



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:15 PM UTC

PDB ID : 3I3J / pdb_00003i3j
Title : Crystal Structure of the Bromodomain of Human EP300
Authors : Filippakopoulos, P.; Picaud, S.; Phillips, C.; Pike, A.C.W.; Muniz, J.; Roos, A.; Chaikuad, A.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)
Deposited on : 2009-06-30
Resolution : 2.33 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

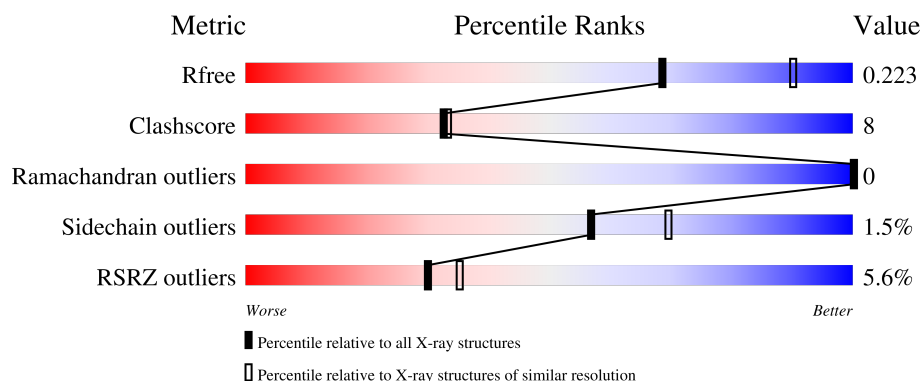
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	124	
1	B	124	
1	C	124	
1	D	124	
1	E	124	

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Mol	Chain	Length	Quality of chain
1	F	124	
1	G	124	
1	H	124	
1	I	124	
1	J	124	
1	K	124	
1	L	124	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PEG	A	1	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11399 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			932	609	145	173	5			
1	B	114	Total	C	N	O	S	0	0	0
			913	598	139	171	5			
1	C	114	Total	C	N	O	S	0	0	0
			944	612	152	175	5			
1	D	113	Total	C	N	O	S	0	0	0
			920	604	139	172	5			
1	E	115	Total	C	N	O	S	0	0	0
			948	616	149	178	5			
1	F	111	Total	C	N	O	S	0	0	0
			890	580	139	166	5			
1	G	113	Total	C	N	O	S	0	0	0
			918	599	143	171	5			
1	H	113	Total	C	N	O	S	0	1	0
			922	602	145	170	5			
1	I	115	Total	C	N	O	S	0	0	0
			944	615	148	176	5			
1	J	113	Total	C	N	O	S	0	0	0
			925	605	142	173	5			
1	K	114	Total	C	N	O	S	0	1	0
			934	609	151	169	5			
1	L	113	Total	C	N	O	S	0	0	0
			906	590	146	165	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1038	SER	-	expression tag	UNP Q09472
A	1039	MET	-	expression tag	UNP Q09472
B	1038	SER	-	expression tag	UNP Q09472
B	1039	MET	-	expression tag	UNP Q09472
C	1038	SER	-	expression tag	UNP Q09472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1039	MET	-	expression tag	UNP Q09472
D	1038	SER	-	expression tag	UNP Q09472
D	1039	MET	-	expression tag	UNP Q09472
E	1038	SER	-	expression tag	UNP Q09472
E	1039	MET	-	expression tag	UNP Q09472
F	1038	SER	-	expression tag	UNP Q09472
F	1039	MET	-	expression tag	UNP Q09472
G	1038	SER	-	expression tag	UNP Q09472
G	1039	MET	-	expression tag	UNP Q09472
H	1038	SER	-	expression tag	UNP Q09472
H	1039	MET	-	expression tag	UNP Q09472
I	1038	SER	-	expression tag	UNP Q09472
I	1039	MET	-	expression tag	UNP Q09472
J	1038	SER	-	expression tag	UNP Q09472
J	1039	MET	-	expression tag	UNP Q09472
K	1038	SER	-	expression tag	UNP Q09472
K	1039	MET	-	expression tag	UNP Q09472
L	1038	SER	-	expression tag	UNP Q09472
L	1039	MET	-	expression tag	UNP Q09472

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		

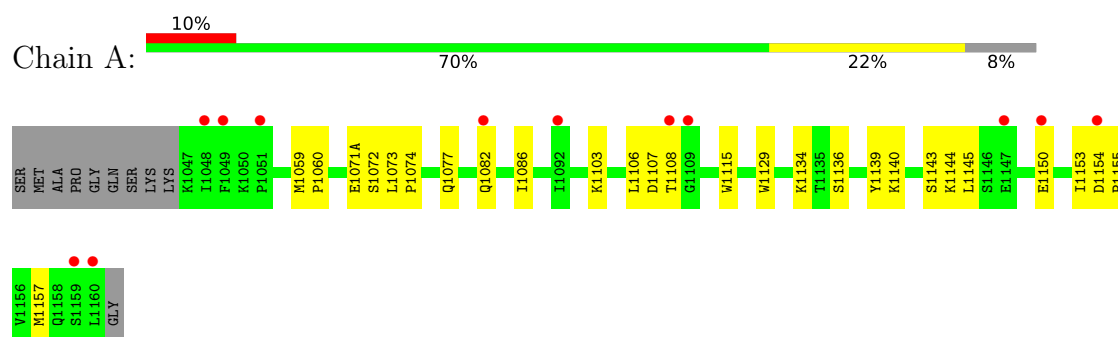
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total 39	O 39	0	0
5	B	14	Total 14	O 14	0	0
5	C	31	Total 31	O 31	0	0
5	D	20	Total 20	O 20	0	0
5	E	32	Total 32	O 32	0	0
5	F	1	Total 1	O 1	0	0
5	G	38	Total 38	O 38	0	0
5	H	15	Total 15	O 15	0	0
5	I	24	Total 24	O 24	0	0
5	J	23	Total 23	O 23	0	0
5	K	28	Total 28	O 28	0	0
5	L	12	Total 12	O 12	0	0

