



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 03:17 am GMT

PDB ID : 2X18
Title : The crystal structure of the PH domain of human AKT3 protein kinase
Authors : Vollmar, M.; Wang, J.; Zhang, Y.; Elkins, J.M.; Burgess-Brown, N.; Chaikuad, A.; Pike, A.C.W.; von Delft, F.; Bountra, C.; Arrowsmith, C.H.; Weigelt, J.; Edwards, A.; Knapp, S.
Deposited on : 2009-12-22
Resolution : 1.46 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

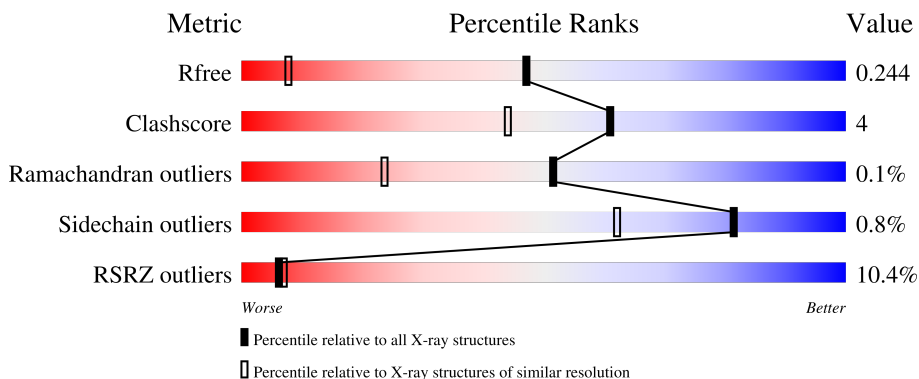
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.46 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.



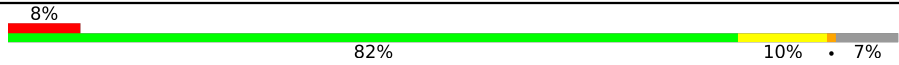
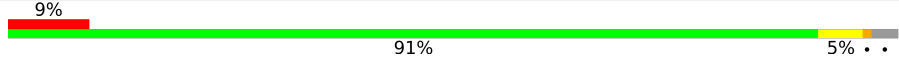

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	119	
1	B	119	
1	C	119	
1	D	119	
1	E	119	

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Mol	Chain	Length	Quality of chain
1	F	119	 <p>8% 82% 10% • 7%</p>
1	G	119	 <p>9% 91% 5% • •</p>
1	H	119	 <p>13% 88% 9% •</p>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9414 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 RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	111	Total 945	C 601	N 169	O 171	S 4	0	9	0
1	B	114	Total 963	C 618	N 163	O 177	S 5	0	6	0
1	C	115	Total 989	C 631	N 173	O 181	S 4	0	8	0
1	D	115	Total 948	C 606	N 160	O 177	S 5	0	7	0
1	E	116	Total 978	C 624	N 169	O 179	S 6	0	5	0
1	F	111	Total 910	C 581	N 161	O 164	S 4	0	5	0
1	G	115	Total 953	C 605	N 166	O 178	S 4	0	5	0
1	H	116	Total 983	C 625	N 172	O 181	S 5	0	4	0

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total	C	O	S	0	0	
			5	1	3	1			
2	E	1	Total	C	O	S	0	0	
			5	1	3	1			
2	F	1	Total	C	O	S	0	0	
			6	2	3	1			
2	H	1	Total	C	N	O	S	0	0
			12	6	2	3	1		

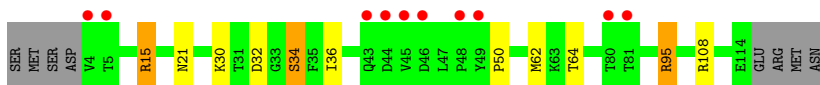
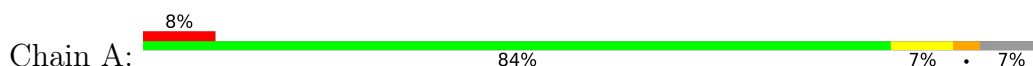
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	223	Total	O	0	0
			223	223		
3	B	227	Total	O	0	0
			227	227		
3	C	229	Total	O	0	0
			229	229		
3	D	245	Total	O	0	0
			245	245		
3	E	189	Total	O	0	0
			189	189		
3	F	192	Total	O	0	0
			192	192		
3	G	200	Total	O	0	0
			200	200		
3	H	212	Total	O	0	0
			212	212		

