Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 03:24 PM EDT

PDB ID	:	3LVP
Title	:	Crystal structure of bisphosphorylated IGF1-R Kinase domain (2P) in complex with a bis-azaindole inhibitor
Authors	:	Maignan, S.; Marquette, J.P.; Guilloteau, J.P.
Deposited on	:	2010-02-22
Resolution	:	3.00 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 (i) 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 (i)) were used in the production of this report:

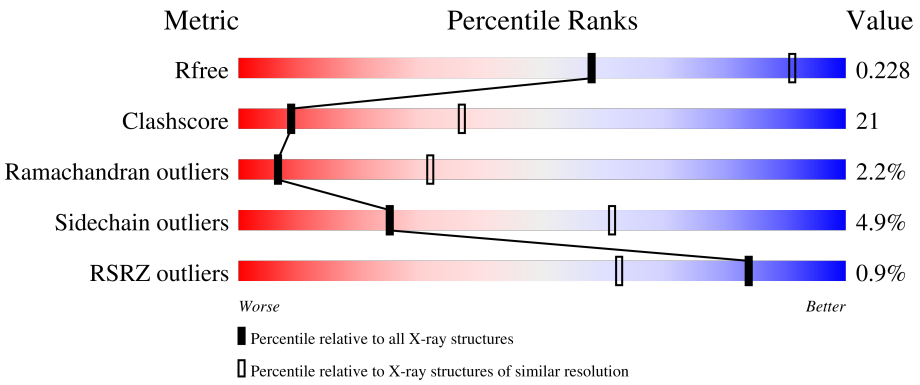
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	336	51% 32% • 14%
1	B	336	52% 33% • 12%
1	C	336	.% 48% 36% • 13%
1	D	336	2% 46% 36% • 16%

2 Entry composition (i)

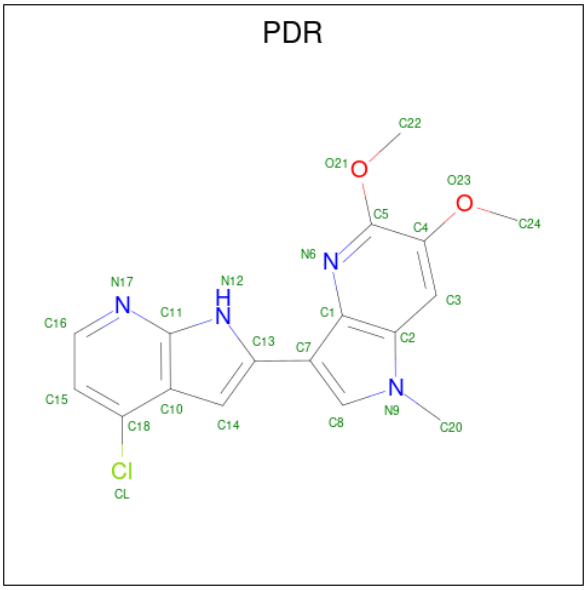
There are 5 unique types of molecules in this entry. The entry contains 9405 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	289	2300	1461	384	432	23	63	0	0
1	B	295	2360	1502	393	443	22	38	0	0
1	C	293	2355	1499	392	442	22	50	0	0
1	D	282	2259	1442	372	424	21	55	0	0

- Molecule 2 is 3-(4-chloro-1H-pyrrolo[2,3-b]pyridin-2-yl)-5,6-dimethoxy-1-methyl-1H-pyrrolo[3,2-b]pyridine (three-letter code: PDR) (formula: $C_{17}H_{15}ClN_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	A	1	24	17	1	4	2	0	0
2	B	1	24	17	1	4	2	0	0

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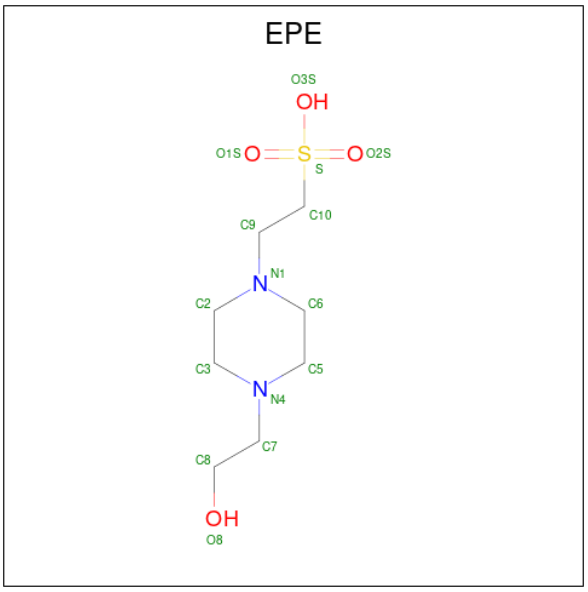
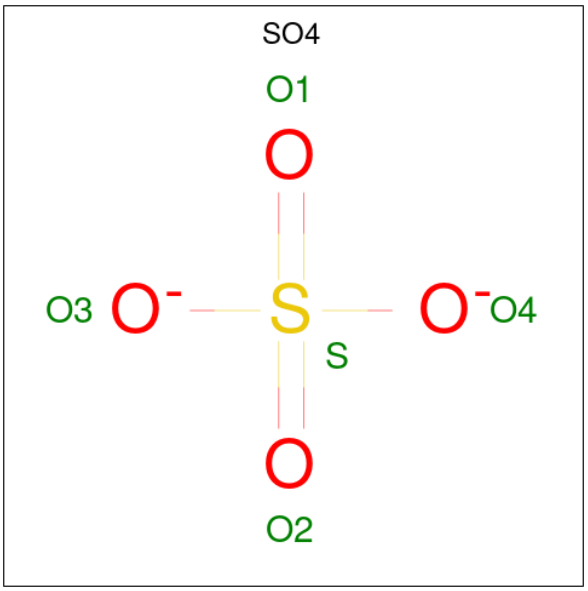
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
2	C	1	24	17	1	4	2	0	0
			Total	C	Cl	N	O		
2	D	1	24	17	1	4	2	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

