



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:07 AM GMT

PDB ID : 2ZM3
Title : Complex Structure of Insulin-like Growth Factor Receptor and Isoquinoline-dione Inhibitor
Authors : Xu, W.; Mayer, S.C.; Boschelli, F.; Johnson, M.; Dwyer, B.
Deposited on : 2008-04-10
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

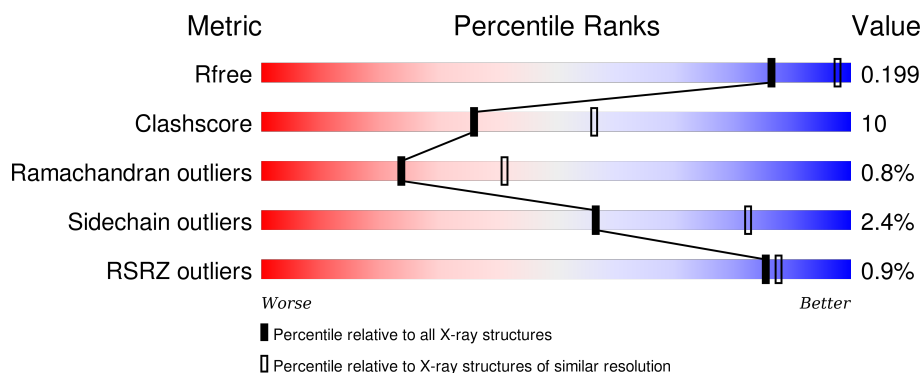
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 14%, green 84%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 84% 14% </div> </div>
1	B	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 20%, green 76%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 76% 20% </div> </div>
1	C	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 23%, green 72%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 72% 23% </div> </div>
1	D	308	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 16%, green 79%, grey 3%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 79% 16% </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10157 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.

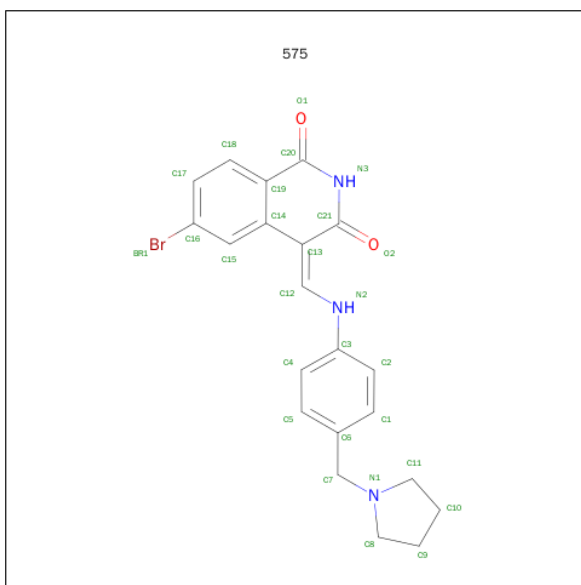
- Molecule 1 is a protein called Insulin-like growth factor 1 receptor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	P	S	0	0	0
			2424	1536	402	462	2	22			
1	B	299	Total	C	N	O	P	S	0	0	0
			2394	1516	397	457	2	22			
1	C	299	Total	C	N	O	P	S	0	0	0
			2397	1517	397	458	3	22			
1	D	296	Total	C	N	O	P	S	0	0	0
			2377	1503	394	455	3	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	979	GLY	-	EXPRESSION TAG	UNP P08069
A	980	SER	-	EXPRESSION TAG	UNP P08069
B	979	GLY	-	EXPRESSION TAG	UNP P08069
B	980	SER	-	EXPRESSION TAG	UNP P08069
C	979	GLY	-	EXPRESSION TAG	UNP P08069
C	980	SER	-	EXPRESSION TAG	UNP P08069
D	979	GLY	-	EXPRESSION TAG	UNP P08069
D	980	SER	-	EXPRESSION TAG	UNP P08069

- Molecule 2 is (4Z)-6-BROMO-4-([4-(PYRROLIDIN-1-YLMETHYL)PHENYL]AMINO) METHYLIDENE)ISOQUINOLINE-1,3(2H,4H)-DIONE (three-letter code: 575) (formula: C₂₁H₂₀BrN₃O₂).