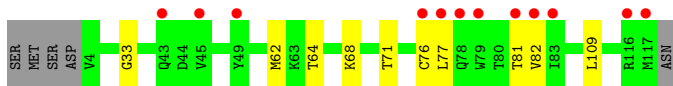
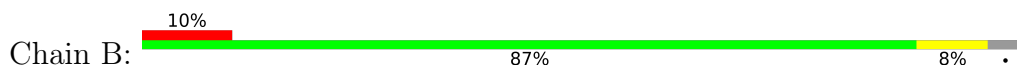
3 Residue-property plots [i](#)

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.

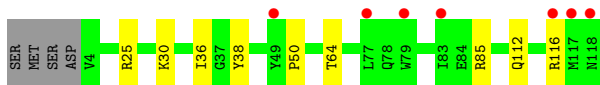
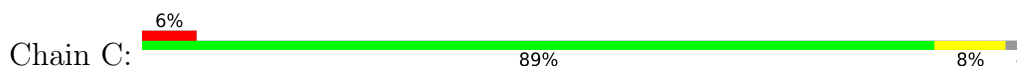
- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



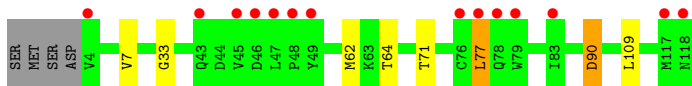
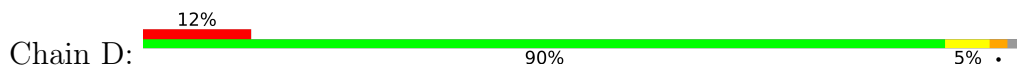
- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



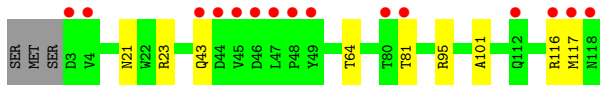
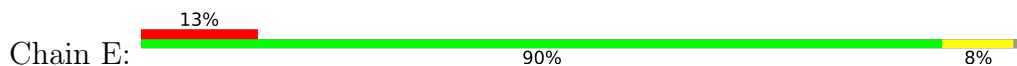
- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



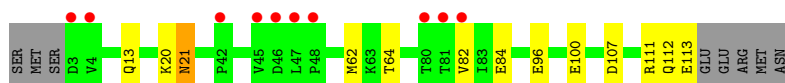
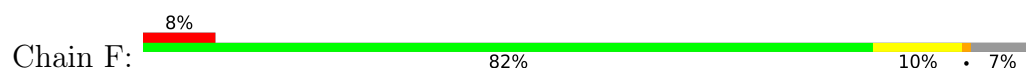
- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



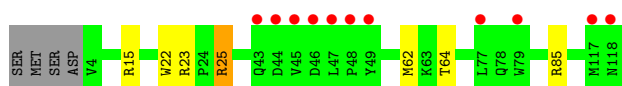
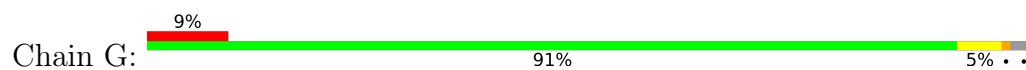
- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



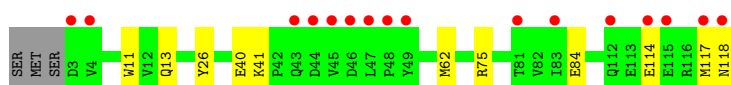
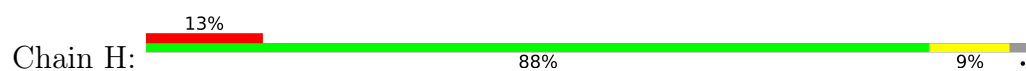
- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