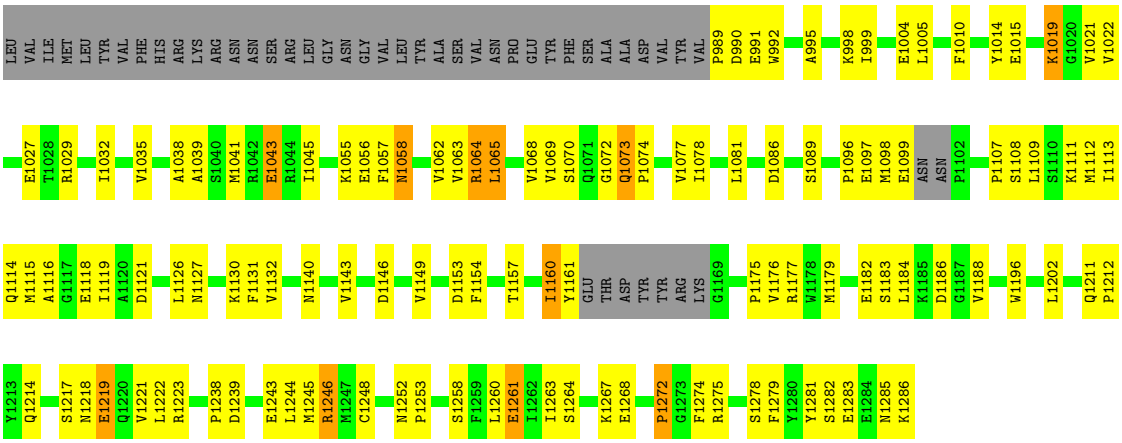
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total O 4 4	0	0
5	B	4	Total O 4 4	0	0
5	C	2	Total O 2 2	0	0
5	D	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

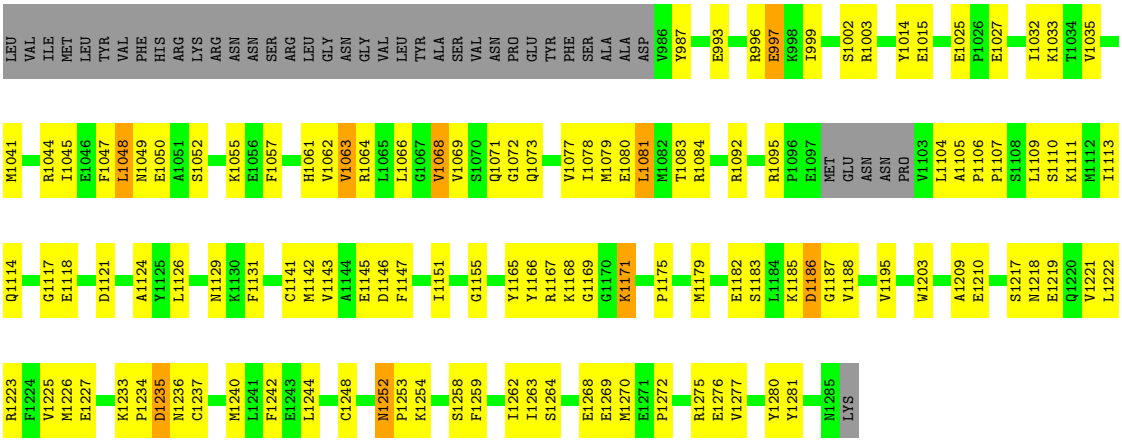
• Molecule 1: Insulin-like growth factor 1 receptor

Chain A: 51% 32% • 14%



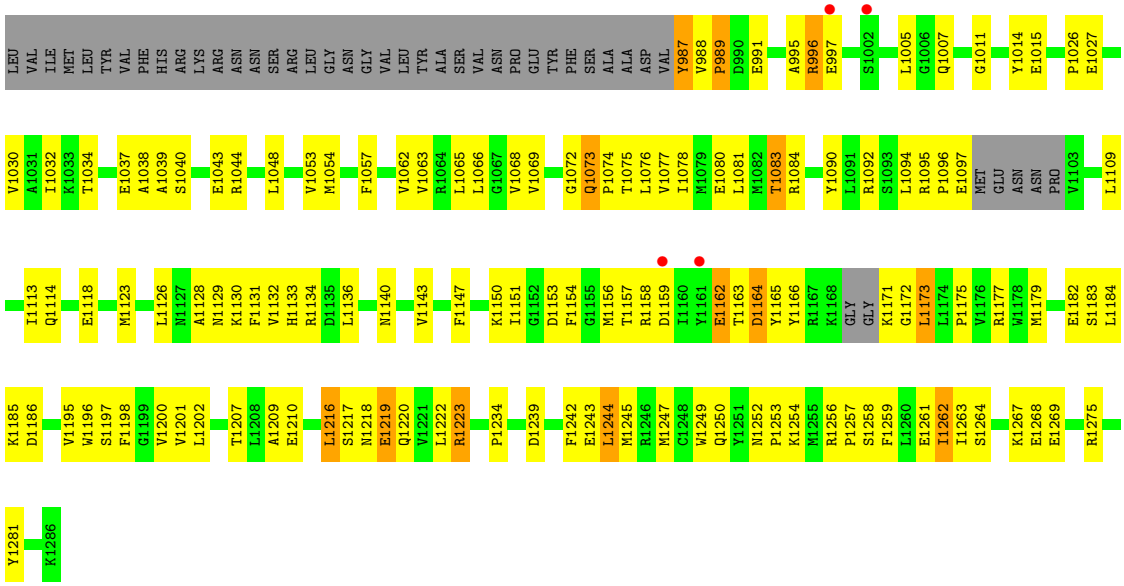
• Molecule 1: Insulin-like growth factor 1 receptor