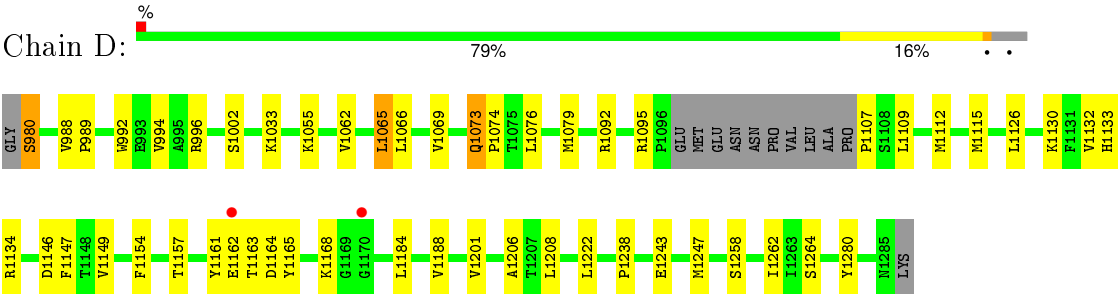


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			27	1	21	3	2		
2	B	1	Total	Br	C	N	O	0	0
			27	1	21	3	2		
2	C	1	Total	Br	C	N	O	0	0
			27	1	21	3	2		
2	D	1	Total	Br	C	N	O	0	0
			27	1	21	3	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total	O	0	0
			134	134		
3	B	106	Total	O	0	0
			106	106		
3	C	103	Total	O	0	0
			103	103		
3	D	114	Total	O	0	0
			114	114		

● Molecule 1: Insulin-like growth factor 1 receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	137.72Å 135.96Å 86.38Å 90.00° 114.27° 90.00°	Depositor
Resolution (Å)	46.37 – 2.50 46.37 – 2.27	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.37-2.50) 90.1 (46.37-2.27)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.27Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.201 , 0.257 0.200 , 0.199	Depositor DCC
R_{free} test set	2421 reflections (5.18%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 60384 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10157	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, 575

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	0.25	0/2427	0.44	0/3271
1	B	0.25	0/2396	0.43	0/3227
1	C	0.24	0/2395	0.43	0/3226
1	D	0.24	0/2374	0.45	0/3195
All	All	0.24	0/9592	0.44	0/12919

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	2424	0	2368	34	0
1	B	2394	0	2335	48	0
1	C	2397	0	2340	61	0
1	D	2377	0	2318	46	0
2	A	27	0	20	2	0
2	B	27	0	20	0	0
2	C	27	0	20	1	0
2	D	27	0	20	0	0
3	A	134	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	106	0	0	3	0
3	C	103	0	0	1	0
3	D	114	0	0	1	0
All	All	10157	0	9441	183	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 10.