- Molecule 1: RAC-GAMMA SERINE/THREONINE-PROTEIN KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.48Å 62.40Å 71.41Å 111.47° 102.75° 94.36°	Depositor
Resolution (Å)	64.03 – 1.46 38.24 – 1.46	Depositor EDS
% Data completeness (in resolution range)	98.1 (64.03-1.46) 97.2 (38.24-1.46)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.46Å)	Xtrriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.189 , 0.234 0.198 , 0.244	Depositor DCC
R_{free} test set	8193 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtrriage
Anisotropy	0.162	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9414	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5578e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: EPE

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	0.77	0/1013	0.88	2/1372 (0.1%)
1	B	0.70	0/1022	0.81	0/1384
1	C	0.78	0/1053	0.91	1/1423 (0.1%)
1	D	2.22	2/1002 (0.2%)	1.29	8/1359 (0.6%)
1	E	0.77	1/1022 (0.1%)	0.87	2/1383 (0.1%)
1	F	0.72	0/961	0.85	0/1302
1	G	0.82	0/1003	0.91	4/1358 (0.3%)
1	H	0.77	0/1026	0.80	0/1387
All	All	1.06	3/8102 (0.0%)	0.93	17/10968 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	77[A]	LEU	CB-CG	46.32	2.86	1.52
1	D	77[B]	LEU	CB-CG	46.32	2.86	1.52
1	E	101	ALA	CA-CB	-5.48	1.41	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77[A]	LEU	CB-CG-CD2	17.08	140.03	111.00
1	D	77[B]	LEU	CB-CG-CD2	17.08	140.03	111.00
1	D	77[A]	LEU	CB-CG-CD1	-15.83	84.09	111.00
1	D	77[B]	LEU	CB-CG-CD1	-15.83	84.09	111.00
1	A	95	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	D	90[A]	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	D	90[B]	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	G	85	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	E	95	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	77[A]	LEU	CA-CB-CG	-5.67	102.27	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77[B]	LEU	CA-CB-CG	-5.67	102.27	115.30
1	C	85	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	15	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	G	25	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	23	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	G	15	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	G	85	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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	945	0	917	12	0
1	B	963	0	940	12	0
1	C	989	0	972	11	0
1	D	948	0	890	8	0
1	E	978	0	936	8	0
1	F	910	0	854	14	0
1	G	953	0	909	12	0
1	H	983	0	945	14	0
2	A	5	0	0	0	0
2	E	5	0	0	0	0
2	F	6	0	2	0	0
2	H	12	0	13	0	0
3	A	223	0	0	0	0
3	B	227	0	0	1	0
3	C	229	0	0	1	0
3	D	245	0	0	2	0
3	E	189	0	0	0	0
3	F	192	0	0	1	0
3	G	200	0	0	1	0
3	H	212	0	0	1	0
All	All	9414	0	7378	68	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 4.