Chain B: 52% 33% • 12%



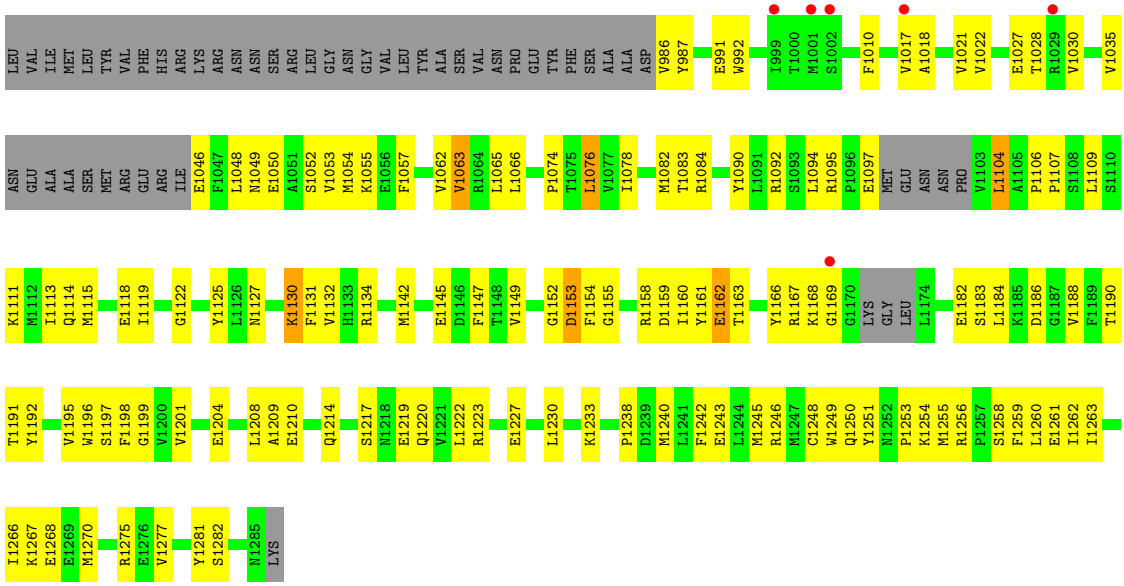
• Molecule 1: Insulin-like growth factor 1 receptor

Chain C: % 48% 36% • 13%



- Molecule 1: Insulin-like growth factor 1 receptor

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.95Å 94.95Å 322.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 53.33 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 98.6 (53.33-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.279 0.217 , 0.228	Depositor DCC
R_{free} test set	1529 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 59.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9405	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PDR, EPE, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.38	0/2347	0.62	0/3159
1	B	0.41	0/2410	0.63	0/3251
1	C	0.42	0/2404	0.62	1/3239 (0.0%)
1	D	0.38	0/2307	0.58	0/3112
All	All	0.40	0/9468	0.61	1/12761 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1216	LEU	CA-CB-CG	5.14	127.12	115.30

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	2300	0	2276	87	0
1	B	2360	0	2328	85	0
1	C	2355	0	2325	110	0
1	D	2259	0	2220	104	0
2	A	24	0	15	1	0
2	B	24	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	15	1	0
2	D	24	0	15	0	0
3	A	12	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	2	0	0	0	0
5	D	3	0	0	0	0
All	All	9405	0	9221	374	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 21.

