



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 09:46 PM EDT

PDB ID : 1RQQ
Title : Crystal Structure of the Insulin Receptor Kinase in Complex with the SH2 Domain of APS
Authors : Hu, J.; Liu, J.; Ghirlando, R.; Saltiel, A.R.; Hubbard, S.R.
Deposited on : 2003-12-06
Resolution : 2.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
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) : 2.23.2

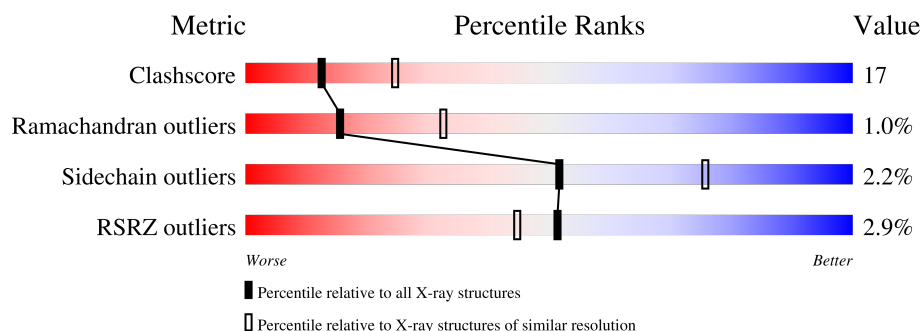
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	306	<div> <div>%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div> </div>
1	B	306	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div> </div>
2	C	114	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>19%</div> <div>27%</div> </div> </div>
2	D	114	<div> <div>3%</div> <div> <div></div> <div>56%</div> <div>16%</div> <div>27%</div> </div> </div>
3	E	18	<div> <div></div> <div> <div></div> <div>44%</div> <div>28%</div> <div>6%</div> <div>22%</div> </div> </div>
3	F	18	<div> <div>6%</div> <div> <div></div> <div>39%</div> <div>33%</div> <div>28%</div> </div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6300 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 Insulin receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	P	S	0	0	0
			2324	1466	396	440	3	19			
1	B	297	Total	C	N	O	P	S	0	0	0
			2318	1463	393	440	3	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	981	SER	CYS	engineered mutation	UNP P06213
A	1158	PTR	TYR	modified residue	UNP P06213
A	1162	PTR	TYR	modified residue	UNP P06213
A	1163	PTR	TYR	modified residue	UNP P06213
A	1251	ASN	LYS	variant	UNP P06213
B	981	SER	CYS	engineered mutation	UNP P06213
B	1158	PTR	TYR	modified residue	UNP P06213
B	1162	PTR	TYR	modified residue	UNP P06213
B	1163	PTR	TYR	modified residue	UNP P06213
B	1251	ASN	LYS	variant	UNP P06213

- Molecule 2 is a protein called adaptor protein APS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	83	Total	C	N	O	S	0	0	0
			657	425	119	110	3			
2	D	83	Total	C	N	O	S	0	0	0
			658	426	119	110	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	397	GLY	-	expression tag	UNP Q9Z200
C	398	SER	-	expression tag	UNP Q9Z200

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	399	HIS	-	expression tag	UNP Q9Z200
C	400	MET	-	expression tag	UNP Q9Z200
D	397	GLY	-	expression tag	UNP Q9Z200
D	398	SER	-	expression tag	UNP Q9Z200
D	399	HIS	-	expression tag	UNP Q9Z200
D	400	MET	-	expression tag	UNP Q9Z200

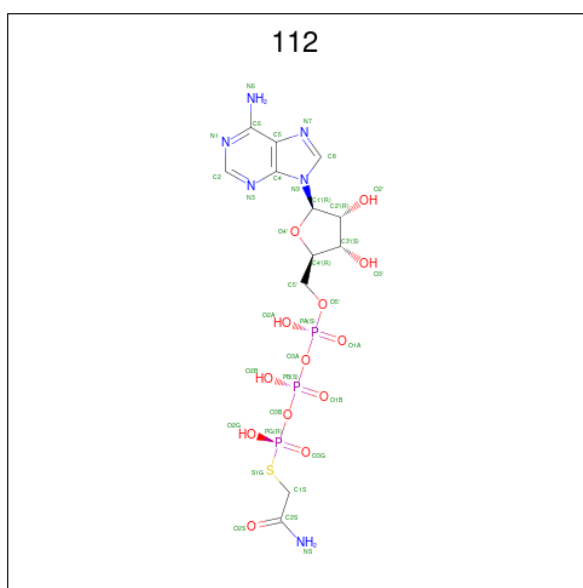
- Molecule 3 is a protein called BISUBSTRATE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	14	Total	C	N	O	S	0	0	0
			98	62	15	19	2			
3	F	13	Total	C	N	O	S	0	0	0
			94	60	14	18	2			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		
4	B	1	Total	Mn	0	0
			1	1		

- Molecule 5 is THIOPHOSPHORIC ACID O-((ADENOSYL-PHOSPHO)PHOSPHO)-S-AC ETAMIDYL-DIESTER (three-letter code: 112) (formula: C₁₂H₁₉N₆O₁₃P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		
5	F	1	Total	C	N	O	P	S	0	0
			35	12	6	13	3	1		

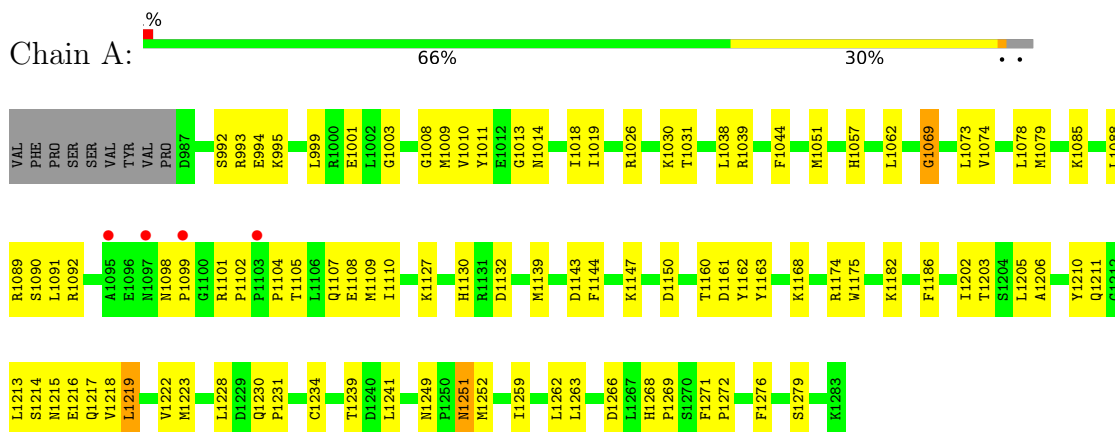
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total	O	0	0
			37	37		
6	B	25	Total	O	0	0
			25	25		
6	C	4	Total	O	0	0
			4	4		
6	D	7	Total	O	0	0
			7	7		
6	E	3	Total	O	0	0
			3	3		
6	F	3	Total	O	0	0
			3	3		