All (183) 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:C:1156:MET:HG2	1:C:1174:LEU:HD21	1.45	0.98
1:C:1073:GLN:HB2	1:C:1074:PRO:HD3	1.53	0.89
1:D:1073:GLN:HB3	1:D:1074:PRO:CD	2.11	0.79
1:B:1162:GLU:O	1:B:1164:ASP:N	2.17	0.77
1:C:989:PRO:HG2	1:C:1055:LYS:HE2	1.66	0.75
1:A:1184:LEU:HD22	1:A:1222:LEU:HD13	1.70	0.74
1:D:1161:PTR:CD2	1:D:1162:GLU:HG2	2.18	0.73
1:A:1133:HIS:HA	1:A:1157:THR:HG22	1.71	0.73
1:D:996:ARG:HB3	1:D:1069:VAL:HG11	1.71	0.72
1:C:1069:VAL:HB	1:C:1076:LEU:HB2	1.71	0.71
1:D:1134:ARG:HH22	1:D:1168:LYS:HZ3	1.38	0.70
1:D:1161:PTR:HD2	1:D:1162:GLU:HG2	1.73	0.70
1:B:1052:SER:HA	1:B:1055:LYS:HD3	1.73	0.70
1:B:1163:THR:O	1:B:1164:ASP:HB2	1.92	0.68
1:A:1069:VAL:HG23	1:A:1078:ILE:HD11	1.76	0.68
1:C:1066:LEU:HB2	1:C:1078:ILE:HG22	1.76	0.67
1:D:1168:LYS:HE3	3:D:1375:HOH:O	1.95	0.67
1:C:1126:LEU:HD11	1:C:1154:PHE:HE1	1.60	0.66
1:B:1114:GLN:HA	1:B:1270:MET:CE	2.26	0.65
1:D:1073:GLN:CB	1:D:1074:PRO:CD	2.77	0.63
1:D:1073:GLN:HB3	1:D:1074:PRO:HD3	1.80	0.62
1:D:1133:HIS:HA	1:D:1157:THR:HG22	1.81	0.62
1:B:1127:ASN:HB3	3:B:219:HOH:O	1.99	0.62
1:A:1073:GLN:OE1	1:A:1074:PRO:HA	2.00	0.61
1:C:1109:LEU:O	1:C:1113:ILE:HG12	2.00	0.61
1:B:1126:LEU:HD11	1:B:1154:PHE:HE2	1.66	0.60
1:A:1161:PTR:O	1:A:1162:GLU:HB2	2.02	0.59
1:B:1041:MET:HE1	1:C:1246:ARG:HB3	1.83	0.59
1:A:1109:LEU:O	1:A:1113:ILE:HG12	2.04	0.58
1:C:1092:ARG:HG2	1:C:1209:ALA:HB3	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1134:ARG:NH2	1:D:1168:LYS:HE2	2.19	0.58
1:B:1121:ASP:HA	1:B:1263:ILE:HD11	1.84	0.57
1:B:1273:GLY:O	1:B:1276:GLU:HG2	2.04	0.57
1:C:996:ARG:NH1	1:C:1072:GLY:HA3	2.19	0.57
1:A:1115:MET:HG2	1:A:1149:VAL:HG21	1.86	0.57
1:C:1013:VAL:HG21	2:C:1:575:BR1	2.60	0.57
1:D:1062:VAL:HG13	1:D:1154:PHE:HZ	1.70	0.57
1:C:1115:MET:HG2	1:C:1149:VAL:HG21	1.86	0.57
1:D:1264:SER:HB3	1:D:1280:TYR:OH	2.05	0.57
1:C:996:ARG:HG2	1:C:1069:VAL:HG11	1.86	0.56
1:D:1161:PTR:O	1:D:1162:GLU:HB2	2.05	0.56
1:D:1069:VAL:HB	1:D:1076:LEU:HB2	1.87	0.56
1:D:1062:VAL:HG13	1:D:1154:PHE:CZ	2.40	0.56
1:D:1065:LEU:HD12	1:D:1066:LEU:N	2.21	0.56
1:B:1166:PTR:O1P	1:B:1166:PTR:HE1	2.06	0.56
1:B:1267:LYS:HA	1:B:1270:MET:HG3	1.88	0.55