All (374) 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:1066:LEU:HB2	1:B:1078:ILE:HG22	1.45	0.98
1:C:1162:GLU:HG2	1:C:1163:THR:H	1.30	0.94
1:A:1073:GLN:HB3	1:A:1074:PRO:CD	2.01	0.91
1:C:996:ARG:HB3	1:C:1069:VAL:HG11	1.56	0.88
1:C:996:ARG:CZ	1:C:1073:GLN:HB2	2.05	0.86
1:C:1081:LEU:HD21	1:C:1083:THR:HG23	1.60	0.83
1:C:1109:LEU:O	1:C:1113:ILE:HG12	1.78	0.83
1:A:1246:ARG:HH11	1:A:1246:ARG:HB3	1.45	0.82
1:A:1073:GLN:HB3	1:A:1074:PRO:HD3	1.62	0.81
1:D:1046:GLU:HA	1:D:1049:ASN:HD22	1.43	0.81
1:A:1140:ASN:HB3	1:A:1153:ASP:HB3	1.61	0.80
1:D:1046:GLU:HA	1:D:1049:ASN:ND2	1.96	0.80
1:A:1041:MET:HG3	1:A:1045:ILE:HD11	1.62	0.80
1:D:1258:SER:O	1:D:1262:ILE:HG12	1.82	0.80
1:B:1221:VAL:O	1:B:1225:VAL:HG12	1.82	0.80
1:A:1186:ASP:HB2	1:A:1188:VAL:HG23	1.65	0.79
1:A:1045:ILE:HD12	1:A:1045:ILE:H	1.47	0.78
1:B:1171:LYS:CB	1:C:1219:GLU:HG3	2.14	0.78
1:B:1113:ILE:HG21	1:B:1269:GLU:HB2	1.66	0.77
1:D:1198:PHE:O	1:D:1201:VAL:HG22	1.85	0.77
1:A:1068:VAL:HG23	1:A:1077:VAL:HG22	1.67	0.76
1:C:1066:LEU:HB2	1:C:1078:ILE:HG22	1.65	0.76
1:B:1171:LYS:HB2	1:C:1219:GLU:HG3	1.67	0.75
1:B:1114:GLN:O	1:B:1118:GLU:HG3	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1252:ASN:C	1:B:1252:ASN:HD22	1.92	0.73
1:B:1109:LEU:O	1:B:1113:ILE:HG12	1.89	0.72
1:C:1158:ARG:HG2	1:C:1166:TYR:CE2	2.25	0.72
1:D:1109:LEU:O	1:D:1113:ILE:HG12	1.90	0.72
1:B:1111:LYS:HE2	1:B:1111:LYS:HA	1.73	0.70
1:D:1230:LEU:HD21	1:D:1249:TRP:HB3	1.74	0.69
1:A:995:ALA:HB3	1:A:998:LYS:HG3	1.73	0.69
1:B:1186:ASP:HB3	1:C:1092:ARG:NH2	2.07	0.69
1:C:1223:ARG:HD2	1:D:1223:ARG:HH21	1.55	0.69
1:A:1073:GLN:CB	1:A:1074:PRO:CD	2.70	0.69
1:B:1264:SER:HB2	1:B:1280:TYR:OH	1.93	0.69
1:B:1252:ASN:HD22	1:B:1253:PRO:N	1.91	0.69
1:D:1104:LEU:H	1:D:1104:LEU:HD22	1.55	0.69
1:D:1217:SER:OG	1:D:1220:GLN:HG3	1.93	0.68
1:C:1252:ASN:HD21	1:C:1254:LYS:HG2	1.58	0.67
1:C:1092:ARG:HG3	1:C:1209:ALA:HB3	1.76	0.67
1:C:1275:ARG:HA	1:C:1281:TYR:HD1	1.58	0.66
1:B:1185:LYS:HA	1:B:1226:MET:HE3	1.76	0.66
1:A:1021:VAL:HG23	1:A:1022:VAL:HG23	1.78	0.66
1:D:1275:ARG:HA	1:D:1281:TYR:CD1	2.32	0.65
1:C:1162:GLU:HG2	1:C:1163:THR:N	2.08	0.65
1:A:1132:VAL:HG23	1:A:1160:ILE:HG22	1.79	0.64
1:B:1252:ASN:ND2	1:B:1254:LYS:H	1.95	0.64
1:A:1239:ASP:O	1:A:1243:GLU:HG3	1.98	0.64
1:C:1114:GLN:O	1:C:1118:GLU:HG3	1.97	0.64
1:D:1132:VAL:HG12	1:D:1158:ARG:O	1.98	0.64
1:D:1186:ASP:O	1:D:1188:VAL:HG23	1.98	0.64
1:C:1252:ASN:HD21	1:C:1254:LYS:CG	2.11	0.63
1:A:1121:ASP:HA	1:A:1263:ILE:HD11	1.80	0.63
1:B:1033:LYS:HD3	1:B:1079:MET:CE	2.29	0.63
1:D:1250:GLN:O	1:D:1256:ARG:HD2	1.99	0.63
1:C:1217:SER:OG	1:C:1220:GLN:HG3	1.99	0.63
1:B:1146:ASP:O	1:B:1147:PHE:HB2	1.99	0.62
1:A:1004:GLU:HG2	1:A:1014:TYR:CE1	2.34	0.62
1:C:1166:TYR:OH	1:C:1171:LYS:HG3	2.00	0.62
1:B:1275:ARG:HA	1:B:1281:TYR:CD1	2.34	0.62
1:A:1279:PHE:O	1:A:1282:SER:HB3	2.01	0.61
1:D:1078:ILE:HD12	1:D:1078:ILE:N	2.14	0.61
1:B:1186:ASP:HB2	1:B:1188:VAL:HG23	1.83	0.61
1:C:1123:MET:HG2	1:C:1151:ILE:HD11	1.83	0.61
1:C:1223:ARG:HB3	1:D:1223:ARG:NH2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1182:GLU:HG2	1:B:1183:SER:N	2.16	0.60
1:A:1176:VAL:HG21	1:A:1218:ASN:HB3	1.83	0.60
1:D:1114:GLN:HE21	1:D:1118:GLU:CD	2.03	0.60
1:C:1073:GLN:HB3	1:C:1074:PRO:CD	2.31	0.60
