



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 AM GMT

PDB ID : 2X4Y
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.; Kvinnlaug, 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
<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

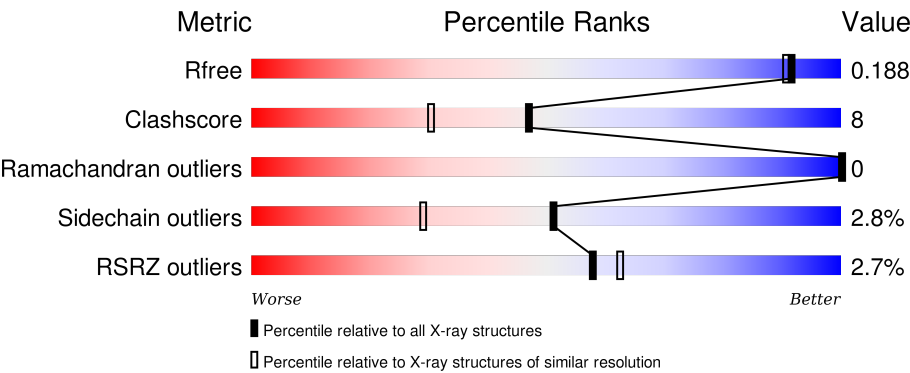
1 Overall quality at a glance i

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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	132	<div><div>%</div><div>82%13%••</div></div>
1	C	132	<div><div>2%</div><div>78%16%•5%</div></div>
1	E	132	<div><div>2%</div><div>86%8%•5%</div></div>
1	G	132	<div><div>%</div><div>83%9%•6%</div></div>
1	I	132	<div><div>%</div><div>86%7%•5%</div></div>

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Mol	Chain	Length	Quality of chain
1	K	132	<p>2% 77% 17% • 5%</p>
1	M	132	<p>2% 83% 11% • 5%</p>
1	O	132	<p>5% 74% 17% • 7%</p>
2	B	21	<p>5% 67% 19% 14%</p>
2	D	21	<p>5% 52% 14% 33%</p>
2	F	21	<p>5% 48% 24% 29%</p>
2	H	21	<p>38% 14% 48%</p>
2	J	21	<p>5% 48% 10% 43%</p>
2	L	21	<p>5% 33% 19% 48%</p>
2	N	21	<p>10% 57% 10% 33%</p>
2	P	21	<p>19% 43% 19% 38%</p>

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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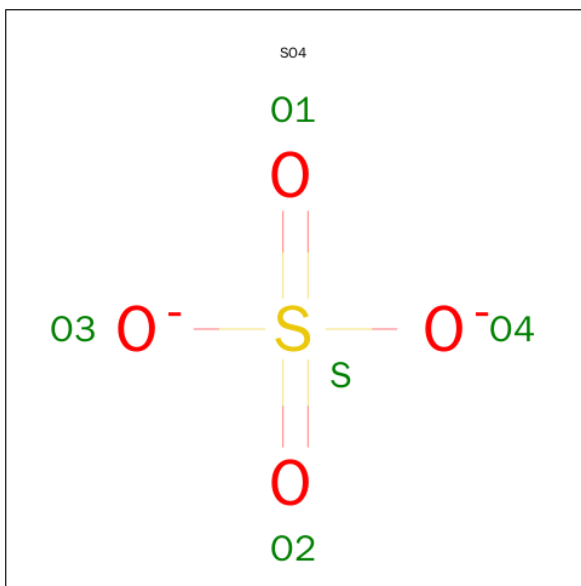
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Chain	Residue	Modelled	Actual	Comment	Reference
M	1075	GLY	-	EXPRESSION TAG	UNP P55201
O	1074	GLY	-	EXPRESSION TAG	UNP P55201
O	1075	GLY	-	EXPRESSION TAG	UNP P55201