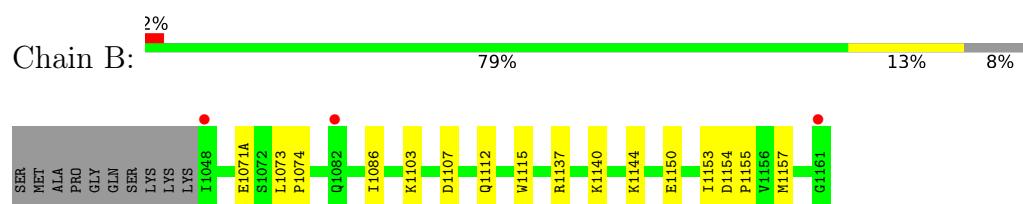
3 Residue-property plots [i](#)

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.

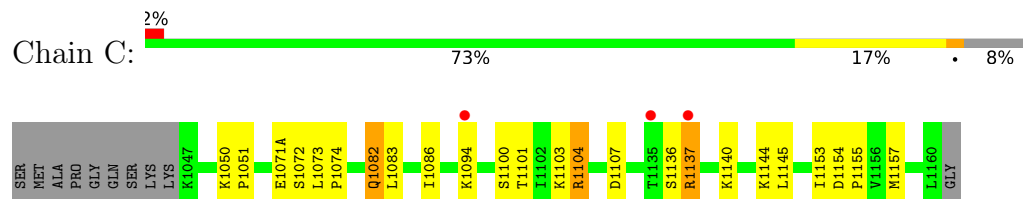
- Molecule 1: Histone acetyltransferase p300



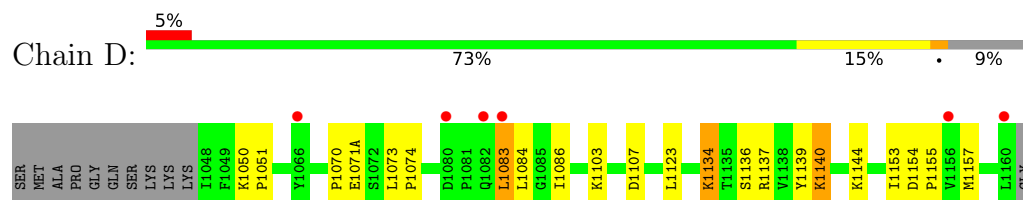
- Molecule 1: Histone acetyltransferase p300



- Molecule 1: Histone acetyltransferase p300



- Molecule 1: Histone acetyltransferase p300

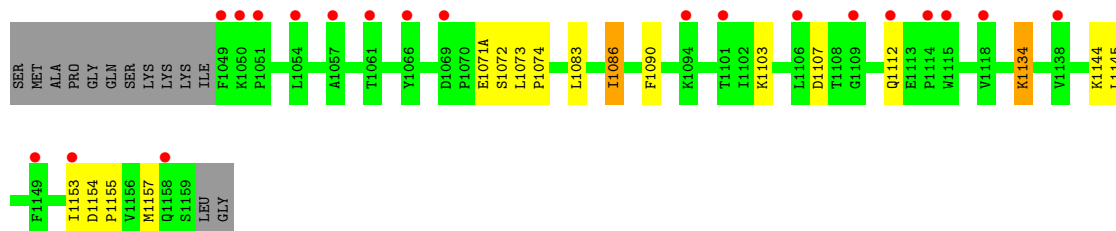
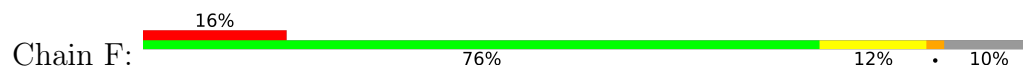


- Molecule 1: Histone acetyltransferase p300

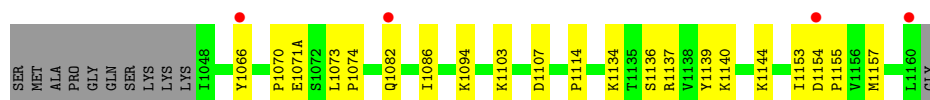
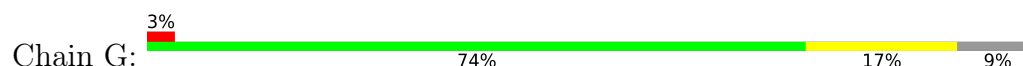




