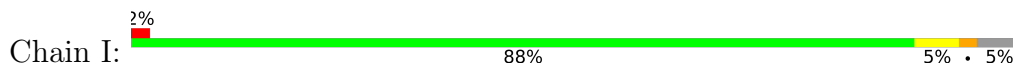
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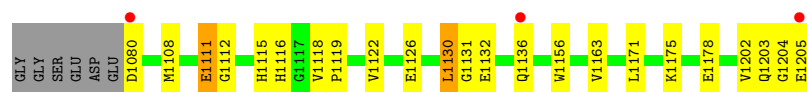
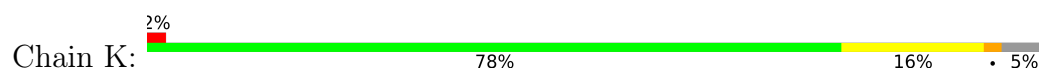
- Molecule 1: PEREGRIN



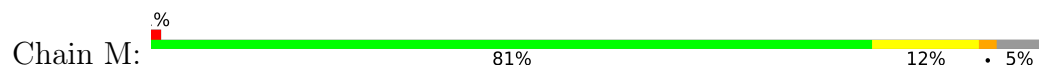
- Molecule 1: PEREGRIN



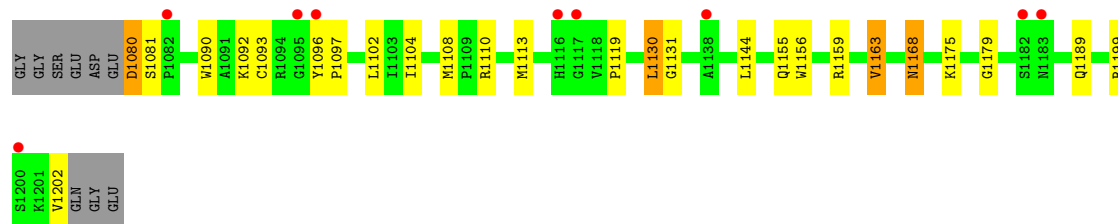
- Molecule 1: PEREGRIN



• Molecule 1: PEREGRIN



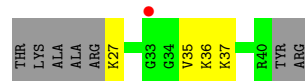
• Molecule 1: PEREGRIN



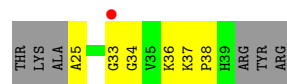
• Molecule 2: HISTONE H3.2



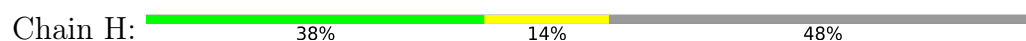
• Molecule 2: HISTONE H3.2



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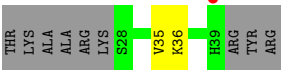


• Molecule 2: HISTONE H3.2

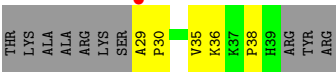
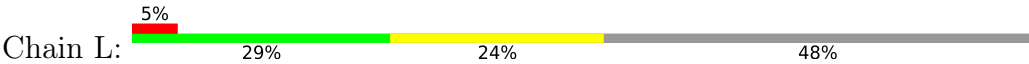




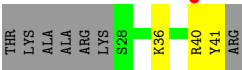
● Molecule 2: HISTONE H3.2



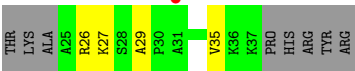
● Molecule 2: HISTONE H3.2



● Molecule 2: HISTONE H3.2



● Molecule 2: HISTONE H3.2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.76Å 97.91Å 102.52Å 86.80° 80.96° 87.24°	Depositor
Resolution (Å)	24.77 – 1.70 24.77 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.0 (24.77-1.70) 94.1 (24.77-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.70Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.190 , 0.227 0.187 , 0.188	Depositor DCC
R_{free} test set	7137 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10140	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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: SO4, M3L