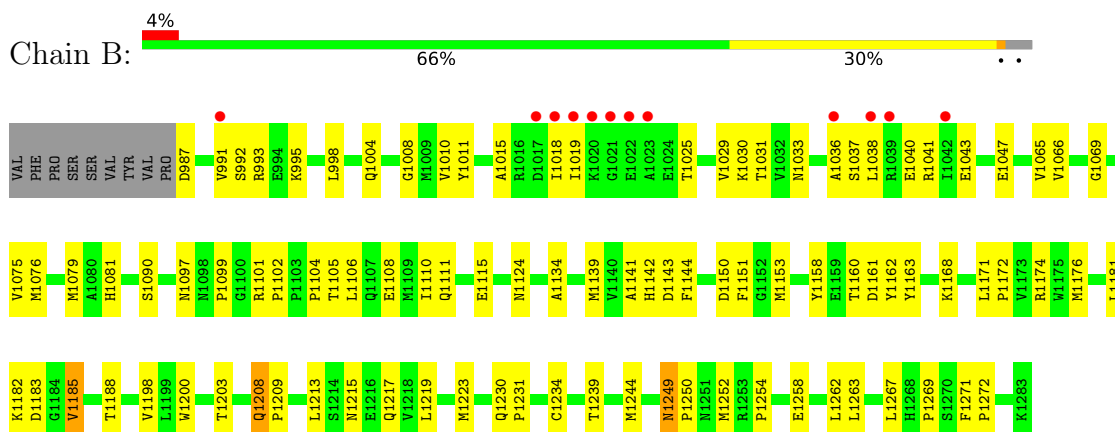
3 Residue-property plots [i](#)

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.

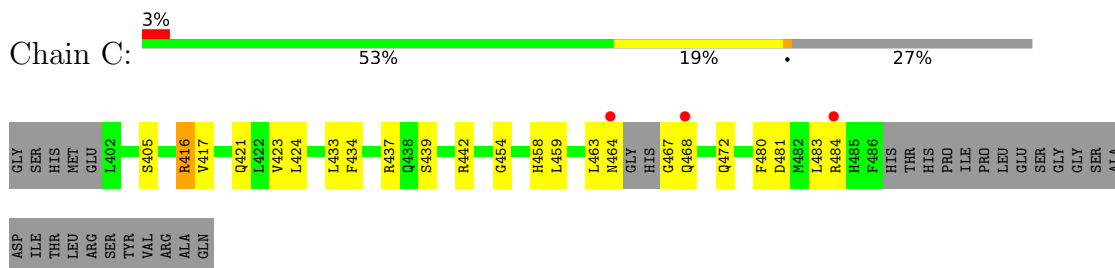
• Molecule 1: Insulin receptor



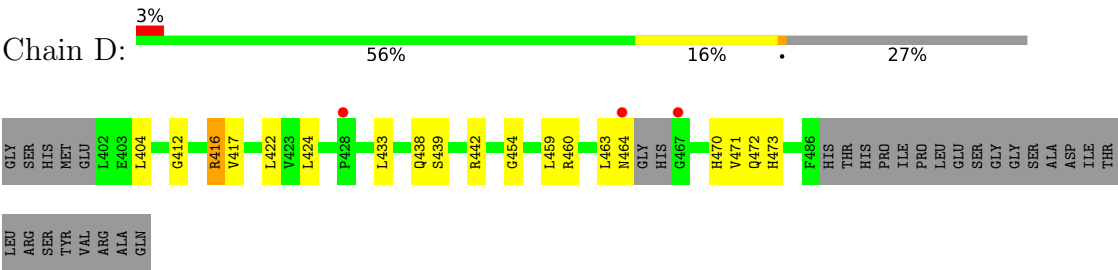
• Molecule 1: Insulin receptor



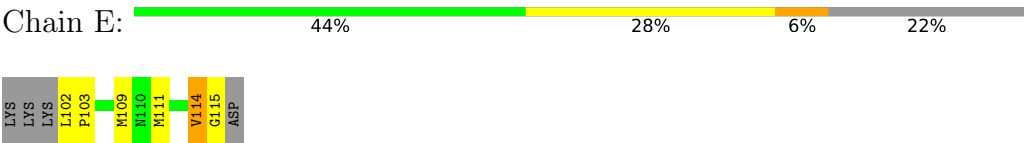
• Molecule 2: adaptor protein APS



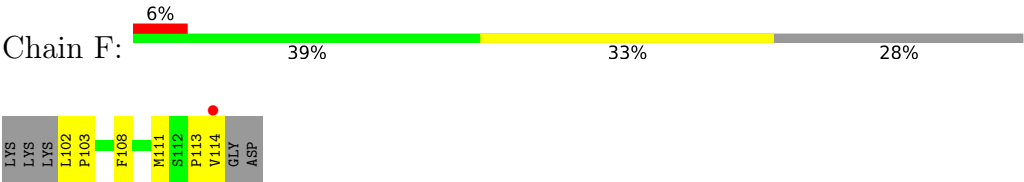
• Molecule 2: adaptor protein APS



• Molecule 3: BISUBSTRATE INHIBITOR



• Molecule 3: BISUBSTRATE INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.22Å 96.44Å 121.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 42.20 – 2.61	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-2.60) 98.5 (42.20-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.94 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.277 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6300	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 112, PTR, MN

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	0.40	0/2324	0.63	0/3147
1	B	0.42	0/2318	0.64	0/3140
2	C	0.43	0/675	0.65	0/912
2	D	0.43	0/677	0.62	0/914
3	E	0.40	0/100	0.72	0/135
3	F	0.37	0/96	0.63	0/130
All	All	0.41	0/6190	0.64	0/8378

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	2324	0	2223	88	0
1	B	2318	0	2212	81	0
2	C	657	0	633	18	0
2	D	658	0	635	14	0
3	E	98	0	93	5	0
3	F	94	0	90	9	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	E	35	0	14	3	0
5	F	35	0	14	4	0
6	A	37	0	0	0	0
6	B	25	0	0	2	0
6	C	4	0	0	0	0
6	D	7	0	0	0	0
6	E	3	0	0	1	0
6	F	3	0	0	0	0
All	All	6300	0	5914	204	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 17.