1:D:1267:LYS:O	1:D:1270:MET:HB2	2.00	0.60
1:B:1025:GLU:HG2	1:B:1027:GLU:O	2.01	0.60
1:D:1184:LEU:HD13	1:D:1222:LEU:HD22	1.84	0.60
1:A:1005:LEU:O	2:A:1:PDR:H24B	2.01	0.60
1:A:1217:SER:O	1:A:1221:VAL:HG23	2.02	0.60
1:B:1203:TRP:HZ3	1:B:1210:GLU:O	1.85	0.59
1:D:1057:PHE:HE1	1:D:1131:PHE:CD2	2.20	0.59
1:B:1050:GLU:OE1	1:B:1155:GLY:HA2	2.02	0.59
1:D:1021:VAL:HG23	1:D:1022:VAL:HG23	1.83	0.59
1:C:1096:PRO:HG2	1:C:1097:GLU:OE1	2.02	0.59
1:D:1066:LEU:HD12	1:D:1078:ILE:HG22	1.84	0.59
1:A:1219:GLU:HG2	1:A:1223:ARG:NH1	2.18	0.58
1:D:1227:GLU:OE1	1:D:1227:GLU:HA	2.04	0.58
1:B:1183:SER:O	1:B:1187:GLY:HA2	2.04	0.58
1:D:1168:LYS:CD	1:D:1169:GLY:H	2.17	0.58
1:B:1252:ASN:C	1:B:1252:ASN:ND2	2.55	0.57
1:C:1014:TYR:HB2	1:C:1032:ILE:HB	1.85	0.57
1:C:1252:ASN:HD22	1:C:1253:PRO:HD2	1.70	0.57
1:A:1004:GLU:HG2	1:A:1014:TYR:HE1	1.68	0.57
1:C:1073:GLN:HB3	1:C:1074:PRO:HD2	1.86	0.57
1:C:1158:ARG:HH21	1:C:1171:LYS:HB2	1.70	0.57
1:D:1248:CYS:O	1:D:1256:ARG:HG2	2.05	0.57
1:D:1054:MET:HB3	1:D:1065:LEU:HB2	1.88	0.56
1:D:1258:SER:OG	1:D:1261:GLU:HG3	2.06	0.56
1:A:1108:SER:O	1:A:1112:MET:HG3	2.05	0.56
1:C:987:TYR:O	1:C:989:PRO:HD3	2.06	0.56
1:D:1168:LYS:HD3	1:D:1169:GLY:H	1.68	0.56
1:A:1114:GLN:O	1:A:1118:GLU:HG3	2.06	0.56
1:C:1185:LYS:HG2	1:C:1186:ASP:OD1	2.05	0.56
1:A:1107:PRO:HB2	1:A:1112:MET:HG2	1.87	0.56
1:C:1048:LEU:HD11	1:C:1075:THR:HG21	1.86	0.56
1:B:1052:SER:HA	1:B:1055:LYS:HD2	1.87	0.55
1:A:1109:LEU:C	1:A:1109:LEU:HD13	2.26	0.55
1:C:995:ALA:C	1:C:997:GLU:H	2.08	0.55
1:A:1072:GLY:O	1:A:1073:GLN:O	2.25	0.55
1:C:1113:ILE:HG21	1:C:1269:GLU:HB2	1.88	0.55
1:A:1032:ILE:HD12	1:A:1078:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1275:ARG:HA	1:D:1281:TYR:HD1	1.71	0.55
1:C:987:TYR:CD1	1:C:987:TYR:N	2.75	0.54
1:A:1109:LEU:O	1:A:1113:ILE:HG12	2.08	0.54
1:B:1045:ILE:HG22	1:B:1049:ASN:ND2	2.23	0.54
1:C:1131:PHE:CE1	1:C:1159:ASP:HB3	2.43	0.54
1:A:1182:GLU:HG2	1:A:1183:SER:N	2.23	0.54
1:C:1202:LEU:HD11	1:C:1244:LEU:HD13	1.89	0.54
1:B:1227:GLU:HA	1:B:1227:GLU:OE1	2.07	0.54
1:C:1007:GLN:HE22	1:C:1011:GLY:HA2	1.72	0.54
1:A:1015:GLU:CD	1:A:1029:ARG:NH1	2.62	0.53
1:C:1128:ALA:C	1:C:1130:LYS:H	2.11	0.53
1:D:1259:PHE:O	1:D:1263:ILE:HG13	2.09	0.53
1:A:1015:GLU:OE2	1:A:1029:ARG:NH1	2.42	0.53
1:C:1196:TRP:O	1:C:1197:SER:C	2.47	0.53
1:A:992:TRP:CD1	1:A:1055:LYS:HD3	2.44	0.53
1:D:987:TYR:CD2	1:D:1048:LEU:HD13	2.44	0.53
1:A:1126:LEU:O	1:A:1131:PHE:HB2	2.09	0.53
1:C:1162:GLU:CG	1:C:1163:THR:H	2.06	0.53
1:B:1062:VAL:O	1:B:1063:VAL:C	2.47	0.53
1:D:1050:GLU:HG3	1:D:1155:GLY:HA2	1.91	0.52
1:D:1196:TRP:O	1:D:1199:GLY:N	2.41	0.52
1:D:1233:LYS:HD2	1:D:1242:PHE:CD2	2.44	0.52
1:C:1080:GLU:OE1	1:C:1150:LYS:NZ	2.34	0.52
1:B:1002:SER:HB2	1:B:1015:GLU:O	2.09	0.52
1:C:1063:VAL:HG23	1:C:1151:ILE:O	2.10	0.52
1:D:1275:ARG:NH2	1:D:1275:ARG:HB2	2.25	0.52
1:A:1175:PRO:O	1:A:1179:MET:HG3	2.10	0.52
1:B:1175:PRO:O	1:B:1179:MET:HG3	2.09	0.52
1:C:1207:THR:HB	1:C:1210:GLU:HG3	1.90	0.52
1:B:1033:LYS:HD3	1:B:1079:MET:HE2	1.92	0.52
1:D:1053:VAL:HG12	1:D:1057:PHE:CE2	2.45	0.52
1:D:1109:LEU:HD23	1:D:1238:PRO:HB3	1.91	0.52
1:D:1275:ARG:HG3	1:D:1281:TYR:CG	2.45	0.52
1:C:1223:ARG:CD	1:D:1223:ARG:HD3	2.40	0.51
1:C:1259:PHE:O	1:C:1262:ILE:HB	2.10	0.51
1:B:1186:ASP:HB3	1:C:1092:ARG:CZ	2.40	0.51