1:C:1037:GLU:HA	1:C:1044:ARG:HH22	1.70	0.55
1:A:1163:THR:HG23	1:A:1165:PTR:CE2	2.36	0.55
1:B:1114:GLN:HA	1:B:1270:MET:HE1	1.88	0.55
1:C:1122:GLY:HA3	1:C:1151:ILE:HD12	1.89	0.55
1:C:1160:ILE:CG2	1:C:1164:ASP:HA	2.36	0.55
1:C:1023:LYS:O	1:C:1024:ASP:HB2	2.07	0.54
1:C:1113:ILE:HD11	1:C:1240:MET:HE1	1.90	0.54
1:A:992:TRP:NE1	1:A:1055:LYS:HD3	2.22	0.54
1:C:1243:GLU:O	1:C:1247:MET:HG3	2.07	0.54
1:D:992:TRP:CE2	1:D:1055:LYS:HG2	2.42	0.54
1:C:989:PRO:HB2	1:C:992:TRP:HD1	1.72	0.54
1:B:1176:VAL:HG23	3:B:106:HOH:O	2.06	0.54
1:C:989:PRO:O	1:C:991:GLU:N	2.33	0.54
1:C:1163:THR:HG23	1:C:1165:PTR:CE2	2.38	0.53
1:A:1222:LEU:O	1:A:1226:MET:HB2	2.08	0.53
1:D:1112:MET:CE	1:D:1206:ALA:HA	2.39	0.53
1:C:1163:THR:HG23	1:C:1165:PTR:CD2	2.38	0.53
1:D:1134:ARG:HH22	1:D:1168:LYS:NZ	2.05	0.53
1:A:1013:VAL:HG21	2:A:1:575:BR1	2.63	0.52
1:D:1184:LEU:HD22	1:D:1222:LEU:HD13	1.91	0.52
1:D:1163:THR:O	1:D:1164:ASP:HB2	2.09	0.52
1:B:1165:PTR:HE1	1:B:1165:PTR:O1P	2.09	0.52
1:C:1134:ARG:NH2	1:C:1156:MET:HG3	2.25	0.52
1:C:1115:MET:HG2	1:C:1149:VAL:CG2	2.40	0.52
1:D:1112:MET:HE3	1:D:1206:ALA:HA	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1034:THR:HG22	1:B:1076:LEU:HD22	1.92	0.51
1:D:1161:PTR:CE2	1:D:1162:GLU:HG2	2.40	0.51
1:B:1001:MET:HG2	1:B:1032:ILE:HD13	1.93	0.51
1:C:1126:LEU:HD11	1:C:1154:PHE:CE1	2.43	0.51
1:A:1161:PTR:O	1:A:1162:GLU:CB	2.58	0.51
1:B:1109:LEU:O	1:B:1113:ILE:HG12	2.10	0.51
1:B:992:TRP:CG	1:B:1055:LYS:HE3	2.47	0.50
1:B:1114:GLN:HA	1:B:1270:MET:HE2	1.93	0.50
1:D:1184:LEU:HD22	1:D:1222:LEU:CD1	2.42	0.50
1:D:1033:LYS:HE2	1:D:1079:MET:HG3	1.93	0.50
1:C:1160:ILE:O	1:C:1160:ILE:HG22	2.11	0.50
1:B:1045:ILE:HG22	1:C:1255:MET:HE3	1.93	0.50
1:A:992:TRP:CE2	1:A:1055:LYS:HD3	2.47	0.50
1:C:1127:ASN:OD1	1:C:1191:THR:HB	2.12	0.49
1:B:992:TRP:CD2	1:B:1055:LYS:HE3	2.47	0.49
1:B:1139:ARG:NH1	1:B:1175:PRO:HG2	2.27	0.49
1:D:1258:SER:O	1:D:1262:ILE:HG12	2.13	0.49
1:B:1041:MET:CE	1:C:1246:ARG:HB3	2.43	0.48
1:B:1241:LEU:O	1:B:1245:MET:HG3	2.14	0.48
1:B:1161:PTR:O	1:B:1161:PTR:CG	2.61	0.48
1:C:989:PRO:CG	1:C:1055:LYS:HE2	2.41	0.48
1:A:984:ALA:HB1	1:A:1070:SER:HB2	1.94	0.47
1:B:1087:LEU:HB3	1:B:1138:ALA:O	2.13	0.47