All (68) 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:G:25:ARG:NH2	1:H:117:MET:O	1.88	1.06
1:D:64[C]:THR:HG21	3:D:2168:HOH:O	1.58	1.04
1:C:64[A]:THR:CG2	1:G:62[A]:MET:SD	2.46	1.03
1:E:64:THR:CG2	1:H:62[B]:MET:SD	2.49	1.00
1:F:13[B]:GLN:NE2	3:F:2030:HOH:O	1.94	0.99
1:B:64[B]:THR:HG21	3:B:2145:HOH:O	1.63	0.97
1:A:64:THR:CG2	1:D:62[B]:MET:SD	2.55	0.95
1:G:23:ARG:CG	1:H:114:GLU:HB3	1.99	0.91
1:C:64[B]:THR:HG21	3:C:2136:HOH:O	1.69	0.91
1:B:62[B]:MET:SD	1:F:64:THR:CG2	2.61	0.89
1:G:64[B]:THR:HG21	3:G:2113:HOH:O	1.74	0.87
1:E:64:THR:HG22	1:H:62[B]:MET:SD	2.14	0.86
1:G:23:ARG:HG2	1:H:114:GLU:HB3	1.59	0.82
1:G:23:ARG:HG3	1:H:114:GLU:HB3	1.73	0.71
1:C:64[A]:THR:HG22	1:G:62[A]:MET:SD	2.31	0.70
1:A:64:THR:HG22	1:D:62[B]:MET:SD	2.32	0.70
1:E:64:THR:HG21	1:H:62[B]:MET:SD	2.32	0.70
1:C:64[A]:THR:HG23	1:G:62[A]:MET:SD	2.31	0.69
1:B:64[B]:THR:HB	1:F:62[B]:MET:HE1	1.75	0.68
1:G:22:TRP:C	1:G:23:ARG:HD3	2.14	0.68
1:A:30:LYS:HE3	1:A:36:ILE:HD12	1.76	0.67
1:A:64:THR:HG21	1:D:62[B]:MET:SD	2.34	0.67
1:B:62[B]:MET:SD	1:F:64:THR:HG22	2.34	0.66
1:C:64[A]:THR:HG21	1:G:62[A]:MET:SD	2.34	0.66
1:F:20[B]:LYS:O	1:F:21[B]:ASN:O	2.16	0.64
1:D:7:VAL:HA	1:H:117:MET:HE1	1.79	0.63
1:G:23:ARG:HD3	1:G:23:ARG:N	2.14	0.61
1:H:13[B]:GLN:OE1	3:H:2030:HOH:O	2.14	0.60
1:C:25[B]:ARG:HG3	1:C:38:TYR:O	2.02	0.59
1:C:30:LYS:HE3	1:C:36[A]:ILE:HD12	1.86	0.57
1:C:112:GLN:O	1:C:116:ARG:HG2	2.04	0.57
1:B:62[B]:MET:SD	1:F:64:THR:HG21	2.45	0.56
1:A:32:ASP:OD1	1:A:34[A]:SER:OG	2.20	0.54
1:F:82:VAL:CG1	1:F:84:GLU:O	2.57	0.52
1:C:30:LYS:HE3	1:C:36[A]:ILE:CD1	2.41	0.51
1:B:77:LEU:CD2	1:B:82:VAL:HG22	2.42	0.50
1:B:77:LEU:HD23	1:B:82:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:HA3	1:B:109:LEU:HD11	1.94	0.49
1:B:64[B]:THR:HB	1:F:62[B]:MET:CE	2.43	0.48
1:A:108[A]:ARG:HG2	1:E:81:THR:HG21	1.95	0.48
1:E:116:ARG:H	1:E:117[B]:MET:HE2	1.79	0.48
1:B:76:CYS:O	1:B:82:VAL:HA	2.13	0.48
1:F:107:ASP:O	1:F:111:ARG:HG2	2.14	0.48
1:F:82:VAL:HG12	1:F:84:GLU:O	2.15	0.46
1:D:64[C]:THR:CG2	3:D:2168:HOH:O	2.34	0.46
1:E:21[B]:ASN:O	1:E:21[B]:ASN:OD1	2.34	0.46
1:B:64[B]:THR:HG22	1:B:71:THR:HB	1.97	0.46
1:C:36[A]:ILE:HG22	1:C:50:PRO:HB3	1.98	0.46
1:H:75:ARG:HG2	1:H:84:GLU:HB3	1.97	0.46
1:A:108[B]:ARG:HG2	1:E:81:THR:HG21	1.97	0.45
1:D:33:GLY:HA3	1:D:109:LEU:HD11	2.00	0.44
1:A:36:ILE:CG2	1:A:50:PRO:HB3	2.48	0.43
1:H:75:ARG:NE	1:H:84:GLU:OE2	2.47	0.43
1:C:36[A]:ILE:HG22	1:C:50:PRO:CB	2.49	0.42
1:A:15:ARG:HA	1:A:21[A]:ASN:O	2.18	0.42
1:D:64[C]:THR:HG22	1:D:71:THR:HB	2.00	0.42
1:F:112:GLN:HA	1:F:113:GLU:HA	1.86	0.42
1:H:26:TYR:CE1	1:H:41:LYS:HG2	2.55	0.42
1:F:96:GLU:HG3	1:F:100:GLU:OE2	2.20	0.41
1:G:23:ARG:NH2	1:H:118:ASN:OXT	2.53	0.41
1:H:11:TRP:CH2	1:H:40:GLU:HA	2.56	0.41
1:B:77:LEU:HA	1:B:81:THR:O	2.20	0.41