All (204) 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:B:992:SER:HB2	1:B:995:LYS:HD3	1.39	0.99
1:A:1014:ASN:HD21	1:A:1026:ARG:HE	1.20	0.88
1:A:1001:GLU:HB3	1:A:1009:MET:HE2	1.58	0.83
1:A:1107:GLN:O	1:A:1110:ILE:HG22	1.80	0.81
1:B:1160:THR:O	1:B:1161:ASP:HB2	1.81	0.81
1:A:1213:LEU:H	1:A:1213:LEU:HD12	1.46	0.81
1:A:1014:ASN:ND2	1:A:1026:ARG:HE	1.83	0.77
1:B:1258:GLU:O	1:B:1262:LEU:HD13	1.85	0.76
2:C:481:ASP:O	2:C:484:ARG:HG2	1.86	0.76
1:B:1111:GLN:O	1:B:1115:GLU:HG3	1.85	0.75
1:A:1130:HIS:HD2	1:A:1132:ASP:H	1.34	0.75
1:A:993:ARG:NH2	1:A:1069:GLY:O	2.21	0.73
1:A:1039:ARG:HB3	1:A:1039:ARG:NH1	2.04	0.72
1:A:992:SER:HB2	1:A:995:LYS:HG3	1.72	0.72
1:A:1276:PHE:O	1:A:1279:SER:HB3	1.90	0.72
1:B:1171:LEU:HB3	1:B:1176:MET:HE3	1.73	0.70
2:C:433:LEU:HD23	2:C:434:PHE:N	2.06	0.70
2:D:463:LEU:HG	2:D:464:ASN:H	1.57	0.70
1:B:1018:ILE:HD12	1:B:1019:ILE:N	2.07	0.69
2:C:437:ARG:HH21	2:C:458:HIS:CD2	2.09	0.69
1:A:1160:THR:O	1:A:1161:ASP:HB2	1.92	0.69
1:A:1214:SER:OG	1:A:1217:GLN:HG3	1.92	0.69
1:B:1076:MET:CE	5:F:117:112:HN61	2.05	0.69
1:A:999:LEU:HD23	1:A:1013:GLY:HA2	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:422:LEU:C	2:D:422:LEU:HD23	2.14	0.68
1:B:1011:TYR:HB2	1:B:1029:VAL:HG23	1.76	0.68
2:D:463:LEU:O	2:D:464:ASN:HB2	1.92	0.68
1:B:1018:ILE:HD11	1:B:1025:THR:HB	1.76	0.68
1:B:1004:GLN:O	3:F:103:PRO:HG3	1.94	0.67
1:B:1038:LEU:HD12	1:B:1041:ARG:HD2	1.76	0.67
1:B:1076:MET:HE3	5:F:117:112:HN61	1.59	0.67
1:B:998:LEU:HD22	1:B:1029:VAL:HG21	1.76	0.67
1:A:1089:ARG:HG2	1:A:1092:ARG:NH1	2.12	0.65
1:A:1026:ARG:HG3	1:A:1078:LEU:HD22	1.79	0.64
1:B:1213:LEU:HD12	1:B:1217:GLN:HB3	1.79	0.64
2:C:463:LEU:HG	2:C:464:ASN:H	1.63	0.63
1:A:1215:ASN:HB3	3:E:109:MET:SD	2.39	0.62
1:B:1018:ILE:HD11	1:B:1025:THR:CB	2.28	0.62
1:B:1011:TYR:HB2	1:B:1029:VAL:CG2	2.28	0.62
2:C:459:LEU:HD13	2:D:471:VAL:HG12	1.82	0.62
1:A:1182:LYS:HB2	1:A:1223:MET:HE3	1.81	0.62
2:C:437:ARG:HH21	2:C:458:HIS:HD2	1.46	0.61
2:C:423:VAL:HG12	2:C:433:LEU:HD22	1.82	0.60
1:B:1203:THR:OG1	1:B:1231:PRO:HG3	2.01	0.60
1:A:1101:ARG:HB2	1:A:1102:PRO:HD2	1.83	0.60
1:A:1271:PHE:HB3	1:A:1272:PRO:HD3	1.83	0.59
1:A:1127:LYS:HE2	1:A:1127:LYS:HA	1.84	0.59
1:A:1249:ASN:OD1	1:A:1251:ASN:ND2	2.36	0.59
1:B:1271:PHE:HB3	1:B:1272:PRO:HD3	1.84	0.59
2:D:412:GLY:O	2:D:438:GLN:HG3	2.02	0.59
1:B:1018:ILE:CD1	1:B:1019:ILE:HG13	2.32	0.58
2:D:422:LEU:HD23	2:D:422:LEU:O	2.04	0.58
1:B:1037:SER:O	1:B:1041:ARG:HG3	2.03	0.58
1:B:1230:GLN:NE2	1:B:1239:THR:HG23	2.19	0.57
1:B:992:SER:HB2	1:B:995:LYS:CD	2.26	0.57
1:A:1216:GLU:H	1:A:1216:GLU:CD	2.08	0.57
1:A:1001:GLU:HG2	1:A:1011:TYR:CE1	2.40	0.57
1:A:1130:HIS:CD2	1:A:1132:ASP:H	2.19	0.57
1:A:1249:ASN:CG	1:A:1251:ASN:HD21	2.08	0.56
1:A:1013:GLY:O	1:A:1026:ARG:HD3	2.05	0.56
1:A:1211:GLN:OE1	1:A:1211:GLN:HA	2.06	0.56
1:A:1014:ASN:HD21	1:A:1026:ARG:NE	1.96	0.55
2:D:416:ARG:HG3	2:D:417:VAL:N	2.21	0.55
1:A:1213:LEU:HD12	1:A:1213:LEU:N	2.18	0.55
1:B:1079:MET:HG3	1:B:1139:MET:HB3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1249:ASN:HB3	1:B:1252:MET:CG	2.37	0.54
1:A:1018:ILE:HG23	1:A:1019:ILE:HG13	1.88	0.54
1:A:1168:LYS:HA	3:E:111:MET:O	2.06	0.54
1:B:1106:LEU:O	1:B:1110:ILE:HG12	2.08	0.54
1:B:1188:THR:HG23	6:B:16:HOH:O	2.06	0.54
2:C:459:LEU:HD21	2:D:472:GLN:HA	1.90	0.54
1:A:1109:MET:HE1	1:A:1203:THR:HA	1.90	0.54
1:B:1047:GLU:HG3	1:B:1151:PHE:HB2	1.89	0.54
2:C:416:ARG:HG3	2:C:417:VAL:N	2.22	0.54
2:C:442:ARG:HH11	2:C:442:ARG:HG3	1.72	0.54
1:A:1003:GLY:O	1:A:1009:MET:HE3	2.09	0.53
1:B:1043:GLU:HA	1:B:1043:GLU:OE1	2.09	0.53
2:C:459:LEU:HD13	2:D:471:VAL:CG1	2.38	0.53
1:B:1079:MET:HG3	1:B:1139:MET:CB	2.39	0.52
1:B:1033:ASN:OD1	1:B:1036:ALA:HB2	2.09	0.52
1:A:1182:LYS:HB2	1:A:1223:MET:CE	2.39	0.52
1:B:1015:ALA:HB3	1:B:1018:ILE:HG12	1.92	0.52
2:D:439:SER:HB3	2:D:442:ARG:O	2.09	0.52
1:A:1001:GLU:HB3	1:A:1009:MET:CE	2.33	0.52
1:A:1057:HIS:O	1:A:1147:LYS:HE2	2.10	0.52
1:B:998:LEU:CD2	1:B:1029:VAL:HG21	2.39	0.52
1:B:1104:PRO:HA	1:B:1108:GLU:OE1	2.09	0.52
1:B:1231:PRO:HG2	1:B:1234:CYS:HB2	1.92	0.52
2:C:442:ARG:HG3	2:C:442:ARG:NH1	2.25	0.52
1:B:1249:ASN:HB3	1:B:1252:MET:HG3	1.91	0.52
1:B:1008:GLY:HA3	1:B:1031:THR:O	2.11	0.51
1:B:1153:MET:HE3	6:B:67:HOH:O	2.11	0.51
1:A:992:SER:HB3	1:A:994:GLU:HG2	1.92	0.51
1:A:1218:VAL:O	1:A:1222:VAL:HG23	2.11	0.51
3:E:102:LEU:N	3:E:103:PRO:HD2	2.26	0.51
1:A:1214:SER:H	1:A:1217:GLN:CD	2.15	0.51
1:B:1105:THR:HB	1:B:1108:GLU:HG3	1.93	0.51
1:A:1044:PHE:CZ	1:A:1074:VAL:HG23	2.46	0.51
1:B:991:VAL:HG23	1:B:1066:VAL:CG2	2.41	0.51
1:B:1230:GLN:CD	1:B:1239:THR:HG23	2.32	0.51
3:F:102:LEU:N	3:F:103:PRO:CD	2.74	0.51
1:A:1010:VAL:HG22	1:A:1030:LYS:HG2	1.93	0.50
1:B:1153:MET:CE	3:F:108:PHE:HE2	2.24	0.50
1:A:1008:GLY:HA3	1:A:1031:THR:O	2.12	0.50
1:B:1018:ILE:HD13	1:B:1019:ILE:HG13	1.94	0.50
1:A:1213:LEU:H	1:A:1213:LEU:CD1	2.18	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1214:SER:H	1:A:1217:GLN:CG	2.24	0.50