1:C:1223:ARG:HD2	1:D:1223:ARG:NH2	2.25	0.51
1:C:1040:SER:O	1:C:1043:GLU:HB2	2.10	0.51
1:C:1219:GLU:O	1:C:1223:ARG:HG3	2.11	0.51
1:B:1182:GLU:HG2	1:B:1183:SER:H	1.76	0.51
1:C:1258:SER:OG	1:C:1261:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1119:ILE:HD11	1:D:1149:VAL:HG11	1.93	0.51
1:A:1282:SER:O	1:A:1286:LYS:HB2	2.11	0.51
1:B:1003:ARG:HG3	1:B:1003:ARG:HH11	1.76	0.51
1:A:1143:VAL:HG22	1:A:1149:VAL:HG22	1.92	0.51
1:A:1264:SER:HA	1:A:1267:LYS:HD3	1.92	0.51
1:A:1109:LEU:HD23	1:A:1238:PRO:CB	2.41	0.51
1:C:1195:VAL:O	1:C:1198:PHE:HB3	2.11	0.50
1:D:1074:PRO:HB2	1:D:1076:LEU:HD21	1.94	0.50
1:A:1160:ILE:HD13	1:A:1161:TYR:H	1.76	0.50
1:C:1197:SER:O	1:C:1200:VAL:HB	2.11	0.50
1:A:1219:GLU:HG2	1:A:1223:ARG:HH12	1.76	0.50
1:B:1151:ILE:HD12	1:B:1151:ILE:N	2.27	0.50
1:B:1252:ASN:HD22	1:B:1253:PRO:CD	2.25	0.50
1:C:1177:ARG:NH2	1:C:1218:ASN:OD1	2.45	0.50
1:D:1092:ARG:HG3	1:D:1209:ALA:HB3	1.94	0.50
1:B:1151:ILE:HD12	1:B:1151:ILE:H	1.76	0.50
1:B:1050:GLU:CD	1:B:1155:GLY:HA2	2.32	0.50
1:C:1223:ARG:HD2	1:D:1223:ARG:HD3	1.93	0.49
1:A:999:ILE:CD1	1:A:1078:ILE:HD13	2.42	0.49
1:D:1190:THR:HG1	1:D:1192:TYR:HD2	1.54	0.49
1:C:1090:TYR:CE2	1:C:1094:LEU:HD11	2.47	0.49
1:A:1068:VAL:HG22	1:A:1069:VAL:N	2.28	0.49
1:A:1073:GLN:HB3	1:A:1074:PRO:HD2	1.90	0.49
1:C:1044:ARG:O	1:C:1048:LEU:HD13	2.12	0.49
1:C:1184:LEU:HD22	1:C:1222:LEU:HD23	1.93	0.49
1:D:1243:GLU:CD	1:D:1246:ARG:HH11	2.14	0.49
1:B:1121:ASP:HA	1:B:1263:ILE:HD11	1.94	0.49
1:C:1034:THR:HG22	1:C:1076:LEU:HB3	1.93	0.49
1:C:1239:ASP:O	1:C:1243:GLU:HG3	2.12	0.49
1:A:1010:PHE:HB3	1:A:1035:VAL:HG12	1.93	0.49
1:D:1084:ARG:NE	1:D:1147:PHE:HE1	2.10	0.49
1:C:1163:THR:OG1	1:C:1164:ASP:N	2.45	0.49
1:D:1132:VAL:O	1:D:1132:VAL:HG13	2.13	0.49
1:D:1182:GLU:HG2	1:D:1183:SER:N	2.28	0.49
1:D:1195:VAL:O	1:D:1198:PHE:HB3	2.13	0.49
1:D:1054:MET:HB2	1:D:1065:LEU:HD22	1.95	0.48
1:A:995:ALA:HB3	1:A:998:LYS:CG	2.43	0.48
1:B:1047:PHE:CE2	1:B:1077:VAL:HG23	2.48	0.48
1:D:1095:ARG:O	1:D:1097:GLU:HG2	2.12	0.48
1:B:1219:GLU:O	1:B:1222:LEU:HB3	2.13	0.48
1:C:1250:GLN:O	1:C:1256:ARG:HD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1084:ARG:NE	1:D:1147:PHE:CE1	2.82	0.48
1:A:992:TRP:CZ3	1:A:1065:LEU:HD23	2.48	0.48
1:B:1167:ARG:C	1:B:1169:GLY:H	2.17	0.48
1:B:1233:LYS:HA	1:B:1242:PHE:CE1	2.48	0.48
1:C:1140:ASN:HB3	1:C:1153:ASP:HB3	1.95	0.48
1:B:1084:ARG:HB2	1:B:1143:VAL:O	2.13	0.48
1:C:1092:ARG:O	1:C:1095:ARG:HG3	2.14	0.48
1:C:1123:MET:HB3	1:C:1259:PHE:CE2	2.49	0.48
1:D:1132:VAL:HG22	1:D:1134:ARG:HG3	1.95	0.48
1:A:1045:ILE:HD12	1:A:1045:ILE:N	2.23	0.47
1:A:991:GLU:OE2	1:A:991:GLU:HA	2.14	0.47
1:C:1179:MET:HE3	1:C:1183:SER:HB3	1.96	0.47
1:B:1084:ARG:NH2	1:B:1145:GLU:O	2.47	0.47
1:C:1109:LEU:O	1:C:1109:LEU:HD22	2.13	0.47
1:B:1061:HIS:CD2	1:B:1118:GLU:HB3	2.49	0.47
1:B:1210:GLU:HA	1:D:1246:ARG:HH12	1.79	0.47
1:C:996:ARG:CZ	1:C:1073:GLN:CB	2.87	0.47
1:C:1068:VAL:HG22	1:C:1069:VAL:N	2.30	0.47
1:C:1062:VAL:HG13	1:C:1154:PHE:HZ	1.80	0.47
1:C:1132:VAL:HG13	1:C:1134:ARG:HG3	1.97	0.47
1:D:1210:GLU:HB3	1:D:1214:GLN:NE2	2.30	0.47
1:D:1222:LEU:HD13	1:D:1222:LEU:C	2.35	0.47
1:D:1010:PHE:O	1:D:1035:VAL:HA	2.15	0.47
1:D:1109:LEU:HD23	1:D:1238:PRO:CB	2.43	0.47
1:A:1109:LEU:HD23	1:A:1238:PRO:HG2	1.97	0.47