1:A:1201:VAL:O	1:A:1205:ILE:HG13	2.14	0.47
1:B:1139:ARG:HH12	1:B:1175:PRO:HG2	1.78	0.47
1:A:1101:ASN:N	3:A:408:HOH:O	2.47	0.47
1:C:1036:ASN:O	1:C:1037:GLU:HB3	2.14	0.47
1:C:1162:GLU:O	1:C:1163:THR:CB	2.63	0.47
1:B:1243:GLU:O	1:B:1247:MET:HG3	2.15	0.47
1:D:1109:LEU:HD13	1:D:1238:PRO:HG2	1.97	0.47
1:D:1243:GLU:O	1:D:1247:MET:HG3	2.14	0.47
1:C:1160:ILE:O	1:C:1160:ILE:CG2	2.63	0.47
1:A:1133:HIS:O	1:A:1134:ARG:HB2	2.15	0.47
1:C:1163:THR:HG22	1:C:1165:PTR:N	2.30	0.47
1:C:1139:ARG:NH2	1:C:1175:PRO:HG3	2.30	0.46
1:B:1184:LEU:HD22	1:B:1222:LEU:HD12	1.97	0.46
1:A:1236:ASN:HB3	1:D:1074:PRO:HD3	1.98	0.46
1:C:992:TRP:CG	1:C:1055:LYS:HE3	2.51	0.46
1:B:1222:LEU:O	1:B:1226:MET:HB2	2.16	0.46
1:C:1063:VAL:HG21	1:C:1142:MET:HG3	1.97	0.46
1:D:1092:ARG:HE	1:D:1095:ARG:NH2	2.13	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1065:LEU:C	1:D:1065:LEU:HD12	2.37	0.45
1:A:1112:MET:CE	1:A:1205:ILE:HG22	2.46	0.45
1:D:1163:THR:HG22	1:D:1165:PTR:N	2.32	0.45
1:C:996:ARG:HG2	1:C:1069:VAL:CG1	2.47	0.45
1:C:996:ARG:HG3	3:C:298:HOH:O	2.17	0.45
1:B:1113:ILE:HG21	1:B:1269:GLU:HB2	1.99	0.45
1:D:992:TRP:CZ2	1:D:1055:LYS:HG2	2.52	0.45
1:D:1134:ARG:HH21	1:D:1168:LYS:HE2	1.82	0.44
1:A:1163:THR:HG22	1:A:1165:PTR:N	2.33	0.44
1:C:1234:PRO:HB2	1:C:1237:CYS:HB2	1.97	0.44
1:B:1095:ARG:HA	1:B:1096:PRO:HD3	1.88	0.44
1:A:1142:MET:HB3	1:A:1142:MET:HE3	1.79	0.44
1:C:996:ARG:HH11	1:C:1072:GLY:HA3	1.83	0.44
1:D:1073:GLN:CB	1:D:1074:PRO:HD2	2.45	0.44
1:D:1073:GLN:HB3	1:D:1074:PRO:HD2	1.93	0.44
1:C:1160:ILE:HG23	1:C:1164:ASP:HA	1.99	0.44
1:D:996:ARG:HB3	1:D:1069:VAL:CG1	2.43	0.44
1:C:1054:MET:CE	1:C:1154:PHE:HD2	2.30	0.44
1:A:989:PRO:HD2	1:A:1055:LYS:HE3	1.98	0.44
1:D:1146:ASP:O	1:D:1147:PHE:HB2	2.18	0.44
1:C:1033:LYS:HE2	1:C:1079:MET:HG3	2.00	0.44
1:A:1166:PTR:O1P	1:A:1166:PTR:HE1	2.17	0.44
1:A:1235:ASP:O	1:A:1236:ASN:HB2	2.18	0.43
1:C:1092:ARG:NH2	1:C:1095:ARG:NH1	2.65	0.43
1:B:1021:VAL:HG23	1:B:1022:VAL:HG23	2.01	0.43
1:B:1054:MET:HE3	1:B:1154:PHE:HD1	1.84	0.43
1:C:1035:VAL:O	1:C:1037:GLU:N	2.51	0.43
1:C:988:VAL:CG2	1:C:1048:LEU:HD22	2.49	0.43
1:C:1052:SER:HA	1:C:1055:LYS:HD2	2.01	0.43
1:A:1126:LEU:HD11	1:A:1154:PHE:HE2	1.84	0.43