- 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 (three-letter code: 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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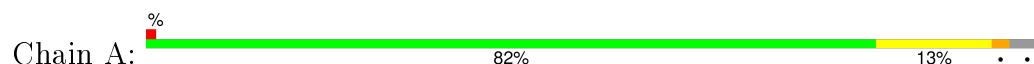
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	N	6	Total 6	O 6	0	0
4	O	62	Total 62	O 62	0	0
4	P	3	Total 3	O 3	0	0

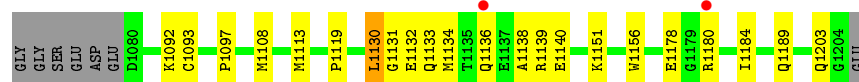
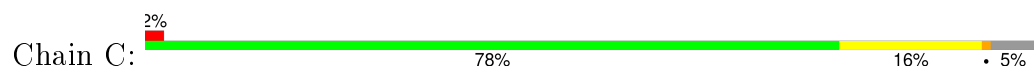
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA 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.

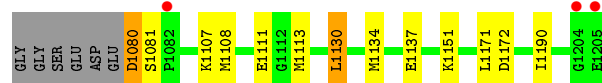
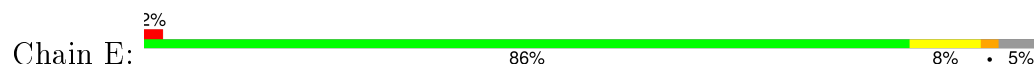
• Molecule 1: PEREGRIN



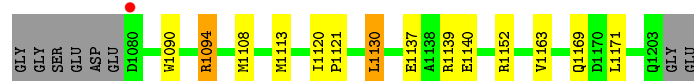
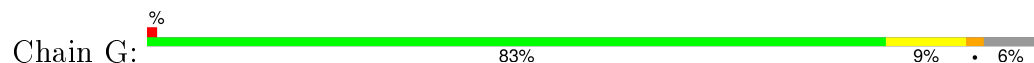
• Molecule 1: PEREGRIN



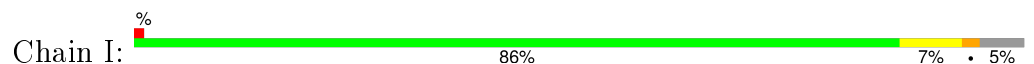
• Molecule 1: PEREGRIN



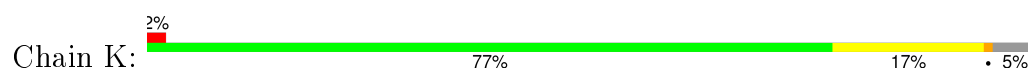
• Molecule 1: PEREGRIN



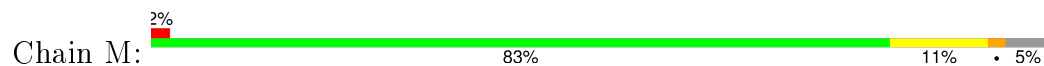
• Molecule 1: PEREGRIN



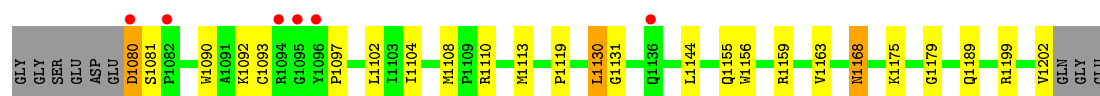
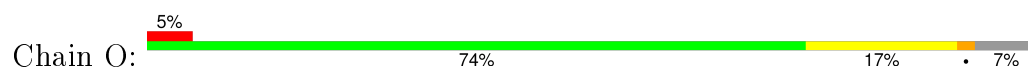
• Molecule 1: PEREGRIN