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	118/119 (99%)	116 (98%)	2 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	118/119 (99%)	114 (97%)	4 (3%)	0	100	100
1	C	121/119 (102%)	118 (98%)	3 (2%)	0	100	100
1	D	120/119 (101%)	117 (98%)	3 (2%)	0	100	100
1	E	119/119 (100%)	117 (98%)	2 (2%)	0	100	100
1	F	114/119 (96%)	109 (96%)	3 (3%)	2 (2%)	8	1
1	G	118/119 (99%)	115 (98%)	3 (2%)	0	100	100
1	H	118/119 (99%)	114 (97%)	4 (3%)	0	100	100
All	All	946/952 (99%)	920 (97%)	24 (2%)	2 (0%)	51	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	21[A]	ASN
1	F	21[B]	ASN

5.3.2 Protein sidechains [i](#)

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	105/111 (95%)	102 (97%)	3 (3%)	42	10
1	B	107/111 (96%)	105 (98%)	2 (2%)	57	23
1	C	109/111 (98%)	109 (100%)	0	100	100
1	D	101/111 (91%)	97 (96%)	4 (4%)	31	4
1	E	105/111 (95%)	104 (99%)	1 (1%)	76	52
1	F	96/111 (86%)	96 (100%)	0	100	100
1	G	103/111 (93%)	103 (100%)	0	100	100
1	H	107/111 (96%)	107 (100%)	0	100	100
All	All	833/888 (94%)	823 (99%)	10 (1%)	81	43

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34[A]	SER
1	A	34[B]	SER
1	A	95	ARG
1	B	68[A]	LYS
1	B	68[B]	LYS
1	D	77[A]	LEU
1	D	77[B]	LEU
1	D	90[A]	ASP
1	D	90[B]	ASP
1	E	43	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	G	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
2	EPE	E	500	-	4,4,15	0.98	0	5,6,20	1.66	1 (20%)
2	EPE	F	500	-	5,5,15	0.72	0	7,7,20	1.17	0
2	EPE	H	500	-	12,12,15	0.95	1 (8%)	14,16,20	2.43	8 (57%)
2	EPE	A	500	-	4,4,15	1.13	0	5,6,20	1.69	1 (20%)

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	EPE	F	500	-	-	3/3/3/19	-
2	EPE	H	500	-	-	1/6/14/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	500	EPE	C10-S	2.68	1.81	1.77

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	500	EPE	O1S-S-C10	-4.50	101.50	106.92
2	H	500	EPE	O2S-S-C10	4.41	112.23	106.92
2	A	500	EPE	O2S-S-O1S	-3.62	108.25	118.02
2	E	500	EPE	O2S-S-O1S	-3.55	108.44	118.02
2	H	500	EPE	C5-N4-C3	3.24	119.65	110.34
2	H	500	EPE	O3S-S-C10	2.78	110.27	105.77
2	H	500	EPE	O3S-S-O2S	-2.46	105.25	111.27
2	H	500	EPE	O3S-S-O1S	2.41	117.16	111.27
2	H	500	EPE	C9-N1-C6	2.15	116.73	111.23
2	H	500	EPE	C5-C6-N1	-2.15	107.87	110.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	500	EPE	C9-C10-S-O1S
2	F	500	EPE	C9-C10-S-O2S
2	F	500	EPE	C9-C10-S-O3S

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Mol	Chain	Res	Type	Atoms
2	H	500	EPE	C10-C9-N1-C6

There are no ring outliers.

No monomer is involved in short contacts.