1:B:1183:ASP:HB2	1:B:1185:VAL:HG13	1.94	0.50
1:A:1130:HIS:HD2	1:A:1132:ASP:N	2.06	0.50
1:A:1088:LEU:HD13	1:A:1202:ILE:HA	1.93	0.49
1:B:1076:MET:HE2	5:F:117:112:N7	2.26	0.49
2:C:439:SER:HB3	2:C:442:ARG:O	2.11	0.49
1:A:1249:ASN:CG	1:A:1251:ASN:ND2	2.66	0.49
1:B:1223:MET:HE3	3:F:114:VAL:HB	1.95	0.49
1:A:1104:PRO:HG2	1:A:1109:MET:CE	2.43	0.49
2:C:472:GLN:HA	2:D:459:LEU:HD21	1.95	0.49
2:D:424:LEU:HD22	2:D:454:GLY:O	2.12	0.49
1:B:1081:HIS:HD2	1:B:1141:ALA:O	1.96	0.49
1:A:992:SER:HB2	1:A:995:LYS:CG	2.42	0.49
2:C:424:LEU:HD22	2:C:454:GLY:O	2.12	0.49
1:A:1230:GLN:CD	1:A:1239:THR:HG23	2.33	0.48
1:B:991:VAL:HG23	1:B:1066:VAL:HG22	1.94	0.48
1:B:1101:ARG:HB2	1:B:1102:PRO:HD2	1.94	0.48
2:D:470:HIS:O	2:D:473:HIS:HB2	2.13	0.48
1:A:1251:ASN:HD22	1:A:1252:MET:N	2.11	0.48
1:A:1269:PRO:O	1:A:1272:PRO:HD2	2.13	0.47
2:C:480:PHE:HA	2:C:483:LEU:HD12	1.95	0.47
1:A:1001:GLU:CB	1:A:1009:MET:HE2	2.37	0.47
1:B:1263:LEU:O	1:B:1267:LEU:HG	2.13	0.47
1:B:991:VAL:HG22	1:B:1065:VAL:O	2.14	0.47
1:B:1162:PTR:C	1:B:1162:PTR:CD1	2.92	0.47
3:E:114:VAL:HG12	3:E:115:GLY:N	2.29	0.47
1:B:1213:LEU:N	1:B:1213:LEU:HD22	2.30	0.47
1:B:1208:GLN:HE21	1:B:1208:GLN:HA	1.79	0.47
1:A:1213:LEU:HB3	1:A:1217:GLN:HB2	1.95	0.46
2:D:422:LEU:C	2:D:422:LEU:CD2	2.84	0.46
1:B:1168:LYS:HA	3:F:111:MET:O	2.16	0.46
1:A:1039:ARG:HB3	1:A:1039:ARG:HH11	1.79	0.46
1:B:1143:ASP:O	1:B:1144:PHE:HB2	2.14	0.46
1:B:1200:TRP:CH2	1:B:1209:PRO:HA	2.51	0.46
1:A:1251:ASN:HD22	1:A:1251:ASN:C	2.19	0.46
1:B:1174:ARG:HH21	1:B:1215:ASN:ND2	2.13	0.46
1:A:1039:ARG:HB3	1:A:1039:ARG:CZ	2.45	0.46
1:A:1210:TYR:H	1:A:1228:LEU:HD21	1.81	0.45
1:B:991:VAL:O	1:B:1066:VAL:HG22	2.16	0.45
1:B:1018:ILE:HD12	1:B:1019:ILE:HG13	1.98	0.45
1:A:1014:ASN:ND2	1:A:1026:ARG:NE	2.59	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1241:LEU:HD21	1:A:1262:LEU:HD23	1.98	0.45
1:B:1223:MET:CE	3:F:114:VAL:HB	2.47	0.45
1:B:1090:SER:HA	1:B:1097:ASN:OD1	2.16	0.45
1:A:1186:PHE:CD1	1:A:1186:PHE:N	2.85	0.45
1:A:1088:LEU:CD1	1:A:1202:ILE:HA	2.47	0.45
1:A:1174:ARG:HB2	1:A:1175:TRP:CZ3	2.52	0.44
1:A:1105:THR:O	1:A:1109:MET:HG3	2.17	0.44
1:A:1268:HIS:CG	1:A:1269:PRO:HD2	2.52	0.44
5:E:117:112:H1S1	5:E:117:112:PB	2.57	0.44
1:B:1106:LEU:O	1:B:1106:LEU:HD23	2.18	0.44
1:A:1085:LYS:HG3	1:A:1206:ALA:HB1	1.99	0.44
1:A:1104:PRO:HG2	1:A:1109:MET:HE3	1.99	0.44
5:E:117:112:PG	6:E:62:HOH:O	2.74	0.44
1:A:1089:ARG:HG3	1:A:1206:ALA:HB3	2.00	0.43
1:B:1244:MET:HB3	1:B:1254:PRO:HD3	1.99	0.43
1:B:1142:HIS:CE1	1:B:1143:ASP:HB3	2.53	0.43
1:B:1171:LEU:HB3	1:B:1176:MET:CE	2.44	0.43
1:A:1219:LEU:HD11	3:E:114:VAL:HG21	2.00	0.43
1:B:1105:THR:HG22	1:B:1106:LEU:N	2.33	0.43
1:B:1037:SER:OG	1:B:1040:GLU:HG3	2.18	0.43
1:A:1009:MET:HG2	1:A:1011:TYR:CZ	2.54	0.43
1:B:1010:VAL:HG22	1:B:1030:LYS:HG2	2.00	0.42
1:B:1124:ASN:C	1:B:1124:ASN:ND2	2.72	0.42
1:A:1039:ARG:HH11	1:A:1039:ARG:CB	2.33	0.42
1:B:1153:MET:HE1	3:F:108:PHE:HE2	1.84	0.42
3:F:108:PHE:CD1	3:F:108:PHE:N	2.86	0.42
1:B:1076:MET:HE2	5:F:117:112:HN61	1.80	0.42
1:A:1031:THR:HG22	1:A:1073:LEU:HD23	2.01	0.42
1:A:1162:PTR:CD1	1:A:1162:PTR:C	2.97	0.42
1:A:1079:MET:HG3	1:A:1139:MET:CB	2.49	0.42
1:A:1092:ARG:NH1	1:A:1205:LEU:O	2.52	0.42
1:B:1106:LEU:HD23	1:B:1106:LEU:C	2.40	0.42
1:A:1143:ASP:O	1:A:1144:PHE:HB2	2.19	0.42
1:B:1176:MET:HB2	1:B:1181:LEU:HD21	2.02	0.42
1:B:1249:ASN:HD22	1:B:1250:PRO:HD2	1.85	0.42
1:B:1269:PRO:O	1:B:1272:PRO:HD2	2.20	0.42
1:A:1039:ARG:NH1	1:A:1039:ARG:CB	2.81	0.41
1:A:1104:PRO:HA	1:A:1108:GLU:OE2	2.20	0.41
1:A:1214:SER:H	1:A:1217:GLN:HG3	1.85	0.41
1:A:1259:ILE:O	1:A:1263:LEU:HG	2.20	0.41
1:B:1181:LEU:HD22	1:B:1219:LEU:HD22	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:467:GLY:O	2:C:468:GLN:HB2	2.20	0.41
1:A:1105:THR:HG23	1:A:1108:GLU:OE2	2.19	0.41
2:C:463:LEU:O	2:C:464:ASN:CB	2.68	0.41
5:E:117:112:H1S1	5:E:117:112:O2B	2.20	0.41
1:A:1214:SER:O	1:A:1218:VAL:HG23	2.19	0.41
1:A:1231:PRO:HD2	1:A:1234:CYS:HB2	2.02	0.41
1:B:1172:PRO:O	1:B:1176:MET:HG3	2.21	0.41
1:B:1029:VAL:HG12	1:B:1075:VAL:HG22	2.02	0.41
1:A:1091:LEU:HD12	1:A:1104:PRO:HD3	2.03	0.41
1:A:1051:MET:HB3	1:A:1062:LEU:HB2	2.02	0.41
1:A:1230:GLN:OE1	1:A:1239:THR:HG23	2.21	0.41
1:B:1134:ALA:HA	1:B:1198:VAL:HG22	2.03	0.41
1:A:1090:SER:O	1:A:1098:ASN:HA	2.21	0.41
1:B:1182:LYS:O	3:F:113:PRO:HB3	2.21	0.40
1:A:1174:ARG:HB2	1:A:1175:TRP:CE3	2.56	0.40
1:B:993:ARG:HG2	1:B:993:ARG:O	2.22	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	292/306 (95%)	273 (94%)	16 (6%)	3 (1%)	15	32
1	B	292/306 (95%)	274 (94%)	15 (5%)	3 (1%)	15	32
2	C	79/114 (69%)	72 (91%)	7 (9%)	0	100	100
2	D	79/114 (69%)	71 (90%)	7 (9%)	1 (1%)	12	24
3	E	12/18 (67%)	10 (83%)	1 (8%)	1 (8%)	1	1
3	F	11/18 (61%)	10 (91%)	1 (9%)	0	100	100
All	All	765/876 (87%)	710 (93%)	47 (6%)	8 (1%)	15	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1099	PRO
1	B	1099	PRO
3	E	114	VAL
1	B	1150	ASP
1	A	1150	ASP
2	D	404	LEU
1	B	1069	GLY
1	A	1069	GLY