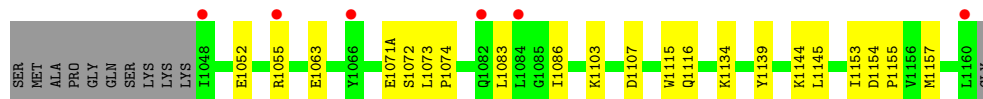
- Molecule 1: Histone acetyltransferase p300



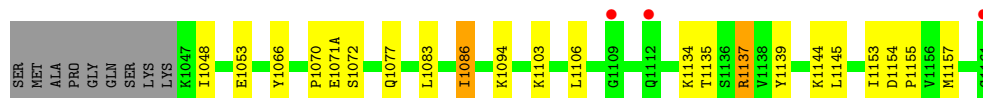
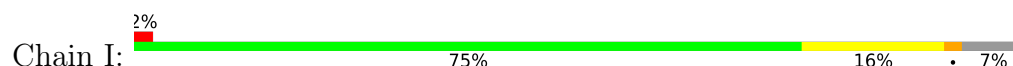
- Molecule 1: Histone acetyltransferase p300



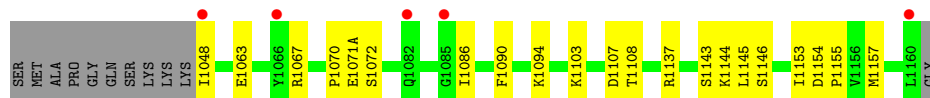
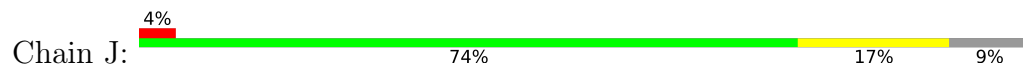
- Molecule 1: Histone acetyltransferase p300



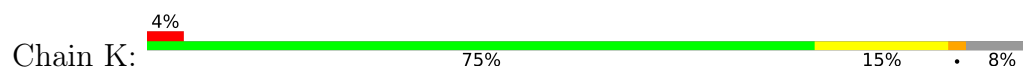
- Molecule 1: Histone acetyltransferase p300

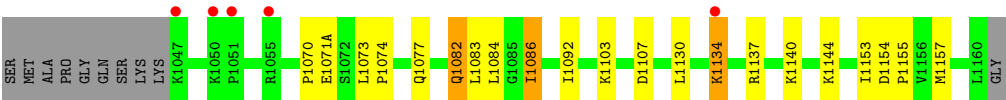


- Molecule 1: Histone acetyltransferase p300

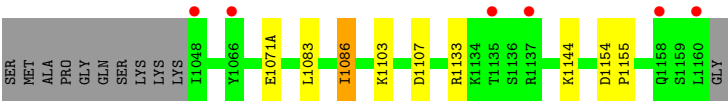
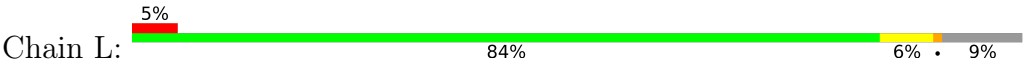


- Molecule 1: Histone acetyltransferase p300





● Molecule 1: Histone acetyltransferase p300



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.90Å 86.19Å 149.90Å 90.00° 96.98° 90.00°	Depositor
Resolution (Å)	32.30 – 2.33 32.30 – 2.33	Depositor EDS
% Data completeness (in resolution range)	91.8 (32.30-2.33) 99.1 (32.30-2.33)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.275 0.230 , 0.223	Depositor DCC
R_{free} test set	1984 reflections (2.85%)	wwPDB-VP
Wilson B-factor (Å ²)	35.5	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11399	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SO4, PEG

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	0.49	0/959	0.83	0/1307
1	B	0.43	0/940	0.80	2/1284 (0.2%)
1	C	0.44	0/971	0.97	3/1322 (0.2%)
1	D	0.45	0/947	0.82	0/1291
1	E	0.46	0/975	0.81	0/1326
1	F	0.44	0/917	0.79	2/1254 (0.2%)
1	G	0.49	0/945	0.83	2/1290 (0.2%)
1	H	0.42	0/949	0.79	0/1296
1	I	0.50	0/971	0.99	5/1322 (0.4%)
1	J	0.43	0/952	0.80	2/1299 (0.2%)
1	K	0.41	0/961	0.76	2/1310 (0.2%)
1	L	0.41	0/933	0.81	2/1274 (0.2%)
All	All	0.45	0/11420	0.83	20/15575 (0.1%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1137	ARG	NE-CZ-NH2	12.73	130.66	119.20
1	C	1137	ARG	NE-CZ-NH2	12.34	130.31	119.20
1	I	1137	ARG	NE-CZ-NH1	-12.13	109.37	121.50
1	C	1137	ARG	NE-CZ-NH1	-12.09	109.41	121.50
1	I	1137	ARG	CD-NE-CZ	9.78	138.09	124.40
1	C	1137	ARG	CD-NE-CZ	9.77	138.07	124.40
1	B	1086	ILE	CA-C-N	5.40	125.22	119.28
1	B	1086	ILE	C-N-CA	5.40	125.22	119.28
1	G	1086	ILE	CA-C-N	5.37	125.19	119.28
1	G	1086	ILE	C-N-CA	5.37	125.19	119.28
1	J	1086	ILE	CA-C-N	5.26	125.07	119.28
1	J	1086	ILE	C-N-CA	5.26	125.07	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1086	ILE	CA-C-N	5.25	125.06	119.28
1	F	1086	ILE	C-N-CA	5.25	125.06	119.28
1	L	1086	ILE	CA-C-N	5.25	125.06	119.28
1	L	1086	ILE	C-N-CA	5.25	125.06	119.28
1	K	1086	ILE	CA-C-N	5.17	125.46	119.47
1	K	1086	ILE	C-N-CA	5.17	125.46	119.47
1	I	1086	ILE	CA-C-N	5.05	125.33	119.47
1	I	1086	ILE	C-N-CA	5.05	125.33	119.47