- Molecule 1: PEREGRIN



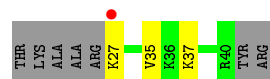
- Molecule 1: PEREGRIN



- Molecule 2: HISTONE H3.2



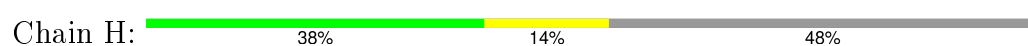
- Molecule 2: HISTONE H3.2



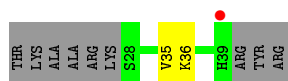
- Molecule 2: HISTONE H3.2



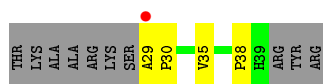
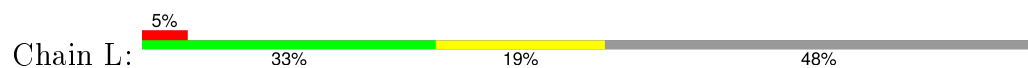
- Molecule 2: HISTONE H3.2



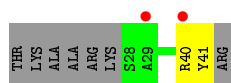
- Molecule 2: HISTONE H3.2



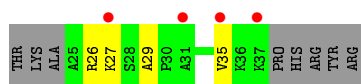
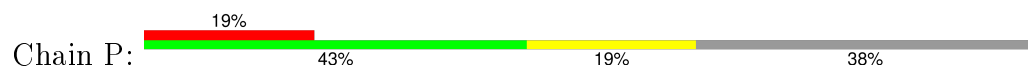
- Molecule 2: HISTONE H3.2



- Molecule 2: HISTONE H3.2



- 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 48.84 – 1.70	Depositor EDS
% Data completeness (in resolution range)	88.0 (24.77-1.70) 92.6 (48.84-1.70)	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 0.186 , 0.188	Depositor DCC
R_{free} test set	7136 reflections (5.03%)	DCC
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 , 52.8	EDS
Estimated twinning fraction	0.016 for -h,-k,-h+l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 141891 reflections	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, 0.375 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: M3L, SO4