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	243/265 (92%)	239 (98%)	4 (2%)	62	82
1	B	242/265 (91%)	238 (98%)	4 (2%)	60	81
2	C	68/97 (70%)	65 (96%)	3 (4%)	28	53
2	D	69/97 (71%)	66 (96%)	3 (4%)	29	54
3	E	11/15 (73%)	11 (100%)	0	100	100
3	F	11/15 (73%)	11 (100%)	0	100	100
All	All	644/754 (85%)	630 (98%)	14 (2%)	52	76

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1038	LEU
1	A	1219	LEU
1	A	1251	ASN
1	A	1266	ASP
1	B	987	ASP
1	B	1185	VAL
1	B	1208	GLN
1	B	1249	ASN
2	C	405	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	416	ARG
2	C	421	GLN
2	D	416	ARG
2	D	433	LEU
2	D	460	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1014	ASN
1	A	1081	HIS
1	A	1124	ASN
1	A	1130	HIS
1	A	1217	GLN
1	A	1230	GLN
1	A	1251	ASN
1	B	1081	HIS
1	B	1124	ASN
1	B	1208	GLN
1	B	1211	GLN
1	B	1215	ASN
1	B	1230	GLN
1	B	1247	GLN
1	B	1249	ASN
2	C	411	HIS
2	C	421	GLN
2	C	438	GLN
2	C	458	HIS
2	C	472	GLN
2	D	411	HIS
2	D	453	GLN
2	D	464	ASN
2	D	472	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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$
1	PTR	B	1162	1	15,16,17	0.81	0	19,22,24	0.97	0
1	PTR	B	1163	1	15,16,17	1.38	1 (6%)	19,22,24	1.08	2 (10%)
1	PTR	B	1158	1	15,16,17	1.16	2 (13%)	19,22,24	0.93	1 (5%)
1	PTR	A	1162	1	15,16,17	0.79	0	19,22,24	0.77	0
1	PTR	A	1158	1	15,16,17	0.89	0	19,22,24	0.76	0
1	PTR	A	1163	1	15,16,17	1.00	1 (6%)	19,22,24	1.11	3 (15%)