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	932	0	889	29	0
1	B	913	0	856	17	0
1	C	944	0	910	16	0
1	D	920	0	874	23	0
1	E	948	0	914	25	0
1	F	890	0	828	16	0
1	G	918	0	871	12	0
1	H	922	0	867	19	0
1	I	944	0	907	20	0
1	J	925	0	881	17	0
1	K	934	0	892	29	0
1	L	906	0	849	5	0
2	A	1	0	0	1	0
2	E	1	0	0	1	0
3	A	7	0	10	1	0
3	E	7	0	10	0	0
4	E	5	0	0	0	0
4	L	5	0	0	1	0
5	A	39	0	0	1	0
5	B	14	0	0	0	0
5	C	31	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	20	0	0	0	0
5	E	32	0	0	0	0
5	F	1	0	0	0	0
5	G	38	0	0	0	0
5	H	15	0	0	0	0
5	I	24	0	0	0	0
5	J	23	0	0	1	0
5	K	28	0	0	0	0
5	L	12	0	0	0	0
All	All	11399	0	10558	171	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 (171) 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:A:1150:GLU:OE2	1:E:1140:LYS:HG2	1.17	1.28
1:A:1150:GLU:OE2	1:E:1140:LYS:CG	2.06	1.02
1:B:1115:TRP:HZ2	1:I:1135:THR:O	1.46	0.97
1:A:1150:GLU:OE1	1:E:1140:LYS:NZ	1.98	0.96
1:D:1134:LYS:HE2	1:K:1092:ILE:CD1	2.01	0.89
1:F:1134:LYS:NZ	1:F:1134:LYS:HB3	1.88	0.89
1:B:1137:ARG:HA	1:H:1115:TRP:CH2	2.10	0.86
1:D:1134:LYS:HE2	1:K:1092:ILE:HD13	1.56	0.85
1:B:1115:TRP:CZ2	1:I:1135:THR:O	2.29	0.85
1:C:1100:SER:O	1:C:1104:ARG:HG2	1.76	0.84
1:K:1134:LYS:HB2	1:K:1134:LYS:NZ	1.93	0.84
1:F:1090:PHE:HE2	1:J:1108:THR:O	1.62	0.83
1:F:1112:GLN:HE22	1:J:1090:PHE:HB3	1.46	0.78
1:A:1150:GLU:CD	1:E:1140:LYS:NZ	2.43	0.76
1:F:1090:PHE:CE2	1:J:1108:THR:O	2.39	0.76
1:A:1150:GLU:OE2	1:E:1140:LYS:CE	2.37	0.71
1:D:1084:LEU:HD22	5:J:384:HOH:O	1.89	0.70
1:K:1134:LYS:HB2	1:K:1134:LYS:HZ3	1.56	0.68
1:A:1150:GLU:OE2	1:E:1140:LYS:HE3	1.96	0.66
1:I:1070:PRO:HG3	1:K:1137:ARG:CZ	2.27	0.65
1:A:1115:TRP:CZ2	1:G:1137:ARG:HA	2.31	0.65
1:F:1134:LYS:HB3	1:F:1134:LYS:HZ1	1.61	0.65
1:D:1083:LEU:HD12	1:J:1063:GLU:HG2	1.80	0.64
1:D:1070:PRO:HG3	1:J:1137:ARG:NH2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1070:PRO:HG3	1:K:1137:ARG:NH2	2.15	0.62
1:D:1083:LEU:O	1:J:1067:ARG:NE	2.26	0.61
1:D:1134:LYS:HE2	1:K:1092:ILE:HD11	1.82	0.61
1:A:1150:GLU:CD	1:E:1140:LYS:CE	2.74	0.61
1:A:1143:SER:HB3	1:E:1135:THR:HG21	1.82	0.60
1:A:1108:THR:HA	1:K:1082:GLN:HE22	1.68	0.59
2:E:2:CL:CL	1:G:1070:PRO:HB3	2.40	0.59
1:A:1077:GLN:NE2	5:A:290:HOH:O	2.25	0.59
1:H:1052:GLU:HA	1:H:1055[B]:ARG:NH1	2.19	0.58
1:B:1140:LYS:HE3	1:H:1116:GLN:NE2	2.17	0.58
1:E:1073:LEU:HB2	1:E:1074:PRO:HD3	1.87	0.56
1:K:1134:LYS:HB2	1:K:1134:LYS:HZ2	1.70	0.56
1:D:1070:PRO:HG3	1:J:1137:ARG:CZ	2.36	0.56
1:I:1071(A):GLU:HG2	1:I:1144:LYS:HG2	1.88	0.55
1:D:1139:TYR:OH	1:K:1130:LEU:HD11	2.06	0.55
1:A:1150:GLU:CD	1:E:1140:LYS:HE3	2.31	0.55
1:K:1134:LYS:NZ	1:K:1134:LYS:CB	2.65	0.53
1:A:1071(A):GLU:HG2	1:A:1144:LYS:HG2	1.91	0.53
1:C:1137:ARG:HD2	5:C:82:HOH:O	2.08	0.53