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	1.05	1/1099 (0.1%)	1.12	0/1485
1	C	0.89	0/1051	1.06	0/1423
1	E	0.99	0/1061	1.06	2/1435 (0.1%)
1	G	0.91	1/1047 (0.1%)	1.03	2/1418 (0.1%)
1	I	0.81	0/1051	1.00	0/1423
1	K	0.87	0/1086	0.97	0/1469
1	M	0.84	0/1061	1.01	2/1435 (0.1%)
1	O	0.67	0/1038	1.01	2/1406 (0.1%)
2	B	0.98	0/127	1.22	2/170 (1.2%)
2	D	0.69	0/93	0.99	0/124
2	F	0.89	0/98	1.14	0/131
2	H	0.81	0/62	1.11	0/84
2	J	0.62	0/73	1.02	0/99
2	L	0.53	0/67	1.19	0/91
2	N	0.53	0/97	0.71	0/131
2	P	0.57	0/79	1.14	0/104
All	All	0.88	2/9190 (0.0%)	1.04	10/12428 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1093	CYS	CB-SG	-5.70	1.62	1.81
1	G	1122	VAL	CA-C	-5.52	1.48	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	1096	TYR	CA-C-N	-8.81	111.80	120.52
1	O	1096	TYR	C-N-CA	-8.81	111.80	120.52
2	B	33	GLY	N-CA-C	-6.91	102.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1184	ILE	N-CA-C	-5.56	105.11	110.72
1	M	1096	TYR	CA-C-N	-5.49	114.94	120.21
1	M	1096	TYR	C-N-CA	-5.49	114.94	120.21
2	B	34	GLY	N-CA-C	-5.39	104.89	112.60
1	E	1122	VAL	N-CA-C	5.23	113.13	108.63
1	G	1122	VAL	CA-C-N	-5.05	115.17	120.38
1	G	1122	VAL	C-N-CA	-5.05	115.17	120.38

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	1059	0	1080	17	0
1	C	1023	0	1045	22	0
1	E	1033	0	1051	10	0
1	G	1019	0	1042	11	0
1	I	1023	0	1045	12	0
1	K	1050	0	1065	20	0
1	M	1033	0	1051	18	0
1	O	1010	0	1034	18	0
2	B	136	0	147	4	0
2	D	103	0	115	4	0
2	F	108	0	120	5	0
2	H	73	0	82	4	0
2	J	83	0	89	3	0
2	L	77	0	84	4	0
2	N	106	0	111	1	0
2	P	91	0	106	4	0
3	A	15	0	0	2	0
3	C	5	0	0	0	0
3	D	5	0	0	1	0
3	E	5	0	0	1	0
3	G	5	0	0	0	0
4	A	154	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	1	0
4	C	113	0	0	7	0
4	D	14	0	0	2	0
4	E	166	0	0	3	0
4	F	19	0	0	4	0
4	G	140	0	0	3	0
4	H	9	0	0	3	0
4	I	119	0	0	4	0
4	J	12	0	0	0	0
4	K	123	0	0	4	0
4	L	6	0	0	0	0
4	M	108	0	0	5	0
4	N	6	0	0	0	0
4	O	62	0	0	2	0
4	P	3	0	0	0	0
All	All	10140	0	9267	142	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 8.