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	111/119 (93%)	0.70	10 (9%) 9 11	6, 11, 32, 48	0
1	B	114/119 (95%)	0.75	12 (10%) 6 6	6, 12, 29, 39	0
1	C	115/119 (96%)	0.72	7 (6%) 21 23	4, 10, 24, 34	0
1	D	115/119 (96%)	0.75	14 (12%) 4 4	5, 11, 28, 41	0
1	E	116/119 (97%)	0.78	15 (12%) 3 4	4, 12, 27, 31	0
1	F	111/119 (93%)	0.64	10 (9%) 9 11	5, 11, 32, 43	0
1	G	115/119 (96%)	0.78	11 (9%) 8 9	5, 10, 27, 35	0
1	H	116/119 (97%)	0.85	16 (13%) 2 3	6, 12, 27, 39	0
All	All	913/952 (95%)	0.75	95 (10%) 6 7	4, 11, 29, 48	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	47	LEU	8.0
1	B	79	TRP	7.0
1	A	45	VAL	6.4
1	H	49	TYR	6.0
1	G	49	TYR	6.0
1	E	45	VAL	6.0
1	E	49	TYR	5.9
1	H	4	VAL	5.6
1	C	49	TYR	5.5
1	E	116	ARG	5.3
1	B	49	TYR	5.0
1	B	78	GLN	5.0
1	C	77	LEU	4.9
1	D	117	MET	4.8
1	D	77[A]	LEU	4.8
1	D	45	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	4	VAL	4.7
1	H	47	LEU	4.7
1	H	48	PRO	4.5
1	G	77	LEU	4.4
1	D	79	TRP	4.4
1	H	118	ASN	4.2
1	B	77	LEU	4.2
1	H	117	MET	4.0
1	C	79	TRP	4.0
1	B	76	CYS	3.9
1	B	45	VAL	3.9
1	H	46	ASP	3.9
1	A	48	PRO	3.8
1	G	118	ASN	3.8
1	G	79	TRP	3.8
1	H	81	THR	3.7
1	A	4	VAL	3.7
1	E	81	THR	3.6
1	D	76[A]	CYS	3.6
1	F	45	VAL	3.6
1	F	46	ASP	3.4
1	E	80	THR	3.4
1	E	43	GLN	3.3
1	F	81	THR	3.3
1	E	48	PRO	3.3
1	F	47	LEU	3.3
1	H	45	VAL	3.2
1	C	116	ARG	3.2
1	E	47	LEU	3.2
1	G	45	VAL	3.2
1	C	118	ASN	3.2
1	B	81	THR	3.1
1	H	83	ILE	3.1
1	H	3	ASP	3.1
1	G	43	GLN	3.1
1	E	117[A]	MET	3.1
1	B	83	ILE	2.9
1	G	48	PRO	2.9
1	B	82	VAL	2.9
1	D	49	TYR	2.8
1	D	43	GLN	2.8
1	D	4	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	3	ASP	2.8
1	H	115	GLU	2.8
1	E	3	ASP	2.8
1	C	117	MET	2.8
1	A	46	ASP	2.7
1	C	83	ILE	2.6
1	E	44	ASP	2.6
1	B	116	ARG	2.6
1	H	43	GLN	2.6
1	B	117	MET	2.6
1	E	118	ASN	2.6
1	D	118	ASN	2.5
1	G	46	ASP	2.5
1	D	46	ASP	2.5
1	A	81	THR	2.5
1	G	117	MET	2.5
1	A	43	GLN	2.5
1	D	47	LEU	2.4
1	B	43	GLN	2.4
1	E	112	GLN	2.4
1	A	5	THR	2.4
1	D	48	PRO	2.4
1	F	48	PRO	2.4
1	F	82	VAL	2.4
1	A	44	ASP	2.4
1	G	44	ASP	2.3
1	E	46	ASP	2.3
1	D	78	GLN	2.3
1	F	42	PRO	2.3
1	D	83	ILE	2.3
1	A	80	THR	2.2
1	H	44	ASP	2.1
1	A	49	TYR	2.1
1	H	112	GLN	2.1
1	F	80	THR	2.1
1	H	114	GLU	2.0
1	E	4	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EPE	E	500	5/15	0.85	0.23	22,41,64,71	0
2	EPE	A	500	5/15	0.92	0.27	23,29,34,51	0
2	EPE	H	500	12/15	0.96	0.21	15,32,41,44	0
2	EPE	F	500	6/15	0.98	0.13	15,20,32,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.