1:D:1160:ILE:HB	1:D:1163:THR:O	2.14	0.47
1:C:1264:SER:O	1:C:1267:LYS:HG2	2.15	0.47
1:D:1106:PRO:HA	1:D:1107:PRO:HD3	1.84	0.47
1:B:997:GLU:CD	1:B:997:GLU:H	2.17	0.46
1:C:1223:ARG:HD2	1:D:1223:ARG:CD	2.45	0.46
1:D:1062:VAL:O	1:D:1063:VAL:C	2.53	0.46
1:A:1154:PHE:HB3	1:A:1157:THR:HB	1.98	0.46
1:C:1005:LEU:HD11	1:C:1015:GLU:HB2	1.98	0.46
1:C:1207:THR:HG22	1:C:1234:PRO:HB3	1.97	0.46
1:B:1166:TYR:HB3	1:C:1173:LEU:HB3	1.98	0.46
1:C:1068:VAL:HG23	1:C:1077:VAL:HG22	1.98	0.46
1:D:1062:VAL:HG13	1:D:1154:PHE:HZ	1.80	0.46
1:D:1078:ILE:HD12	1:D:1078:ILE:H	1.81	0.46
1:A:1160:ILE:HD13	1:A:1161:TYR:N	2.31	0.46
1:D:1028:THR:O	1:D:1030:VAL:HG13	2.16	0.46
1:A:1211:GLN:O	1:A:1214:GLN:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1154:PHE:HB3	1:C:1157:THR:OG1	2.16	0.46
1:B:1117:GLY:HA3	1:B:1270:MET:CE	2.45	0.46
1:C:1048:LEU:HD11	1:C:1075:THR:CG2	2.46	0.46
1:C:1084:ARG:NE	1:C:1147:PHE:CE1	2.84	0.46
1:C:1172:GLY:O	1:C:1173:LEU:O	2.34	0.46
1:D:1160:ILE:O	1:D:1163:THR:O	2.34	0.46
1:D:1130:LYS:HG3	1:D:1161:TYR:HD1	1.82	0.45
1:D:1243:GLU:OE1	1:D:1246:ARG:NH1	2.47	0.45
1:A:1039:ALA:C	1:A:1041:MET:H	2.19	0.45
1:A:1096:PRO:O	1:A:1098:MET:N	2.50	0.45
1:C:1039:ALA:HB1	1:C:1043:GLU:OE1	2.16	0.45
1:B:1217:SER:O	1:B:1218:ASN:C	2.55	0.45
1:C:1126:LEU:HD11	1:C:1154:PHE:HE2	1.81	0.45
1:D:1167:ARG:HG2	1:D:1188:VAL:HG22	1.97	0.45
1:A:989:PRO:O	1:A:990:ASP:HB3	2.16	0.45
1:A:999:ILE:HD12	1:A:1078:ILE:HD13	1.98	0.45
1:B:1048:LEU:HD12	1:B:1048:LEU:HA	1.81	0.45
1:C:988:VAL:O	1:C:988:VAL:HG13	2.16	0.45
1:C:1252:ASN:HD22	1:C:1253:PRO:CD	2.29	0.45
1:D:1184:LEU:HB3	1:D:1222:LEU:CD2	2.47	0.45
1:A:1219:GLU:O	1:A:1222:LEU:HB3	2.17	0.45
1:C:1247:MET:O	1:C:1250:GLN:HG2	2.16	0.45
1:D:1275:ARG:HG3	1:D:1281:TYR:CD1	2.52	0.45
1:B:1092:ARG:HD2	1:B:1095:ARG:HH21	1.81	0.45
1:A:1258:SER:OG	1:A:1261:GLU:HB2	2.17	0.45
1:B:987:TYR:OH	1:B:1068:VAL:HG11	2.16	0.45
1:B:999:ILE:HD12	1:B:1078:ILE:HG12	1.99	0.45
1:C:1084:ARG:HB2	1:C:1143:VAL:HB	1.98	0.45
1:B:996:ARG:NH1	1:B:1072:GLY:O	2.47	0.44
1:C:1158:ARG:HG2	1:C:1166:TYR:CZ	2.53	0.44
1:C:1262:ILE:HG22	1:C:1263:ILE:N	2.31	0.44
1:D:1082:MET:HG3	1:D:1142:MET:HB3	1.99	0.44
1:B:1077:VAL:C	1:B:1078:ILE:HD12	2.37	0.44
1:B:1234:PRO:HD2	1:B:1237:CYS:SG	2.57	0.44
1:D:1162:GLU:H	1:D:1162:GLU:HG3	1.41	0.44
1:D:1230:LEU:CD2	1:D:1249:TRP:HB3	2.46	0.44
1:D:1268:GLU:C	1:D:1270:MET:H	2.21	0.44
1:C:1182:GLU:OE2	1:C:1256:ARG:NH1	2.47	0.44
1:D:1253:PRO:C	1:D:1255:MET:H	2.21	0.44
1:C:1092:ARG:HG2	1:C:1095:ARG:NH2	2.33	0.44
1:B:1057:PHE:CE1	1:B:1126:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1184:LEU:HB3	1:A:1222:LEU:HD22	1.99	0.44
1:B:1218:ASN:N	1:B:1218:ASN:HD22	2.15	0.44
1:D:1158:ARG:NH1	1:D:1168:LYS:HE3	2.33	0.44
1:B:1185:LYS:HG3	1:B:1226:MET:CE	2.47	0.44
1:B:1003:ARG:HG3	1:B:1003:ARG:NH1	2.33	0.44
1:B:1057:PHE:HE1	1:B:1131:PHE:CD2	2.36	0.44
1:D:1052:SER:O	1:D:1055:LYS:HG3	2.17	0.44
1:A:1109:LEU:HD13	1:A:1109:LEU:O	2.18	0.43
1:A:1014:TYR:HB2	1:A:1032:ILE:HB	2.00	0.43
1:D:1242:PHE:O	1:D:1245:MET:HB2	2.18	0.43
1:A:1057:PHE:HE1	1:A:1131:PHE:CD2	2.36	0.43
1:A:1274:PHE:CD1	1:A:1278:SER:HB3	2.53	0.43
1:C:996:ARG:NE	1:C:1073:GLN:HB2	2.33	0.43
1:C:1027:GLU:OE1	1:C:1027:GLU:HA	2.18	0.43
1:A:1184:LEU:HD22	1:A:1222:LEU:HD23	1.98	0.43