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	0.92	1/1099 (0.1%)	0.91	0/1485
1	C	0.72	0/1051	0.81	0/1423
1	E	0.79	0/1061	0.84	1/1435 (0.1%)
1	G	0.74	0/1047	0.80	0/1418
1	I	0.71	1/1051 (0.1%)	0.76	0/1423
1	K	0.72	0/1086	0.78	0/1469
1	M	0.70	0/1061	0.75	0/1435
1	O	0.58	0/1038	0.70	0/1406
2	B	0.79	0/127	0.96	0/170
2	D	0.63	0/93	0.87	0/124
2	F	0.74	0/98	0.79	0/131
2	H	0.67	0/62	0.85	0/84
2	J	0.57	0/73	0.62	0/99
2	L	0.50	0/67	0.63	0/91
2	N	0.50	0/97	0.56	0/131
2	P	0.52	0/79	0.70	0/104
All	All	0.73	2/9190 (0.0%)	0.79	1/12428 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1093	CYS	CB-SG	-11.65	1.62	1.82
1	I	1093	CYS	CB-SG	-5.79	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1172	ASP	CB-CG-OD1	-5.51	113.34	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	1059	0	1080	16	0
1	C	1023	0	1045	22	0
1	E	1033	0	1051	11	0
1	G	1019	0	1042	11	0
1	I	1023	0	1045	11	0
1	K	1050	0	1065	20	0
1	M	1033	0	1051	15	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
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	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	138	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 (138) 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: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: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:N	1:E:1080:ASP:OD2	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:K:1080:ASP:N	4:K:2002:HOH:O	2.27	0.67
1:I:1108:MET:HE3	1:I:1113:MET:HG2	1.75	0.67
1:K:1116:HIS:HD2	1:K:1202[A]:VAL:HG13	1.58	0.67
2:D:37:LYS:HE2	4:D:2009:HOH:O	1.94	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:1080:ASP:N	1:O:1080:ASP:OD2	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:K:1111:GLU:H	1:K:1111:GLU:CD	2.05	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
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:M:1175:LYS:NZ	4:M:2076:HOH:O	2.37	0.58
1:A:1086:LEU:HD13	1:A:1115:HIS:CD2	2.38	0.57
1:O:1097:PRO:HG3	1:O:1179:GLY:HA2	1.88	0.56
1:M:1189:GLN:NE2	4:M:2093:HOH:O	2.39	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:O:1168:ASN:C	1:O:1168:ASN:HD22	2.10	0.55
1:O:1108:MET:HE3	1:O:1113:MET:HG2	1.89	0.55
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:K:1108:MET:HE3	1:K:1113:MET:HG2	1.90	0.52
1:I:1096:TYR:CD1	2:J:36:M3L:HM33	2.44	0.52
1:A:1079:GLU:O	1:A:1079:GLU:HG2	2.08	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:I:1108:MET:HE3	1:I:1113:MET:CG	2.41	0.51
1:I:1160:THR:HG23	4:I:2047:HOH:O	2.10	0.51
1:C:1108:MET:CE	1:C:1113:MET:HG2	2.41	0.50
1:C:1119:PRO:HD3	2:D:27:LYS:HD3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1181:LYS:HE3	4:I:2092:HOH:O	2.10	0.50
1:M:1168:ASN:HD22	1:M:1168:ASN:C	2.15	0.50
1:C:1130:LEU:HD22	1:C:1134:MET:CG	2.43	0.49
1:E:1108:MET:HE3	1:E:1113:MET:HG2	1.94	0.48
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: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
1:A:1200:SER:OG	1:A:1205:GLU:HB2	2.13	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: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
1:K:1204:GLY:O	1:K:1205:GLU:HB2	2.15	0.47
2:B:27:LYS:HG3	2:P:27:LYS:HG2	1.96	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:E:1171:LEU:C	1:E:1171:LEU:HD23	2.36	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
1:C:1108:MET:HE3	1:C:1113:MET:CG	2.47	0.44
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:OD1	1:I:1080:ASP:N	2.50	0.43
1:C:1097:PRO:HB2	4:C:2018:HOH:O	2.18	0.43
1:O:1144:LEU:HD12	1:O:1155:GLN:O	2.18	0.43
1:G:1171:LEU:HD23	1:G:1171:LEU:C	2.38	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:C:1097:PRO:HA	1:C:1178:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1108:MET:HE2	1:C:1113:MET:HG2	2.00	0.42
1:G:1108:MET:HE3	1:G:1113:MET:HG2	2.02	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:C:1151:LYS:HB2	1:C:1151:LYS:HE3	1.92	0.41
1:O:1189:GLN:NE2	4:O:2055:HOH:O	2.54	0.41
1:E:1108:MET:CE	1:E:1113:MET:HG2	2.50	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: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:C:1131:GLY:HA3	1:C:1156:TRP:CE2	2.56	0.41
1:A:1161:LYS:NZ	3:A:2208:SO4:O2	2.52	0.40
1:M:1131:GLY:HA3	1:M:1156:TRP:CE2	2.57	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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	54	32
1	C	112/117 (96%)	109 (97%)	3 (3%)	52	31
1	E	113/117 (97%)	110 (97%)	3 (3%)	52	31
1	G	112/117 (96%)	108 (96%)	4 (4%)	42	19
1	I	112/117 (96%)	109 (97%)	3 (3%)	52	31
1	K	116/117 (99%)	114 (98%)	2 (2%)	68	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	M	113/117 (97%)	107 (95%)	6 (5%)	28	9
1	O	111/117 (95%)	108 (97%)	3 (3%)	52	31
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%)	51	29

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	1130	LEU
1	C	1139	ARG
1	C	1180	ARG
1	E	1080	ASP
1	E	1111	GLU
1	E	1130	LEU
1	G	1094	ARG
1	G	1130	LEU
1	G	1139	ARG
1	G	1169	GLN
1	I	1080	ASP
1	I	1130	LEU
1	I	1180	ARG
1	K	1130	LEU
1	K	1139	ARG
1	M	1080	ASP
1	M	1130	LEU
1	M	1137	GLU
1	M	1139	ARG
1	M	1168	ASN