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
1	PTR	B	1162	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1163	1	-	0/10/11/13	0/1/1/1
1	PTR	B	1158	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1162	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1158	1	-	0/10/11/13	0/1/1/1
1	PTR	A	1163	1	-	0/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1163	PTR	P-OH	4.26	1.65	1.59
1	B	1158	PTR	P-OH	2.46	1.63	1.59
1	A	1163	PTR	P-OH	2.27	1.62	1.59
1	B	1158	PTR	P-O2P	-2.09	1.46	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1163	PTR	P-OH-CZ	2.76	132.59	123.75
1	A	1163	PTR	O3P-P-O2P	2.26	116.26	107.64
1	A	1163	PTR	O2P-P-OH	-2.20	98.37	105.24
1	B	1158	PTR	CB-CA-C	-2.20	107.35	111.47
1	A	1163	PTR	P-OH-CZ	2.19	130.76	123.75
1	B	1163	PTR	OH-P-O1P	-2.06	101.53	109.31

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
1	B	1162	PTR	1	0
1	A	1162	PTR	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
5	112	E	117	4,3	27,37,37	0.97	1 (3%)	27,57,57	1.07	2 (7%)
5	112	F	117	4,3	27,37,37	0.91	1 (3%)	27,57,57	1.19	4 (14%)

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
5	112	E	117	4,3	-	3/19/44/44	0/3/3/3
5	112	F	117	4,3	-	4/19/44/44	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	117	112	PG-O2G	-3.22	1.48	1.56
5	F	117	112	PG-O2G	-2.23	1.51	1.56

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	117	112	O2S-C2S-NS	-2.80	114.84	122.50
5	E	117	112	O2S-C2S-NS	-2.54	115.56	122.50
5	F	117	112	C5-C6-N6	2.42	124.03	120.35
5	E	117	112	C5-C6-N6	2.33	123.90	120.35
5	F	117	112	PA-O5'-C5'	2.21	134.67	121.68
5	F	117	112	C2S-C1S-S1G	2.10	117.82	111.31

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	E	117	112	C5'-O5'-PA-O1A
5	E	117	112	C5'-O5'-PA-O3A
5	F	117	112	C5'-O5'-PA-O1A
5	F	117	112	C5'-O5'-PA-O3A
5	E	117	112	C5'-O5'-PA-O2A
5	F	117	112	C5'-O5'-PA-O2A
5	F	117	112	PG-O3B-PB-O1B