1:B:1163:THR:HG1	1:B:1164:ASP:H	1.65	0.43
1:D:994:VAL:O	1:D:1069:VAL:HG22	2.19	0.43
1:C:1126:LEU:CD1	1:C:1154:PHE:HE1	2.31	0.43
1:B:1146:ASP:O	1:B:1147:PHE:HB2	2.18	0.42
1:B:1130:LYS:HA	1:B:1130:LYS:HD3	1.91	0.42
1:C:1163:THR:O	1:C:1164:ASP:HB2	2.19	0.42
1:A:988:VAL:HA	1:A:989:PRO:HD3	1.91	0.42
3:A:230:HOH:O	1:D:980:SER:HB2	2.19	0.42
1:B:986:VAL:HG22	1:C:1265:SER:CB	2.49	0.42
1:B:1025:GLU:HA	1:B:1026:PRO:HD3	1.90	0.42
1:D:1130:LYS:HA	1:D:1130:LYS:HD3	1.75	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1161:PTR:HD2	1:D:1162:GLU:CG	2.47	0.42
1:A:1163:THR:O	1:A:1164:ASP:HB2	2.20	0.42
1:A:1241:LEU:HA	1:A:1241:LEU:HD23	1.88	0.42
1:C:996:ARG:NH2	1:C:1074:PRO:HD2	2.35	0.42
1:C:988:VAL:HA	1:C:989:PRO:HD3	1.84	0.42
1:D:1115:MET:HG2	1:D:1149:VAL:HG21	2.01	0.42
1:D:988:VAL:HA	1:D:989:PRO:HD3	1.87	0.42
1:A:1236:ASN:O	1:D:1073:GLN:HG2	2.20	0.42
1:B:1069:VAL:HG23	1:B:1078:ILE:HD11	2.01	0.42
1:C:1241:LEU:O	1:C:1245:MET:HG3	2.19	0.42
1:C:1121:ASP:HA	1:C:1263:ILE:HD11	2.01	0.42
1:A:1112:MET:HE3	1:A:1205:ILE:HG22	2.02	0.41
1:B:1276:GLU:HG3	1:B:1277:VAL:HG13	2.03	0.41
1:B:1045:ILE:HG22	1:C:1255:MET:CE	2.50	0.41
2:A:1:575:H15	2:A:1:575:H12	1.91	0.41
1:B:988:VAL:HA	1:B:989:PRO:HD3	1.89	0.41
1:A:1069:VAL:HB	1:A:1076:LEU:HB2	2.02	0.41
1:A:1130:LYS:HD3	1:A:1130:LYS:HA	1.93	0.41
1:B:1196:TRP:CE3	1:B:1249:TRP:HA	2.56	0.41
1:B:1193:SER:HB2	3:B:350:HOH:O	2.20	0.41
1:B:993:GLU:HA	1:B:1068:VAL:O	2.20	0.41
1:D:1107:PRO:HD3	1:D:1208:LEU:HD21	2.03	0.41
1:C:1146:ASP:O	1:C:1147:PHE:HB2	2.21	0.40
1:A:1034:THR:HG22	1:A:1076:LEU:CD2	2.51	0.40
1:B:1174:LEU:HA	1:B:1175:PRO:HD3	1.91	0.40
1:C:1026:PRO:HB2	1:C:1027:GLU:H	1.75	0.40
1:A:1022:VAL:HG12	1:A:1023:LYS:N	2.37	0.40
1:B:992:TRP:CH2	1:B:1055:LYS:HB3	2.56	0.40
1:C:1106:PRO:HA	1:C:1107:PRO:HD3	1.84	0.40
1:C:1196:TRP:CE3	1:C:1249:TRP:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	296/308 (96%)	287 (97%)	8 (3%)	1 (0%)	46	68
1	B	292/308 (95%)	282 (97%)	8 (3%)	2 (1%)	26	46
1	C	292/308 (95%)	277 (95%)	10 (3%)	5 (2%)	11	19
1	D	289/308 (94%)	278 (96%)	10 (4%)	1 (0%)	46	68
All	All	1169/1232 (95%)	1124 (96%)	36 (3%)	9 (1%)	24	41