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Mol	Chain	Res	Type
1	M	1182	SER
1	O	1080	ASP
1	O	1130	LEU
1	O	1168	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1133	GLN
1	A	1169	GLN
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	1116	HIS
1	G	1133	GLN
1	G	1203	GLN
1	I	1189	GLN
1	I	1203	GLN
1	K	1116	HIS
1	K	1136	GLN
1	K	1203	GLN
1	M	1115	HIS
1	M	1116	HIS
1	M	1133	GLN
1	M	1168	ASN
1	M	1189	GLN
1	M	1203	GLN
1	O	1115	HIS
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	B	36	2	10,11,12	1.00	0	12,14,16	1.24	1 (8%)
2	M3L	D	36	2	10,11,12	1.24	1 (10%)	12,14,16	0.95	1 (8%)
2	M3L	F	36	2	10,11,12	1.18	2 (20%)	12,14,16	0.92	0
2	M3L	H	36	2	10,11,12	1.06	0	12,14,16	0.91	0
2	M3L	J	36	2	10,11,12	0.97	0	12,14,16	0.75	0
2	M3L	L	36	2	10,11,12	1.14	1 (10%)	12,14,16	1.12	2 (16%)
2	M3L	N	36	2	10,11,12	1.09	0	12,14,16	1.00	1 (8%)
2	M3L	P	36	2	10,11,12	0.93	0	12,14,16	1.16	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	B	36	2	-	0/8/10/12	0/0/0/0
2	M3L	D	36	2	-	0/8/10/12	0/0/0/0
2	M3L	F	36	2	-	0/8/10/12	0/0/0/0
2	M3L	H	36	2	-	0/8/10/12	0/0/0/0
2	M3L	J	36	2	-	0/8/10/12	0/0/0/0
2	M3L	L	36	2	-	0/8/10/12	0/0/0/0
2	M3L	N	36	2	-	0/8/10/12	0/0/0/0
2	M3L	P	36	2	-	0/8/10/12	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	36	M3L	CM2-NZ	-2.37	1.43	1.50
2	L	36	M3L	CE-NZ	-2.14	1.44	1.51
2	F	36	M3L	CM1-NZ	-2.06	1.44	1.50
2	D	36	M3L	CB-CA	-2.02	1.51	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	36	M3L	O-C-CA	-2.88	117.99	125.49
2	N	36	M3L	O-C-CA	-2.79	118.21	125.49
2	L	36	M3L	O-C-CA	-2.55	118.85	125.49
2	D	36	M3L	O-C-CA	-2.34	119.39	125.49
2	P	36	M3L	O-C-CA	-2.33	119.43	125.49
2	P	36	M3L	CE-CD-CG	2.01	118.69	110.64
2	L	36	M3L	CM3-NZ-CM1	2.22	114.69	108.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	2206	-	4,4,4	0.51	0	6,6,6	0.63	0
3	SO4	A	2207	-	4,4,4	0.31	0	6,6,6	0.55	0
3	SO4	A	2208	-	4,4,4	0.50	0	6,6,6	0.66	0
3	SO4	C	2205	-	4,4,4	0.24	0	6,6,6	0.20	0
3	SO4	D	1041	-	4,4,4	0.41	0	6,6,6	0.33	0
3	SO4	E	2206	-	4,4,4	0.27	0	6,6,6	0.54	0
3	SO4	G	2204	-	4,4,4	0.46	0	6,6,6	0.15	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
3	SO4	A	2206	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2207	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2208	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2205	-	-	0/0/0/0	0/0/0/0
3	SO4	D	1041	-	-	0/0/0/0	0/0/0/0
3	SO4	E	2206	-	-	0/0/0/0	0/0/0/0
3	SO4	G	2204	-	-	0/0/0/0	0/0/0/0