All (142) 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:K:1130:LEU:HD12	2:L:35:VAL:HG21	1.41	1.00
1:C:1184:ILE:HD11	3:D:1041:SO4:O3	1.64	0.97
1:K:1115:HIS:O	1:K:1118:VAL:HG12	1.70	0.91
1:C:1203:GLN:HB3	4:C:2107:HOH:O	1.70	0.90
1:G:1130:LEU:HD12	2:H:35:VAL:HG21	1.55	0.87
1:C:1108:MET:HE3	1:C:1113:MET:HG2	1.60	0.83
1:O:1090:TRP:HB2	1:O:1163:VAL:HG13	1.58	0.83
1:A:1133:GLN:HB3	4:A:2050:HOH:O	1.79	0.81
1:K:1178[B]:GLU:HG2	4:K:2078:HOH:O	1.78	0.81
1:K:1108:MET:HE2	1:K:1122:VAL:HG22	1.63	0.79
1:O:1163:VAL:HG11	1:O:1175:LYS:HE2	1.65	0.77
1:C:1133:GLN:HG3	4:C:2035:HOH:O	1.84	0.76
1:E:1080:ASP:OD2	1:E:1080:ASP:N	2.17	0.74
1:I:1130:LEU:HD12	2:J:35:VAL:HG21	1.68	0.73
1:G:1090:TRP:HB2	1:G:1163:VAL:HG13	1.69	0.72
1:C:1132:GLU:OE1	1:E:1107:LYS:HE2	1.90	0.70
1:A:1108:MET:HE3	1:A:1113:MET:HG2	1.75	0.68
1:E:1108:MET:HE3	1:E:1113:MET:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1080:ASP:N	4:K:2002:HOH:O	2.27	0.67
2:D:37:LYS:HE2	4:D:2009:HOH:O	1.94	0.67
1:K:1116:HIS:HD2	1:K:1202[A]:VAL:HG13	1.58	0.67
1:I:1108:MET:HE3	1:I:1113:MET:HG2	1.77	0.66
1:A:1125:LEU:HD11	3:A:2206:SO4:O1	1.96	0.66
2:H:33:GLY:HA3	4:H:2006:HOH:O	1.96	0.66
1:A:1133:GLN:O	1:A:1137:GLU:HG2	1.96	0.65
2:B:40:ARG:HD2	4:B:2018:HOH:O	1.97	0.65
1:K:1111:GLU:H	1:K:1111:GLU:CD	2.05	0.64
1:C:1136:GLN:HG3	4:C:2036:HOH:O	1.97	0.64
4:K:2017:HOH:O	2:L:38:PRO:HD2	1.98	0.64
2:H:33:GLY:CA	4:H:2006:HOH:O	2.45	0.63
1:C:1130:LEU:HD12	2:D:35:VAL:HG21	1.80	0.62
2:F:34:GLY:N	4:F:2013:HOH:O	1.97	0.62
1:M:1094:ARG:HG3	4:M:2017:HOH:O	2.00	0.62
2:F:25:ALA:N	4:F:2001:HOH:O	2.33	0.61
1:O:1097:PRO:HB2	4:O:2008:HOH:O	2.01	0.61
1:O:1080:ASP:OD2	1:O:1080:ASP:N	2.34	0.61
1:K:1116:HIS:CD2	1:K:1202[A]:VAL:HG13	2.36	0.60
1:M:1108:MET:CE	1:M:1113:MET:HG2	2.30	0.60
1:K:1115:HIS:CE1	1:K:1202[A]:VAL:HG11	2.36	0.60
1:M:1168:ASN:ND2	1:M:1171:LEU:H	2.00	0.59
1:C:1189:GLN:NE2	4:C:2090:HOH:O	2.34	0.59
1:O:1168:ASN:C	1:O:1168:ASN:HD22	2.10	0.59
2:H:34:GLY:N	4:H:2006:HOH:O	2.08	0.59
1:A:1139:ARG:CZ	4:A:2052:HOH:O	2.50	0.59
1:I:1136:GLN:HG3	4:I:2040:HOH:O	2.03	0.59
1:G:1090:TRP:HB2	1:G:1163:VAL:CG1	2.31	0.59
1:G:1137:GLU:OE2	4:G:2052:HOH:O	2.17	0.58
1:C:1130:LEU:HD22	1:C:1134:MET:HG3	1.85	0.58
2:D:37:LYS:HG3	4:D:2010:HOH:O	2.03	0.58
1:A:1130:LEU:HD12	2:B:35:VAL:HG21	1.83	0.58
1:C:1108:MET:HE3	1:C:1113:MET:CG	2.33	0.57
1:A:1086:LEU:HD13	1:A:1115:HIS:CD2	2.38	0.57
1:M:1189:GLN:NE2	4:M:2093:HOH:O	2.39	0.56
1:O:1097:PRO:HG3	1:O:1179:GLY:HA2	1.88	0.56
1:O:1119:PRO:HB2	2:P:29:ALA:HA	1.87	0.56
1:O:1130:LEU:HD12	2:P:35:VAL:HG21	1.88	0.56
1:E:1137:GLU:HG3	4:E:2049:HOH:O	2.05	0.56