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1073	GLN
1	A	1162	GLU
1	C	990	ASP
1	C	1163	THR
1	C	1026	PRO
1	C	1036	ASN
1	B	1163	THR
1	B	1026	PRO
1	C	1024	ASP

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	261/265 (98%)	255 (98%)	6 (2%)	58	83
1	B	257/265 (97%)	252 (98%)	5 (2%)	65	87
1	C	257/265 (97%)	250 (97%)	7 (3%)	52	79
1	D	255/265 (96%)	248 (97%)	7 (3%)	52	79
All	All	1030/1060 (97%)	1005 (98%)	25 (2%)	57	82

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	994	VAL
1	A	1048	LEU
1	A	1162	GLU
1	A	1201	VAL
1	A	1222	LEU
1	A	1276	GLU
1	B	980	SER
1	B	1000	THR
1	B	1003	ARG
1	B	1132	VAL
1	B	1176	VAL
1	C	990	ASP
1	C	1000	THR
1	C	1068	VAL
1	C	1163	THR
1	C	1168	LYS
1	C	1176	VAL
1	C	1201	VAL
1	D	980	SER
1	D	1002	SER
1	D	1065	LEU
1	D	1126	LEU
1	D	1132	VAL
1	D	1188	VAL
1	D	1201	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1036	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	A	1161	1	11,12,17	0.53	0	12,15,24	0.63	1 (8%)
1	PTR	A	1165	1	14,16,17	1.90	1 (7%)	18,22,24	0.67	0
1	PTR	A	1166	1	14,16,17	1.87	1 (7%)	18,22,24	0.69	0
1	PTR	B	1161	1	11,12,17	0.37	0	12,15,24	0.67	0
1	PTR	B	1165	1	14,16,17	1.84	1 (7%)	18,22,24	0.72	0
1	PTR	B	1166	1	14,16,17	1.85	1 (7%)	18,22,24	0.84	1 (5%)
1	PTR	C	1161	1	14,16,17	1.85	1 (7%)	18,22,24	0.64	0
1	PTR	C	1165	1	14,16,17	1.91	1 (7%)	18,22,24	0.70	0
1	PTR	C	1166	1	14,16,17	1.87	1 (7%)	18,22,24	0.68	0
1	PTR	D	1161	1	14,16,17	1.90	1 (7%)	18,22,24	0.68	0
1	PTR	D	1165	1	14,16,17	1.87	1 (7%)	18,22,24	0.63	0
1	PTR	D	1166	1	14,16,17	1.87	1 (7%)	18,22,24	0.67	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
1	PTR	A	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	A	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	A	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1161	1	-	0/4/6/13	0/1/1/1
1	PTR	B	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	B	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1161	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	C	1166	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1161	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1165	1	-	0/9/11/13	0/1/1/1
1	PTR	D	1166	1	-	0/9/11/13	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1165	PTR	OH-CZ	-7.03	1.23	1.40
1	A	1165	PTR	OH-CZ	-7.00	1.23	1.40
1	D	1161	PTR	OH-CZ	-6.98	1.23	1.40
1	D	1165	PTR	OH-CZ	-6.89	1.24	1.40
1	C	1166	PTR	OH-CZ	-6.87	1.24	1.40
1	A	1166	PTR	OH-CZ	-6.85	1.24	1.40
1	D	1166	PTR	OH-CZ	-6.83	1.24	1.40
1	C	1161	PTR	OH-CZ	-6.81	1.24	1.40
1	B	1166	PTR	OH-CZ	-6.67	1.24	1.40
1	B	1165	PTR	OH-CZ	-6.60	1.24	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1166	PTR	O-C-CA	-2.14	119.92	125.49
1	A	1161	PTR	O-C-CA	-2.08	120.07	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1161	PTR	2	0
1	A	1165	PTR	2	0
1	A	1166	PTR	1	0
1	B	1161	PTR	1	0
1	B	1165	PTR	1	0
1	B	1166	PTR	1	0
1	C	1165	PTR	3	0
1	D	1161	PTR	5	0
1	D	1165	PTR	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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	575	A	1	-	30,30,30	1.22	6 (20%)	42,42,42	1.39	5 (11%)
2	575	B	1	-	30,30,30	1.24	6 (20%)	42,42,42	1.38	6 (14%)
2	575	C	1	-	30,30,30	1.27	6 (20%)	42,42,42	1.39	7 (16%)
2	575	D	1	-	30,30,30	1.24	6 (20%)	42,42,42	1.27	4 (9%)