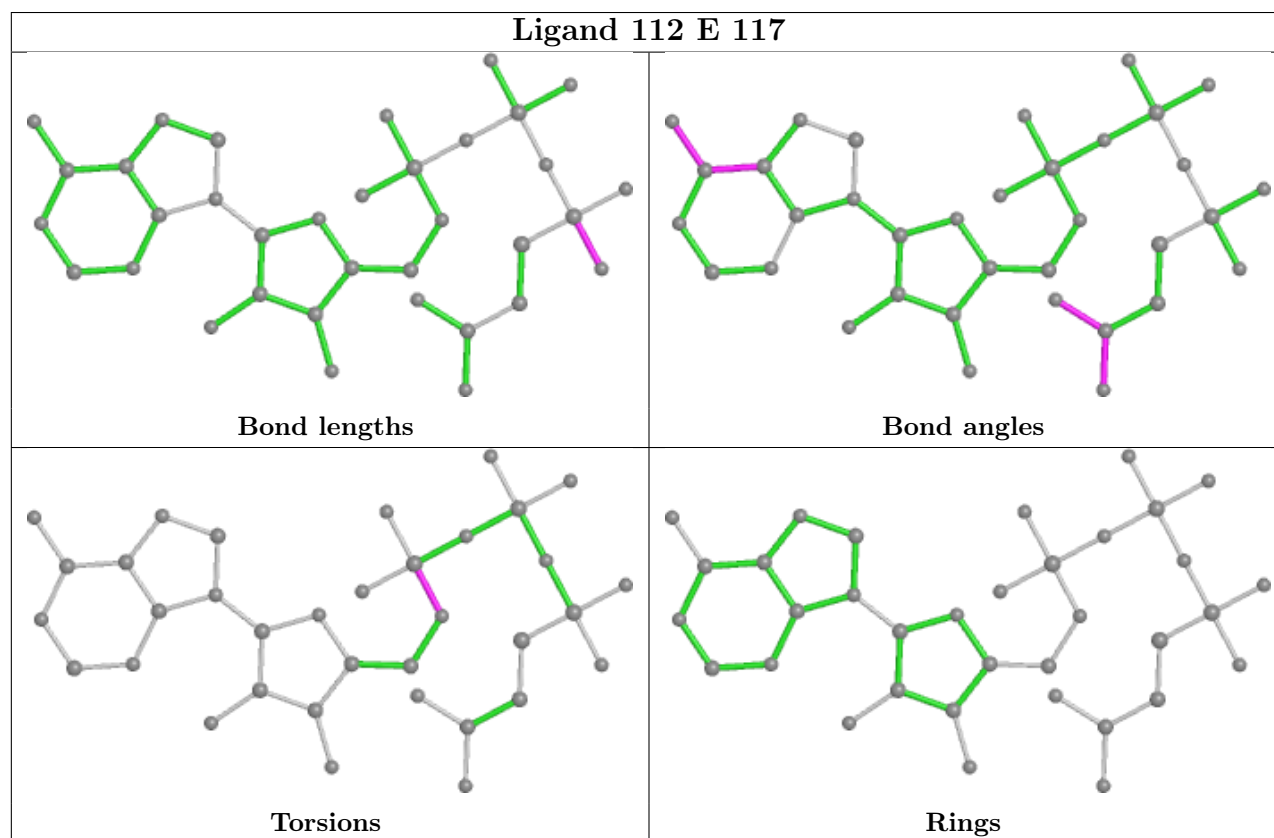
There are no ring outliers.

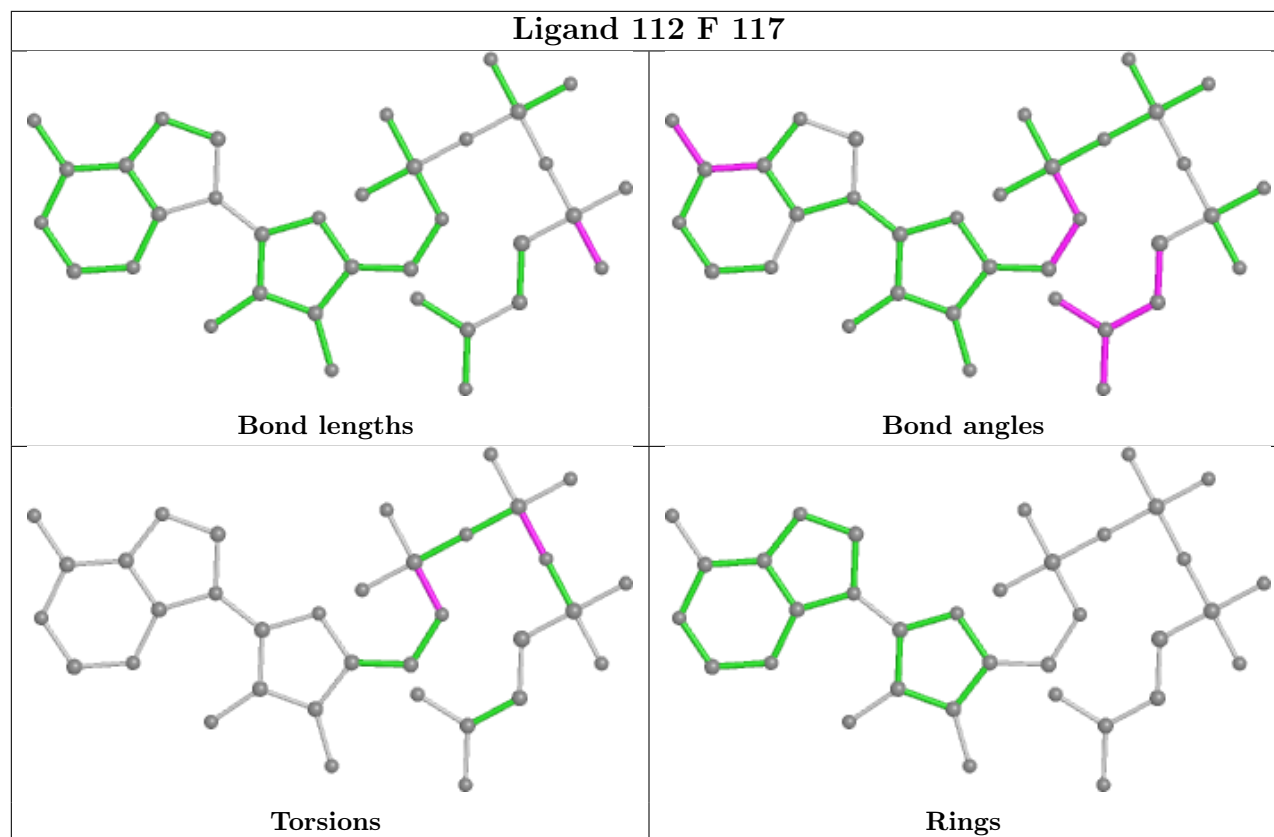
2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	117	112	3	0
5	F	117	112	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	294/306 (96%)	-0.13	4 (1%) 75 71	27, 49, 70, 84	0
1	B	294/306 (96%)	0.04	12 (4%) 37 30	26, 49, 71, 80	0
2	C	83/114 (72%)	-0.16	3 (3%) 42 35	32, 47, 77, 90	0
2	D	83/114 (72%)	-0.05	3 (3%) 42 35	33, 49, 73, 91	0
3	E	14/18 (77%)	-0.13	0 100 100	46, 56, 64, 66	0
3	F	13/18 (72%)	0.14	1 (7%) 13 10	49, 52, 61, 66	0
All	All	781/876 (89%)	-0.06	23 (2%) 51 45	26, 49, 72, 91	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1018	ILE	3.8
2	D	467	GLY	3.3
1	B	1019	ILE	3.3
1	B	1042	ILE	3.1
1	B	1021	GLY	3.0
1	B	991	VAL	2.8
1	B	1020	LYS	2.8
1	B	1023	ALA	2.7
2	C	484	ARG	2.7
1	B	1038	LEU	2.6
1	B	1017	ASP	2.6
2	C	468	GLN	2.6
1	B	1022	GLU	2.5
1	B	1036	ALA	2.5
1	B	1039	ARG	2.4
1	A	1103	PRO	2.4
1	A	1095	ALA	2.3
1	A	1099	PRO	2.2
2	D	464	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	464	ASN	2.1
2	D	428	PRO	2.0
3	F	114	VAL	2.0
1	A	1097	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	A	1162	16/17	0.96	0.12	38,42,51,51	0
1	PTR	A	1163	16/17	0.96	0.15	34,38,48,48	0
1	PTR	B	1162	16/17	0.96	0.12	38,42,48,49	0
1	PTR	B	1158	16/17	0.97	0.14	33,35,40,41	0
1	PTR	B	1163	16/17	0.97	0.11	40,45,54,55	0
1	PTR	A	1158	16/17	0.98	0.13	32,34,39,40	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