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	A	2206	SO4	1	0
3	A	2208	SO4	1	0
3	D	1041	SO4	1	0
3	E	2206	SO4	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	127/132 (96%)	0.10	1 (0%) 87 90	12, 21, 40, 57	0
1	C	125/132 (94%)	-0.07	2 (1%) 74 79	15, 28, 43, 55	0
1	E	126/132 (95%)	-0.09	3 (2%) 62 66	13, 23, 41, 59	0
1	G	124/132 (93%)	-0.16	1 (0%) 87 90	15, 25, 43, 50	0
1	I	125/132 (94%)	-0.11	1 (0%) 87 90	17, 28, 46, 53	0
1	K	126/132 (95%)	-0.13	3 (2%) 62 66	15, 26, 44, 56	0
1	M	126/132 (95%)	0.02	2 (1%) 74 79	16, 30, 49, 59	0
1	O	123/132 (93%)	0.26	6 (4%) 33 36	23, 35, 56, 64	0
2	B	17/21 (80%)	0.22	1 (5%) 26 27	20, 28, 40, 46	0
2	D	13/21 (61%)	0.41	1 (7%) 16 18	31, 36, 48, 52	0
2	F	14/21 (66%)	0.44	1 (7%) 19 21	26, 33, 41, 45	0
2	H	10/21 (47%)	0.67	0 100 100	30, 34, 46, 47	0
2	J	11/21 (52%)	0.32	1 (9%) 11 13	30, 33, 49, 56	0
2	L	10/21 (47%)	0.69	1 (10%) 9 9	33, 36, 42, 45	0
2	N	13/21 (61%)	0.53	2 (15%) 3 3	33, 39, 46, 52	0
2	P	12/21 (57%)	1.19	4 (33%) 0 0	39, 43, 49, 60	0
All	All	1102/1224 (90%)	0.03	30 (2%) 58 62	12, 28, 48, 64	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	1082	PRO	6.0
1	E	1205	GLU	4.3
1	E	1204	GLY	4.2
1	K	1205	GLU	3.6
1	M	1205	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	1082	PRO	3.4
1	O	1095	GLY	3.3
2	P	35	VAL	3.2
2	F	25	ALA	2.9
1	O	1096	TYR	2.9
1	O	1094	ARG	2.8
1	C	1180	ARG	2.8
1	O	1080	ASP	2.7
1	A	1080	ASP	2.6
2	P	31	ALA	2.6
1	K	1080	ASP	2.5
2	J	39	HIS	2.5
1	M	1125	LEU	2.4
2	N	40	ARG	2.4
2	P	27	LYS	2.4
2	D	27	LYS	2.3
1	I	1204	GLY	2.3
2	L	29	ALA	2.3
2	B	24	ALA	2.3
2	P	37	LYS	2.1
1	G	1080	ASP	2.1
1	K	1082	PRO	2.1
1	O	1136	GLN	2.0
2	N	29	ALA	2.0
1	C	1136	GLN	2.0

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

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	M3L	F	36	12/13	0.96	0.08	-	18,21,24,28	0
2	M3L	B	36	12/13	0.98	0.11	-	15,20,23,25	0
2	M3L	L	36	12/13	0.96	0.08	-	21,26,33,34	0
2	M3L	N	36	12/13	0.94	0.10	-	26,28,32,33	0
2	M3L	H	36	12/13	0.97	0.07	-	20,26,32,32	0
2	M3L	J	36	12/13	0.95	0.08	-	24,25,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	M3L	P	36	12/13	0.93	0.13	-	37,41,52,53	0
2	M3L	D	36	12/13	0.94	0.09	-	24,29,33,34	0

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(\AA^2)	Q<0.9
3	SO4	A	2207	5/5	0.96	0.10	0.22	28,29,31,31	5
3	SO4	D	1041	5/5	0.98	0.12	-0.16	44,46,48,51	5
3	SO4	A	2208	5/5	0.97	0.10	-0.33	29,32,33,35	5
3	SO4	G	2204	5/5	0.97	0.06	-1.33	28,33,36,38	4
3	SO4	A	2206	5/5	0.99	0.08	-1.36	29,34,36,37	0
3	SO4	C	2205	5/5	0.98	0.07	-1.87	30,33,36,38	5
3	SO4	E	2206	5/5	0.99	0.08	-	30,31,36,37	4

6.5 Other polymers [i](#)

There are no such residues in this entry.