1:O:1090:TRP:HB2	1:O:1163:VAL:CG1	2.32	0.55
1:M:1168:ASN:HD22	1:M:1168:ASN:C	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1152:ARG:HD3	4:G:2069:HOH:O	2.06	0.54
1:M:1130:LEU:HD22	1:M:1130:LEU:O	2.06	0.54
1:O:1092:LYS:NZ	1:O:1093:CYS:O	2.40	0.54
1:K:1115:HIS:O	1:K:1118:VAL:CG1	2.51	0.53
1:G:1108:MET:HE2	1:G:1122:VAL:HG22	1.89	0.53
1:A:1079:GLU:O	1:A:1079:GLU:HG2	2.08	0.52
1:I:1096:TYR:CD1	2:J:36:M3L:HM33	2.44	0.52
1:O:1131:GLY:HA3	1:O:1156:TRP:CE2	2.44	0.52
1:I:1189:GLN:NE2	4:I:2103:HOH:O	2.42	0.52
1:C:1133:GLN:HB3	4:C:2041:HOH:O	2.10	0.52
1:E:1137:GLU:CG	4:E:2049:HOH:O	2.57	0.51
2:F:33:GLY:HA3	4:F:2013:HOH:O	2.10	0.51
1:E:1171:LEU:C	1:E:1171:LEU:HD23	2.36	0.51
1:I:1160:THR:HG23	4:I:2047:HOH:O	2.10	0.51
1:C:1119:PRO:HD3	2:D:27:LYS:HD3	1.94	0.50
1:I:1181:LYS:HE3	4:I:2092:HOH:O	2.10	0.50
1:C:1130:LEU:HD22	1:C:1134:MET:CG	2.43	0.49
1:M:1080:ASP:OD2	1:M:1080:ASP:N	2.46	0.48
1:A:1139:ARG:NE	4:A:2052:HOH:O	2.46	0.48
1:A:1200:SER:OG	1:A:1205:GLU:HB2	2.13	0.48
1:G:1140:GLU:OE2	4:G:2054:HOH:O	2.20	0.48
2:N:40:ARG:HD2	2:N:41:TYR:CE2	2.49	0.48
2:F:33:GLY:CA	4:F:2013:HOH:O	2.61	0.48
1:C:1092:LYS:NZ	1:C:1093:CYS:O	2.47	0.48
1:K:1203:GLN:NE2	4:K:2122:HOH:O	2.47	0.47
1:G:1171:LEU:C	1:G:1171:LEU:HD23	2.38	0.47
1:K:1163:VAL:HG11	1:K:1171:LEU:HD11	1.96	0.47
1:A:1180:ARG:HG3	1:A:1181:LYS:N	2.29	0.47
1:M:1175:LYS:CE	4:M:2076:HOH:O	2.62	0.47
1:K:1132:GLU:O	1:K:1136:GLN:HG2	2.15	0.47
2:B:27:LYS:HG3	2:P:27:LYS:HG2	1.96	0.47
1:K:1204:GLY:O	1:K:1205:GLU:HB2	2.15	0.47
1:M:1130:LEU:HD22	1:M:1134:MET:HG3	1.98	0.46
1:K:1118:VAL:HG11	1:K:1202[B]:VAL:CG1	2.45	0.46
1:I:1108:MET:CE	1:I:1113:MET:HG2	2.43	0.46
1:A:1096:TYR:CD1	2:B:36:M3L:HM33	2.51	0.46
1:O:1102:LEU:HD23	1:O:1104:ILE:HD11	1.98	0.46
1:M:1175:LYS:HE3	4:M:2076:HOH:O	2.15	0.46
1:A:1184:ILE:HG23	4:A:2111:HOH:O	2.17	0.45
1:K:1131:GLY:HA3	1:K:1156:TRP:CE2	2.52	0.44
1:O:1081:SER:O	1:O:1159:ARG:NE	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1110:ARG:HB3	4:M:2029:HOH:O	2.18	0.44
1:I:1130:LEU:HD12	2:J:35:VAL:CG2	2.44	0.44
1:C:1138:ALA:HB1	1:C:1140:GLU:HG2	2.00	0.44
1:A:1094[A]:ARG:HD2	4:A:2021:HOH:O	2.17	0.44
1:C:1130:LEU:O	1:C:1134:MET:HG3	2.19	0.43
1:I:1080:ASP:N	1:I:1080:ASP:OD1	2.50	0.43
1:C:1097:PRO:HB2	4:C:2018:HOH:O	2.18	0.43
1:M:1108:MET:HE3	1:M:1113:MET:HG2	1.99	0.43
1:O:1144:LEU:HD12	1:O:1155:GLN:O	2.18	0.43
2:F:37:LYS:HA	2:F:38:PRO:HD3	1.88	0.43
1:K:1119:PRO:HB2	2:L:29:ALA:HA	2.01	0.42
1:O:1108:MET:HE3	1:O:1113:MET:HG2	2.00	0.42
1:C:1097:PRO:HA	1:C:1178:GLU:OE2	2.19	0.42
3:E:2206:SO4:O4	4:E:2165:HOH:O	2.19	0.42
1:K:1112:GLY:HA2	1:K:1122:VAL:CG2	2.50	0.42