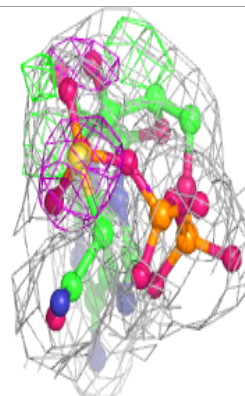
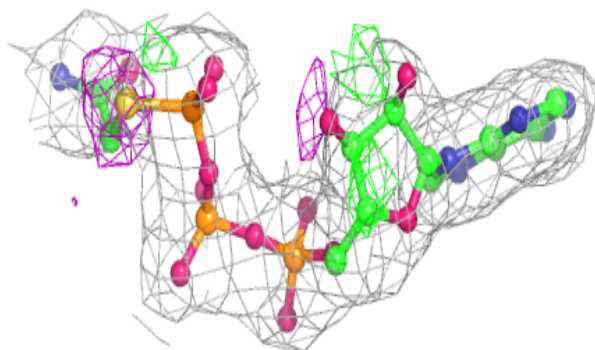
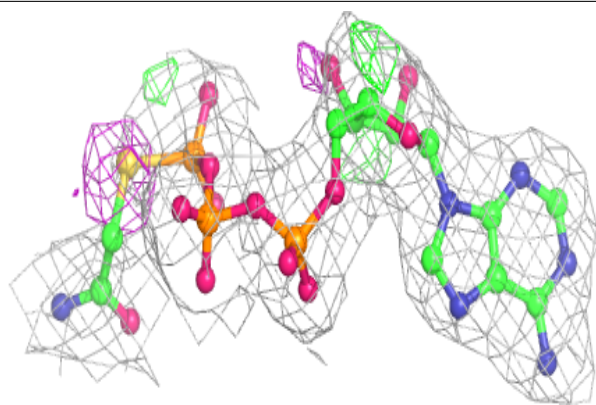
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	112	F	117	35/35	0.94	0.19	34,46,53,62	0
5	112	E	117	35/35	0.96	0.13	36,44,52,53	0
4	MN	B	202	1/1	0.99	0.14	35,35,35,35	0
4	MN	A	201	1/1	1.00	0.13	35,35,35,35	0

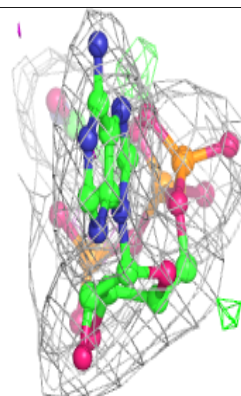
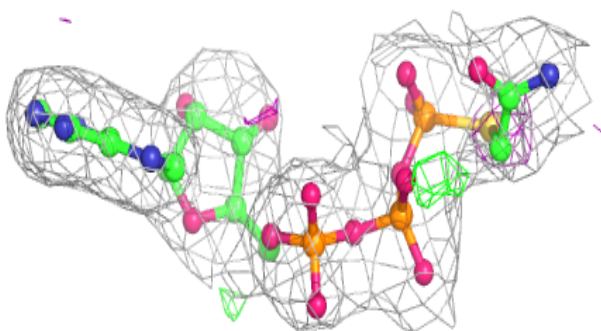
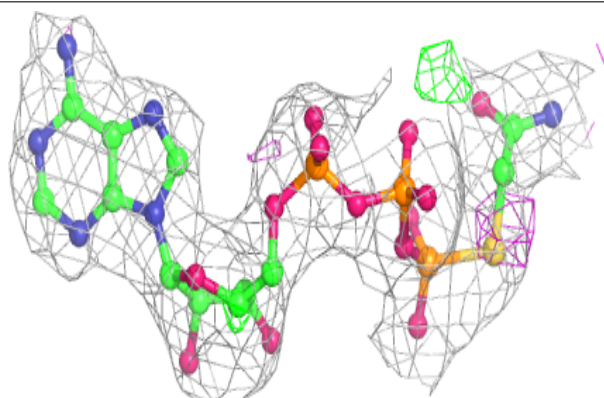
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 112 F 117:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 112 E 117:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.