1:L:1071(A):GLU:HG2	1:L:1144:LYS:HG2	1.91	0.52
1:J:1071(A):GLU:HG2	1:J:1144:LYS:HG2	1.91	0.52
1:B:1140:LYS:HE3	1:H:1116:GLN:HE21	1.72	0.52
1:B:1071(A):GLU:HG2	1:B:1144:LYS:HG2	1.92	0.52
1:H:1071(A):GLU:HG2	1:H:1144:LYS:HG2	1.91	0.51
1:E:1136:SER:O	1:E:1140:LYS:HD3	2.10	0.51
1:B:1150:GLU:OE2	1:K:1140:LYS:HE3	2.12	0.50
3:A:1:PEG:O2	1:E:1141:TYR:HE1	1.95	0.50
1:B:1137:ARG:N	1:H:1115:TRP:CZ2	2.80	0.50
1:G:1103:LYS:HE2	1:G:1107:ASP:OD2	2.11	0.50
1:I:1066:TYR:CD1	1:K:1083:LEU:HD13	2.47	0.50
1:F:1083:LEU:HD23	1:H:1063:GLU:HG2	1.93	0.50
1:A:1150:GLU:OE2	1:E:1140:LYS:CD	2.60	0.49
1:G:1071(A):GLU:HG2	1:G:1144:LYS:HG2	1.93	0.49
1:D:1103:LYS:HE2	1:D:1107:ASP:OD2	2.13	0.49
1:D:1137:ARG:CZ	1:J:1070:PRO:HG3	2.42	0.49
1:C:1073:LEU:HB2	1:C:1074:PRO:HD3	1.95	0.49
1:C:1136:SER:O	1:C:1140:LYS:HD3	2.12	0.49
1:J:1143:SER:O	1:J:1146:SER:HB3	2.13	0.49
1:I:1066:TYR:HD2	1:K:1084:LEU:HD23	1.79	0.48
1:A:1108:THR:HA	1:K:1082:GLN:NE2	2.28	0.48
1:H:1103:LYS:HE2	1:H:1107:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1071(A):GLU:HG2	1:F:1144:LYS:HG2	1.95	0.48
1:I:1103:LYS:HZ1	1:K:1082:GLN:HE22	1.62	0.48
1:F:1134:LYS:HB3	1:F:1134:LYS:HZ2	1.74	0.47
1:A:1106:LEU:HA	2:A:3:CL:CL	2.51	0.47
1:C:1082:GLN:HG2	1:C:1083:LEU:N	2.29	0.47
1:B:1112:GLN:HG3	1:I:1135:THR:HG21	1.96	0.47
1:K:1073:LEU:HB2	1:K:1074:PRO:HD3	1.96	0.47
1:L:1103:LYS:HE2	1:L:1107:ASP:OD2	2.15	0.47
1:E:1071(A):GLU:HG2	1:E:1144:LYS:HG2	1.97	0.47
1:J:1103:LYS:HE2	1:J:1107:ASP:OD2	2.13	0.47
1:C:1103:LYS:HE2	1:C:1107:ASP:OD2	2.15	0.47
1:H:1154:ASP:HB2	1:H:1155:PRO:HD3	1.96	0.47
1:D:1134:LYS:CE	1:K:1092:ILE:HD13	2.39	0.46
1:B:1154:ASP:HB2	1:B:1155:PRO:HD3	1.96	0.46
1:I:1077:GLN:OE1	1:K:1077:GLN:OE1	2.34	0.46
1:G:1073:LEU:HB2	1:G:1074:PRO:HD3	1.98	0.46
1:B:1103:LYS:HE2	1:B:1107:ASP:OD2	2.16	0.46
1:C:1101:THR:HA	1:C:1104:ARG:HG3	1.97	0.46
1:K:1154:ASP:HB2	1:K:1155:PRO:HD3	1.98	0.46
1:K:1071(A):GLU:HG2	1:K:1144:LYS:HG2	1.98	0.46
1:D:1154:ASP:HB2	1:D:1155:PRO:HD3	1.97	0.45
1:J:1154:ASP:HB2	1:J:1155:PRO:HD3	1.97	0.45
1:F:1083:LEU:CD2	1:H:1063:GLU:HG2	2.47	0.45
1:F:1154:ASP:HB2	1:F:1155:PRO:HD3	1.98	0.45
1:K:1086:ILE:HG13	1:K:1086:ILE:O	2.16	0.45
1:L:1154:ASP:HB2	1:L:1155:PRO:HD3	1.98	0.45
1:B:1137:ARG:CA	1:H:1115:TRP:CH2	2.93	0.45
1:C:1086:ILE:HG13	1:C:1086:ILE:O	2.16	0.45
1:L:1133:ARG:HD3	4:L:2:SO4:O2	2.15	0.45
1:A:1086:ILE:O	1:A:1086:ILE:HG13	2.17	0.45
1:G:1154:ASP:HB2	1:G:1155:PRO:HD3	1.99	0.45
1:E:1103:LYS:HE2	1:E:1107:ASP:OD2	2.16	0.45
1:I:1137:ARG:CZ	1:K:1070:PRO:HG3	2.47	0.45
1:C:1071(A):GLU:HG2	1:C:1144:LYS:HG2	1.98	0.45
1:A:1134:LYS:HA	1:A:1139:TYR:CD1	2.51	0.45
1:E:1072:SER:HA	1:E:1145:LEU:HD11	1.99	0.45