1:G:1094:ARG:H	1:G:1094:ARG:HG2	1.61	0.42
1:O:1110:ARG:O	2:P:26:ARG:HD2	2.20	0.42
1:C:1133:GLN:CB	4:C:2041:HOH:O	2.68	0.42
1:G:1163:VAL:HG21	1:G:1171:LEU:HD11	2.01	0.42
2:L:29:ALA:HA	2:L:30:PRO:HD3	1.92	0.42
1:A:1094[A]:ARG:NH1	4:A:2019:HOH:O	2.48	0.42
1:A:1194:ARG:HD3	4:A:2059:HOH:O	2.18	0.42
1:E:1080:ASP:HB2	1:E:1081:SER:H	1.41	0.41
1:E:1190:ILE:HG23	1:M:1174:GLU:HG3	2.02	0.41
1:I:1113:MET:HE3	1:I:1113:MET:HB2	1.92	0.41
1:C:1151:LYS:HB2	1:C:1151:LYS:HE3	1.92	0.41
1:C:1113:MET:HE3	1:C:1113:MET:HB2	1.91	0.41
1:O:1189:GLN:NE2	4:O:2055:HOH:O	2.54	0.41
1:M:1108:MET:HE3	1:M:1113:MET:SD	2.60	0.41
1:M:1130:LEU:HD22	1:M:1130:LEU:C	2.46	0.41
1:G:1120:ILE:HA	1:G:1121:PRO:HD3	1.95	0.41
1:K:1175:LYS:O	1:K:1178[B]:GLU:HG3	2.21	0.41
1:C:1131:GLY:HA3	1:C:1156:TRP:CE2	2.56	0.41
1:M:1168:ASN:HD22	1:M:1171:LEU:H	1.68	0.41
1:O:1199:ARG:O	1:O:1202:VAL:HB	2.20	0.41
1:M:1115:HIS:O	1:M:1116:HIS:C	2.62	0.40
1:A:1161:LYS:NZ	3:A:2208:SO4:O2	2.52	0.40
1:I:1108:MET:HE3	1:I:1108:MET:HB2	1.90	0.40
1:E:1130:LEU:HD22	1:E:1134:MET:HG3	2.04	0.40
1:E:1151:LYS:HD3	1:E:1151:LYS:HA	1.95	0.40
1:M:1131:GLY:HA3	1:M:1156:TRP:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	128/132 (97%)	126 (98%)	2 (2%)	0	100	100
1	C	123/132 (93%)	121 (98%)	2 (2%)	0	100	100
1	E	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
1	G	122/132 (92%)	120 (98%)	2 (2%)	0	100	100
1	I	123/132 (93%)	121 (98%)	2 (2%)	0	100	100
1	K	127/132 (96%)	125 (98%)	2 (2%)	0	100	100
1	M	124/132 (94%)	121 (98%)	3 (2%)	0	100	100
1	O	121/132 (92%)	115 (95%)	6 (5%)	0	100	100
2	B	15/21 (71%)	15 (100%)	0	0	100	100
2	D	11/21 (52%)	11 (100%)	0	0	100	100
2	F	12/21 (57%)	12 (100%)	0	0	100	100
2	H	8/21 (38%)	8 (100%)	0	0	100	100
2	J	9/21 (43%)	9 (100%)	0	0	100	100
2	L	8/21 (38%)	8 (100%)	0	0	100	100
2	N	11/21 (52%)	11 (100%)	0	0	100	100
2	P	10/21 (48%)	10 (100%)	0	0	100	100
All	All	1076/1224 (88%)	1054 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/117 (100%)	114 (97%)	3 (3%)	40	23
1	C	112/117 (96%)	108 (96%)	4 (4%)	31	14
1	E	113/117 (97%)	110 (97%)	3 (3%)	39	23
1	G	112/117 (96%)	109 (97%)	3 (3%)	39	23
1	I	112/117 (96%)	110 (98%)	2 (2%)	51	36
1	K	116/117 (99%)	113 (97%)	3 (3%)	40	23
1	M	113/117 (97%)	108 (96%)	5 (4%)	25	10
1	O	111/117 (95%)	107 (96%)	4 (4%)	31	14
2	B	11/14 (79%)	11 (100%)	0	100	100
2	D	9/14 (64%)	9 (100%)	0	100	100
2	F	9/14 (64%)	9 (100%)	0	100	100
2	H	6/14 (43%)	6 (100%)	0	100	100
2	J	7/14 (50%)	7 (100%)	0	100	100
2	L	6/14 (43%)	6 (100%)	0	100	100
2	N	9/14 (64%)	9 (100%)	0	100	100
2	P	7/14 (50%)	7 (100%)	0	100	100
All	All	970/1048 (93%)	943 (97%)	27 (3%)	38	21