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	575	A	1	-	-	0/8/32/32	0/4/4/4
2	575	B	1	-	-	0/8/32/32	0/4/4/4
2	575	C	1	-	-	0/8/32/32	0/4/4/4
2	575	D	1	-	-	0/8/32/32	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	575	C12-C13	-2.69	1.35	1.40
2	C	1	575	C12-C13	-2.58	1.35	1.40
2	D	1	575	C12-C13	-2.57	1.35	1.40
2	A	1	575	C12-C13	-2.52	1.35	1.40
2	B	1	575	C12-N2	2.00	1.37	1.32
2	A	1	575	C12-N2	2.00	1.37	1.32
2	D	1	575	C7-N1	2.01	1.51	1.47
2	D	1	575	C12-N2	2.04	1.37	1.32
2	A	1	575	C11-N1	2.09	1.51	1.47
2	C	1	575	C12-N2	2.13	1.38	1.32
2	B	1	575	C11-N1	2.15	1.51	1.47
2	B	1	575	C7-N1	2.23	1.51	1.47
2	C	1	575	C11-N1	2.25	1.51	1.47
2	C	1	575	C7-N1	2.26	1.51	1.47
2	A	1	575	C7-N1	2.28	1.51	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	575	C11-N1	2.37	1.52	1.47
2	B	1	575	C8-N1	2.47	1.52	1.47
2	A	1	575	C8-N1	2.52	1.52	1.47
2	D	1	575	C8-N1	2.60	1.52	1.47
2	C	1	575	C8-N1	2.77	1.52	1.47
2	C	1	575	C13-C21	2.90	1.50	1.44
2	A	1	575	C13-C21	2.95	1.50	1.44
2	B	1	575	C13-C21	2.97	1.50	1.44
2	D	1	575	C13-C21	3.07	1.50	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	575	C12-C13-C21	-3.06	116.91	119.39
2	A	1	575	C10-C11-N1	-2.27	101.33	103.91
2	C	1	575	C12-C13-C21	-2.24	117.57	119.39
2	B	1	575	C10-C11-N1	-2.23	101.38	103.91
2	C	1	575	C11-N1-C8	2.06	106.20	104.08
2	D	1	575	O1-C20-N3	2.18	123.21	120.59
2	C	1	575	C6-C7-N1	2.36	117.74	113.16
2	C	1	575	C7-N1-C11	2.42	116.79	113.10
2	C	1	575	C14-C13-C12	2.47	122.79	120.39
2	B	1	575	C6-C7-N1	2.48	117.96	113.16
2	A	1	575	C21-N3-C20	2.61	128.72	125.49
2	C	1	575	C21-N3-C20	2.67	128.79	125.49
2	D	1	575	C21-N3-C20	2.69	128.82	125.49
2	B	1	575	C21-N3-C20	2.77	128.92	125.49
2	A	1	575	C7-N1-C11	2.88	117.49	113.10
2	D	1	575	C11-N1-C8	3.01	107.17	104.08
2	B	1	575	C7-N1-C11	3.03	117.72	113.10
2	A	1	575	C6-C7-N1	3.14	119.24	113.16
2	C	1	575	C13-C12-N2	3.82	130.75	123.91
2	B	1	575	C13-C12-N2	4.03	131.13	123.91
2	D	1	575	C13-C12-N2	4.19	131.42	123.91
2	A	1	575	C13-C12-N2	4.78	132.47	123.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	575	2	0
2	C	1	575	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	300/308 (97%)	-0.52	3 (1%) 84 86	17, 27, 50, 80	0
1	B	296/308 (96%)	-0.44	2 (0%) 89 90	19, 31, 54, 77	0
1	C	296/308 (96%)	-0.37	4 (1%) 78 80	20, 31, 57, 73	0
1	D	293/308 (95%)	-0.44	2 (0%) 89 90	19, 30, 48, 70	0
All	All	1185/1232 (96%)	-0.44	11 (0%) 85 88	17, 30, 53, 80	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1023	LYS	3.4
1	D	1170	GLY	3.3
1	B	1023	LYS	3.2
1	C	1073	GLN	2.7
1	A	1162	GLU	2.6
1	C	1024	ASP	2.4
1	C	997	GLU	2.4
1	D	1162	GLU	2.4
1	C	1056	GLU	2.3
1	A	1024	ASP	2.1
1	B	1024	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	PTR	D	1166	16/17	0.95	0.13	-	26,33,42,46	0
1	PTR	A	1166	16/17	0.97	0.11	-	23,32,42,43	0
1	PTR	C	1166	16/17	0.95	0.12	-	28,33,49,49	0
1	PTR	B	1165	16/17	0.93	0.12	-	31,40,54,57	0
1	PTR	A	1165	16/17	0.96	0.10	-	26,33,45,49	0
1	PTR	B	1161	12/17	0.85	0.28	-	40,58,69,71	0
1	PTR	C	1165	16/17	0.96	0.12	-	32,38,46,49	0
1	PTR	D	1161	16/17	0.86	0.20	-	35,59,84,94	0
1	PTR	A	1161	12/17	0.86	0.21	-	29,48,57,60	0
1	PTR	C	1161	16/17	0.75	0.27	-	41,65,84,95	0
1	PTR	D	1165	16/17	0.96	0.10	-	26,33,48,51	0
1	PTR	B	1166	16/17	0.96	0.14	-	25,34,42,44	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	575	C	1	27/27	0.96	0.14	0.79	27,33,39,63	0
2	575	D	1	27/27	0.95	0.14	0.65	24,27,41,55	0
2	575	B	1	27/27	0.96	0.13	0.33	27,31,38,53	0
2	575	A	1	27/27	0.96	0.10	-0.65	18,22,31,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.