1:F:1103:LYS:HE2	1:F:1107:ASP:OD2	2.16	0.45
1:C:1154:ASP:HB2	1:C:1155:PRO:HD3	1.99	0.44
1:I:1066:TYR:CE1	1:K:1083:LEU:HD13	2.52	0.44
1:B:1137:ARG:CA	1:H:1115:TRP:CZ2	3.01	0.44
1:D:1086:ILE:O	1:D:1086:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:1103:LYS:HE2	1:K:1107:ASP:OD2	2.17	0.44
1:F:1086:ILE:HG13	1:F:1086:ILE:O	2.18	0.44
1:F:1072:SER:HA	1:F:1145:LEU:HD11	2.00	0.44
1:A:1129:TRP:CH2	1:E:1135:THR:O	2.71	0.44
1:G:1094:LYS:HD3	1:G:1094:LYS:HA	1.79	0.44
1:A:1154:ASP:HB2	1:A:1155:PRO:HD3	1.99	0.43
1:J:1072:SER:HA	1:J:1145:LEU:HD11	2.00	0.43
1:K:1134:LYS:HZ3	1:K:1134:LYS:CB	2.27	0.43
1:A:1153:ILE:HG13	1:A:1157:MET:HG2	1.99	0.43
1:I:1153:ILE:HG13	1:I:1157:MET:HG2	2.01	0.43
1:E:1154:ASP:HB2	1:E:1155:PRO:HD3	1.99	0.43
1:D:1071(A):GLU:HG2	1:D:1144:LYS:HG2	2.00	0.43
1:B:1137:ARG:HA	1:H:1115:TRP:CZ2	2.50	0.43
1:H:1072:SER:HA	1:H:1145:LEU:HD11	2.01	0.43
1:A:1073:LEU:HB2	1:A:1074:PRO:HD3	2.01	0.43
1:C:1072:SER:HA	1:C:1145:LEU:HD11	2.01	0.42
1:I:1154:ASP:HB2	1:I:1155:PRO:HD3	2.01	0.42
1:D:1123:LEU:HA	1:K:1134:LYS:HE2	2.01	0.42
1:D:1153:ILE:HG13	1:D:1157:MET:HG2	2.01	0.42
1:L:1086:ILE:O	1:L:1086:ILE:HG13	2.19	0.42
1:C:1101:THR:HA	1:C:1104:ARG:CG	2.50	0.42
1:D:1073:LEU:HB2	1:D:1074:PRO:HD3	2.01	0.42
1:C:1050:LYS:HA	1:C:1051:PRO:HD3	1.94	0.42
1:I:1134:LYS:HA	1:I:1139:TYR:CD1	2.54	0.42
1:C:1153:ILE:HG13	1:C:1157:MET:HG2	2.02	0.42
1:A:1134:LYS:HA	1:A:1139:TYR:CG	2.55	0.42
1:F:1073:LEU:HB2	1:F:1074:PRO:HD3	2.01	0.42
1:F:1073:LEU:HB3	1:H:1073:LEU:HB3	2.02	0.42
1:A:1103:LYS:HE2	1:A:1107:ASP:OD2	2.19	0.42
1:F:1153:ILE:HG13	1:F:1157:MET:HG2	2.02	0.42
1:I:1086:ILE:O	1:I:1086:ILE:HG13	2.19	0.42
1:E:1094:LYS:HD3	1:E:1094:LYS:HA	1.79	0.42
1:A:1072:SER:HA	1:A:1145:LEU:HD11	2.00	0.41
1:A:1136:SER:O	1:A:1140:LYS:HD3	2.20	0.41
1:C:1094:LYS:HD3	1:C:1094:LYS:HA	1.78	0.41
1:D:1137:ARG:NH2	1:J:1070:PRO:HG3	2.35	0.41
1:G:1153:ILE:HG13	1:G:1157:MET:HG2	2.02	0.41
1:E:1160:LEU:O	1:E:1161:GLY:C	2.64	0.41
1:B:1115:TRP:HZ2	1:I:1135:THR:C	2.24	0.41
1:B:1153:ILE:HG13	1:B:1157:MET:HG2	2.02	0.41
1:G:1114:PRO:HB2	1:G:1157:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1072:SER:HA	1:I:1145:LEU:HD11	2.01	0.41
1:A:1073:LEU:HB3	1:C:1073:LEU:HB3	2.02	0.41
1:G:1136:SER:O	1:G:1140:LYS:HD3	2.21	0.41
1:H:1153:ILE:HG13	1:H:1157:MET:HG2	2.01	0.41
1:I:1094:LYS:HD3	1:I:1094:LYS:HA	1.86	0.41
1:A:1150:GLU:CD	1:E:1140:LYS:HZ2	2.15	0.41
1:B:1073:LEU:HB2	1:B:1074:PRO:HD3	2.03	0.41
1:D:1136:SER:O	1:D:1140:LYS:HD3	2.19	0.41
1:E:1153:ILE:HG13	1:E:1157:MET:HG2	2.02	0.41
1:E:1086:ILE:HG13	1:E:1086:ILE:O	2.21	0.41
1:H:1086:ILE:O	1:H:1086:ILE:HG13	2.20	0.41
1:H:1134:LYS:HA	1:H:1139:TYR:CD1	2.56	0.41