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1080	ASP
1	A	1130	LEU
1	A	1139	ARG
1	C	1113	MET
1	C	1130	LEU
1	C	1139	ARG
1	C	1180	ARG
1	E	1080	ASP
1	E	1111	GLU
1	E	1130	LEU
1	G	1130	LEU
1	G	1163	VAL
1	G	1169	GLN
1	I	1080	ASP

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Mol	Chain	Res	Type
1	I	1130	LEU
1	K	1111	GLU
1	K	1126	GLU
1	K	1130	LEU
1	M	1080	ASP
1	M	1130	LEU
1	M	1137	GLU
1	M	1168	ASN
1	M	1182	SER
1	O	1080	ASP
1	O	1130	LEU
1	O	1163	VAL
1	O	1168	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1115	HIS
1	A	1133	GLN
1	A	1141	HIS
1	A	1189	GLN
1	A	1203	GLN
2	B	39	HIS
1	C	1116	HIS
1	C	1203	GLN
1	E	1133	GLN
1	E	1189	GLN
1	E	1197	GLN
1	E	1203	GLN
1	G	1115	HIS
1	G	1116	HIS
1	G	1203	GLN
1	I	1115	HIS
1	I	1189	GLN
1	I	1203	GLN
1	K	1116	HIS
1	K	1133	GLN
1	K	1136	GLN
1	K	1203	GLN
1	M	1115	HIS
1	M	1116	HIS
1	M	1133	GLN