1:J:1153:ILE:HG13	1:J:1157:MET:HG2	2.02	0.41
1:G:1134:LYS:HA	1:G:1139:TYR:CD1	2.56	0.41
1:K:1153:ILE:HG13	1:K:1157:MET:HG2	2.02	0.41
1:H:1073:LEU:HB2	1:H:1074:PRO:HD3	2.03	0.40
1:D:1134:LYS:HA	1:D:1139:TYR:CD1	2.56	0.40
1:E:1083:LEU:HD13	1:G:1066:TYR:CD1	2.57	0.40
1:A:1059:MET:N	1:A:1060:PRO:CD	2.85	0.40
1:E:1134:LYS:HA	1:E:1139:TYR:CD1	2.56	0.40
1:I:1103:LYS:NZ	1:K:1082:GLN:NE2	2.70	0.40
1:D:1083:LEU:O	1:J:1067:ARG:CG	2.69	0.40
1:J:1094:LYS:HD3	1:J:1094:LYS:HA	1.84	0.40
1:D:1050:LYS:HA	1:D:1051:PRO:HD3	1.95	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	112/124 (90%)	112 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	112/124 (90%)	112 (100%)	0	0	100	100
1	C	112/124 (90%)	112 (100%)	0	0	100	100
1	D	111/124 (90%)	110 (99%)	1 (1%)	0	100	100
1	E	113/124 (91%)	113 (100%)	0	0	100	100
1	F	109/124 (88%)	109 (100%)	0	0	100	100
1	G	111/124 (90%)	111 (100%)	0	0	100	100
1	H	112/124 (90%)	112 (100%)	0	0	100	100
1	I	113/124 (91%)	113 (100%)	0	0	100	100
1	J	111/124 (90%)	111 (100%)	0	0	100	100
1	K	113/124 (91%)	113 (100%)	0	0	100	100
1	L	111/124 (90%)	111 (100%)	0	0	100	100
All	All	1340/1488 (90%)	1339 (100%)	1 (0%)	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	100/116 (86%)	99 (99%)	1 (1%)	68	79
1	B	96/116 (83%)	96 (100%)	0	100	100
1	C	104/116 (90%)	102 (98%)	2 (2%)	50	63
1	D	98/116 (84%)	95 (97%)	3 (3%)	35	45
1	E	104/116 (90%)	103 (99%)	1 (1%)	68	79
1	F	94/116 (81%)	93 (99%)	1 (1%)	65	77
1	G	99/116 (85%)	98 (99%)	1 (1%)	68	79
1	H	97/116 (84%)	96 (99%)	1 (1%)	68	79
1	I	102/116 (88%)	98 (96%)	4 (4%)	28	37
1	J	100/116 (86%)	99 (99%)	1 (1%)	68	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	99/116 (85%)	97 (98%)	2 (2%)	48	61
1	L	94/116 (81%)	93 (99%)	1 (1%)	65	77
All	All	1187/1392 (85%)	1169 (98%)	18 (2%)	57	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1082	GLN
1	C	1082	GLN
1	C	1104	ARG
1	D	1083	LEU
1	D	1134	LYS
1	D	1140	LYS
1	E	1053	GLU
1	F	1134	LYS
1	G	1082	GLN
1	H	1083	LEU
1	I	1048	ILE
1	I	1053	GLU
1	I	1083	LEU
1	I	1106	LEU
1	J	1048	ILE
1	K	1082	GLN
1	K	1134	LYS
1	L	1083	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1082	GLN
1	C	1082	GLN
1	D	1126	ASN
1	F	1112	GLN
1	G	1082	GLN
1	K	1082	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
3	PEG	A	1	-	6,6,6	0.60	0	5,5,5	2.08	3 (60%)
4	SO4	E	1	-	4,4,4	0.30	0	6,6,6	0.14	0
4	SO4	L	2	-	4,4,4	0.27	0	6,6,6	0.12	0
3	PEG	E	1162	-	6,6,6	0.50	0	5,5,5	1.50	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	PEG	A	1	-	-	4/4/4/4	-
3	PEG	E	1162	-	-	4/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	PEG	O2-C3-C4	2.74	122.21	110.11
3	A	1	PEG	C3-O2-C2	2.37	123.64	113.26
3	A	1	PEG	O2-C2-C1	2.34	120.43	110.11

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	PEG	C1-C2-O2-C3
3	E	1162	PEG	O1-C1-C2-O2
3	A	1	PEG	C4-C3-O2-C2
3	E	1162	PEG	O2-C3-C4-O4
3	A	1	PEG	O2-C3-C4-O4
3	E	1162	PEG	C4-C3-O2-C2
3	A	1	PEG	O1-C1-C2-O2
3	E	1162	PEG	C1-C2-O2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	PEG	1	0
4	L	2	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	114/124 (91%)	0.45	12 (10%) 11 13	23, 41, 90, 121	0
1	B	114/124 (91%)	0.37	3 (2%) 57 63	40, 61, 101, 120	0
1	C	114/124 (91%)	0.29	3 (2%) 57 63	25, 45, 88, 108	0
1	D	113/124 (91%)	0.38	6 (5%) 32 37	30, 51, 95, 114	0
1	E	115/124 (92%)	0.21	3 (2%) 57 63	23, 44, 86, 102	0
1	F	111/124 (89%)	1.43	20 (18%) 3 4	49, 88, 135, 178	0
1	G	113/124 (91%)	0.22	4 (3%) 47 53	24, 45, 92, 102	0
1	H	113/124 (91%)	0.62	6 (5%) 32 37	35, 64, 96, 111	1 (0%)
1	I	115/124 (92%)	0.31	3 (2%) 57 63	22, 44, 81, 112	0
1	J	113/124 (91%)	0.44	5 (4%) 39 45	36, 52, 95, 100	0
1	K	114/124 (91%)	0.45	5 (4%) 39 45	29, 55, 101, 144	1 (0%)
1	L	113/124 (91%)	0.52	6 (5%) 32 37	39, 70, 116, 145	0
All	All	1362/1488 (91%)	0.47	76 (5%) 30 35	22, 55, 102, 178	2 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1066	TYR	5.8
1	F	1109	GLY	4.3
1	J	1066	TYR	4.2
1	H	1066	TYR	4.1
1	F	1057	ALA	4.1
1	C	1094	LYS	3.6
1	F	1149	PHE	3.5
1	F	1051	PRO	3.4
1	H	1084	LEU	3.3
1	A	1048	ILE	3.3
1	C	1137	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	1106	LEU	3.2
1	F	1050	LYS	3.2
1	F	1138	VAL	3.2
1	L	1160	LEU	3.2
1	L	1135	THR	3.2
1	F	1153	ILE	3.1
1	D	1066	TYR	3.1
1	J	1160	LEU	3.0
1	E	1134	LYS	2.9
1	F	1118	VAL	2.8
1	B	1082	GLN	2.8
1	G	1082	GLN	2.8
1	D	1160	LEU	2.7
1	H	1082	GLN	2.7
1	F	1061	THR	2.6
1	A	1150	GLU	2.6
1	F	1158	GLN	2.6
1	A	1051	PRO	2.6
1	F	1049	PHE	2.5
1	D	1082	GLN	2.5
1	E	1137	ARG	2.5
1	K	1050	LYS	2.5
1	L	1066	TYR	2.5
1	A	1160	LEU	2.5
1	I	1161	GLY	2.5
1	J	1082	GLN	2.4
1	K	1055[A]	ARG	2.4
1	F	1112	GLN	2.4
1	A	1108	THR	2.4
1	H	1048	ILE	2.4
1	A	1092	ILE	2.4
1	K	1134	LYS	2.3
1	H	1055[A]	ARG	2.3
1	G	1066	TYR	2.3
1	B	1161	GLY	2.3
1	F	1054	LEU	2.3
1	J	1085	GLY	2.3
1	K	1047	LYS	2.3
1	L	1048	ILE	2.3
1	A	1049	PHE	2.2
1	D	1083	LEU	2.2
1	A	1082	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1109	GLY	2.2
1	I	1109	GLY	2.2
1	A	1147	GLU	2.2
1	F	1115	TRP	2.2
1	H	1160	LEU	2.2
1	G	1154	ASP	2.2
1	J	1048	ILE	2.2
1	K	1051	PRO	2.2
1	C	1135	THR	2.2
1	A	1154	ASP	2.1
1	I	1112	GLN	2.1
1	F	1094	LYS	2.1
1	G	1160	LEU	2.1
1	D	1156	VAL	2.1
1	A	1159	SER	2.1
1	E	1055	ARG	2.1
1	L	1137	ARG	2.1
1	D	1080	ASP	2.0
1	F	1069	ASP	2.0
1	F	1101	THR	2.0
1	L	1158	GLN	2.0
1	B	1048	ILE	2.0
1	F	1114	PRO	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	A	1	7/7	0.72	0.24	48,48,48,48	0
4	SO4	E	1	5/5	0.80	0.10	42,49,65,96	0
3	PEG	E	1162	7/7	0.82	0.15	66,66,66,66	0
4	SO4	L	2	5/5	0.84	0.10	52,57,109,127	0
2	CL	E	2	1/1	0.90	0.14	67,67,67,67	0
2	CL	A	3	1/1	0.93	0.23	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.