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Mol	Chain	Res	Type
1	M	1168	ASN
1	M	1189	GLN
1	M	1203	GLN
1	O	1133	GLN
1	O	1136	GLN
1	O	1168	ASN
1	O	1169	GLN
1	O	1197	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	M3L	N	36	2	10,11,12	1.13	1 (10%)	9,14,16	0.61	0
2	M3L	J	36	2	10,11,12	1.02	0	9,14,16	0.60	0
2	M3L	D	36	2	10,11,12	1.20	1 (10%)	9,14,16	0.72	0
2	M3L	F	36	2	10,11,12	1.22	2 (20%)	9,14,16	0.83	0
2	M3L	P	36	2	10,11,12	0.97	0	9,14,16	0.79	0
2	M3L	B	36	2	10,11,12	1.03	0	9,14,16	1.02	0
2	M3L	L	36	2	10,11,12	1.17	1 (10%)	9,14,16	0.86	1 (11%)
2	M3L	H	36	2	10,11,12	1.11	0	9,14,16	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	N	36	2	-	0/9/10/12	-
2	M3L	J	36	2	-	0/9/10/12	-
2	M3L	D	36	2	-	0/9/10/12	-
2	M3L	F	36	2	-	0/9/10/12	-
2	M3L	P	36	2	-	0/9/10/12	-
2	M3L	B	36	2	-	0/9/10/12	-
2	M3L	L	36	2	-	1/9/10/12	-
2	M3L	H	36	2	-	0/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	36	M3L	CM2-NZ	-2.40	1.43	1.50
2	L	36	M3L	CE-NZ	-2.36	1.44	1.51
2	N	36	M3L	CE-NZ	-2.16	1.44	1.51
2	D	36	M3L	CE-NZ	-2.14	1.44	1.51
2	F	36	M3L	CM1-NZ	-2.08	1.44	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	36	M3L	CM3-NZ-CM1	2.18	114.69	108.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	36	M3L	CD-CE-NZ-CM1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	J	36	M3L	1	0
2	B	36	M3L	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	1041	-	4,4,4	0.29	0	6,6,6	0.28	0
3	SO4	E	2206	-	4,4,4	0.24	0	6,6,6	0.51	0
3	SO4	G	2204	-	4,4,4	0.37	0	6,6,6	0.25	0
3	SO4	A	2206	-	4,4,4	0.42	0	6,6,6	0.58	0
3	SO4	A	2208	-	4,4,4	0.19	0	6,6,6	0.46	0
3	SO4	A	2207	-	4,4,4	0.25	0	6,6,6	0.52	0
3	SO4	C	2205	-	4,4,4	0.29	0	6,6,6	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1041	SO4	1	0
3	E	2206	SO4	1	0
3	A	2206	SO4	1	0
3	A	2208	SO4	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	127/132 (96%)	-0.18	3 (2%) 59 64	10, 21, 40, 57	3 (2%)
1	C	125/132 (94%)	0.11	3 (2%) 59 64	15, 28, 43, 55	0
1	E	126/132 (95%)	-0.13	4 (3%) 50 54	13, 23, 41, 59	0
1	G	124/132 (93%)	-0.05	0 100 100	15, 25, 43, 50	0
1	I	125/132 (94%)	0.10	2 (1%) 70 75	17, 28, 46, 53	0
1	K	126/132 (95%)	0.07	3 (2%) 59 64	12, 26, 44, 56	3 (2%)
1	M	126/132 (95%)	0.19	1 (0%) 82 85	16, 30, 49, 59	0
1	O	123/132 (93%)	0.69	9 (7%) 21 23	23, 35, 56, 64	0
2	B	17/21 (80%)	0.45	1 (5%) 28 31	20, 28, 40, 46	0
2	D	13/21 (61%)	0.92	1 (7%) 19 21	31, 36, 48, 52	0
2	F	14/21 (66%)	0.83	1 (7%) 22 24	26, 33, 41, 45	0
2	H	10/21 (47%)	0.73	0 100 100	30, 34, 46, 47	0
2	J	11/21 (52%)	0.84	1 (9%) 15 15	30, 33, 49, 56	0
2	L	10/21 (47%)	0.83	1 (10%) 12 13	33, 36, 42, 45	0
2	N	13/21 (61%)	0.97	1 (7%) 19 21	33, 39, 46, 52	0
2	P	12/21 (57%)	1.12	1 (8%) 17 18	39, 43, 49, 60	0
All	All	1102/1224 (90%)	0.17	32 (2%) 53 58	10, 28, 48, 64	6 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1095	GLY	3.7
1	O	1082	PRO	3.5
1	K	1205	GLU	3.2
1	C	1204	GLY	3.1
1	O	1096	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	1082	PRO	2.9
1	E	1205	GLU	2.7
1	M	1205	GLU	2.7
1	O	1138	ALA	2.6
1	O	1200	SER	2.5
2	J	39	HIS	2.5
1	O	1117	GLY	2.5
1	I	1204	GLY	2.4
1	O	1183	ASN	2.4
2	B	24	ALA	2.3
1	C	1180	ARG	2.3
1	C	1136	GLN	2.3
1	I	1183	ASN	2.3
1	E	1204	GLY	2.3
2	L	29	ALA	2.3
2	P	31	ALA	2.3
1	K	1080	ASP	2.3
1	O	1182	SER	2.2
1	K	1136	GLN	2.2
1	O	1116	HIS	2.2
1	A	1080	ASP	2.2
2	D	33	GLY	2.1
1	A	1082	PRO	2.1
2	F	33	GLY	2.0
1	A	1180	ARG	2.0
2	N	40	ARG	2.0
1	E	1081	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	M3L	P	36	12/13	0.89	0.11	37,41,52,53	0
2	M3L	N	36	12/13	0.91	0.10	26,28,32,33	0
2	M3L	D	36	12/13	0.93	0.09	24,29,33,34	0
2	M3L	L	36	12/13	0.93	0.08	21,26,33,34	0
2	M3L	J	36	12/13	0.95	0.08	24,25,32,32	0
2	M3L	H	36	12/13	0.95	0.07	20,26,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	M3L	F	36	12/13	0.96	0.07	18,21,24,28	0
2	M3L	B	36	12/13	0.97	0.06	15,20,23,25	0

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($\text{\AA}^2$)	Q<0.9
3	SO4	A	2207	5/5	0.93	0.09	28,29,31,31	5
3	SO4	D	1041	5/5	0.93	0.11	44,46,48,51	5
3	SO4	C	2205	5/5	0.94	0.07	30,33,36,38	5
3	SO4	A	2206	5/5	0.96	0.09	29,34,36,37	0
3	SO4	A	2208	5/5	0.96	0.08	29,32,33,35	5
3	SO4	G	2204	5/5	0.96	0.06	28,33,36,38	4
3	SO4	E	2206	5/5	0.98	0.06	30,31,36,37	4

6.5 Other polymers [i](#)

There are no such residues in this entry.