1:B:993:GLU:OE1	1:B:1071:GLN:HG2	2.18	0.43
1:B:1014:TYR:HB2	1:B:1032:ILE:HB	2.00	0.43
1:D:1074:PRO:HB2	1:D:1076:LEU:CD2	2.49	0.43
1:D:1196:TRP:O	1:D:1197:SER:C	2.55	0.43
1:A:1010:PHE:N	1:A:1010:PHE:CD1	2.86	0.43
1:C:1156:MET:HA	1:C:1158:ARG:NH1	2.33	0.43
1:D:1233:LYS:HB2	1:D:1242:PHE:CZ	2.53	0.43
1:C:1177:ARG:NH1	1:C:1216:LEU:O	2.47	0.43
1:A:1115:MET:O	1:A:1119:ILE:HG13	2.18	0.43
1:C:1197:SER:O	1:C:1201:VAL:HG23	2.17	0.43
1:C:1200:VAL:HA	1:C:1249:TRP:HZ2	1.83	0.43
1:D:986:VAL:HG22	1:D:987:TYR:N	2.34	0.43
1:C:1158:ARG:NH2	1:C:1171:LYS:HB2	2.34	0.43
1:B:1168:LYS:O	1:B:1168:LYS:HG2	2.19	0.42
1:C:1037:GLU:HG3	1:C:1038:ALA:H	1.83	0.42
1:D:1053:VAL:C	1:D:1055:LYS:H	2.21	0.42
1:C:1005:LEU:CD1	1:C:1015:GLU:HB2	2.49	0.42
1:B:996:ARG:HH21	1:B:1069:VAL:HG11	1.84	0.42
1:B:1106:PRO:HA	1:B:1107:PRO:HD3	1.84	0.42
1:C:1257:PRO:HA	1:C:1261:GLU:OE1	2.19	0.42
1:A:1130:LYS:HB3	1:A:1160:ILE:HD12	2.01	0.42
1:A:1252:ASN:HA	1:A:1253:PRO:HD3	1.84	0.42
1:B:1185:LYS:CA	1:B:1226:MET:HE3	2.46	0.42
1:D:1127:ASN:OD1	1:D:1191:THR:OG1	2.36	0.42
1:A:1039:ALA:C	1:A:1041:MET:N	2.73	0.42
1:A:1064:ARG:HB2	1:A:1064:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:TRP:CD1	1:A:1196:TRP:C	2.92	0.42
1:B:1080:GLU:O	2:B:2:PDR:H16	2.19	0.42
1:C:1030:VAL:HG23	1:C:1032:ILE:HD11	2.02	0.42
1:D:1083:THR:OG1	1:D:1145:GLU:HB2	2.20	0.42
1:D:1109:LEU:HD13	1:D:1109:LEU:C	2.39	0.42
1:D:1208:LEU:O	1:D:1209:ALA:HB3	2.20	0.42
1:D:1018:ALA:O	1:D:1027:GLU:HA	2.20	0.42
1:A:1184:LEU:HD22	1:A:1222:LEU:CD2	2.49	0.42
1:B:1258:SER:O	1:B:1262:ILE:HG13	2.20	0.42
1:D:1219:GLU:OE2	1:D:1223:ARG:NH1	2.51	0.42
1:D:1122:GLY:O	1:D:1125:TYR:HB3	2.20	0.42
1:A:1260:LEU:HD23	1:A:1260:LEU:HA	1.89	0.42
1:B:1244:LEU:HD23	1:B:1244:LEU:O	2.20	0.42
1:C:1163:THR:HG1	1:C:1165:TYR:HD1	1.67	0.42
1:D:1082:MET:HG3	1:D:1142:MET:CB	2.50	0.42
1:D:1233:LYS:HB2	1:D:1242:PHE:CE2	2.55	0.42
1:B:993:GLU:HA	1:B:1068:VAL:O	2.19	0.41
1:C:1175:PRO:O	1:C:1179:MET:HG3	2.20	0.41
1:A:1116:ALA:CB	1:A:1202:LEU:HD21	2.50	0.41
1:B:1077:VAL:CG1	1:B:1078:ILE:N	2.83	0.41
1:B:1081:LEU:HD13	1:B:1083:THR:HG22	2.02	0.41
1:C:1157:THR:O	1:C:1158:ARG:HD2	2.20	0.41
1:A:1078:ILE:O	1:A:1078:ILE:HG13	2.19	0.41
1:A:1108:SER:H	1:A:1111:LYS:HB2	1.85	0.41
1:D:1251:TYR:O	1:D:1253:PRO:HD3	2.20	0.41
1:A:1062:VAL:O	1:A:1063:VAL:C	2.58	0.41
1:C:1133:HIS:NE2	1:C:1153:ASP:O	2.50	0.41
1:C:1136:LEU:HG	1:C:1201:VAL:HG21	2.02	0.41
1:D:1049:ASN:O	1:D:1052:SER:HB3	2.20	0.41
1:A:1058:ASN:C	1:A:1058:ASN:HD22	2.24	0.41
1:B:1035:VAL:HG11	1:B:1044:ARG:HG2	2.02	0.41
1:D:1090:TYR:CE2	1:D:1094:LEU:HD11	2.55	0.41
1:D:1158:ARG:HG3	1:D:1166:TYR:CZ	2.56	0.41
1:D:1210:GLU:HB3	1:D:1214:GLN:HE22	1.85	0.41
1:A:1019:LYS:HD3	1:A:1027:GLU:HG2	2.01	0.41
1:A:1245:MET:O	1:A:1248:CYS:N	2.53	0.41
1:C:1054:MET:HB2	1:C:1065:LEU:HD22	2.03	0.41
1:D:1266:ILE:O	1:D:1270:MET:HG2	2.20	0.41
1:B:1141:CYS:C	1:B:1142:MET:HG2	2.41	0.41
1:C:1053:VAL:HG12	1:C:1057:PHE:CE2	2.55	0.41
1:A:1275:ARG:HA	1:A:1281:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1167:ARG:C	1:B:1169:GLY:N	2.74	0.41
1:B:1235:ASP:O	1:B:1236:ASN:HB2	2.21	0.41
1:C:1083:THR:O	2:C:3:PDR:H20	2.21	0.41
1:D:1152:GLY:O	1:D:1153:ASP:O	2.39	0.41
1:D:1201:VAL:HA	1:D:1204:GLU:HB2	2.03	0.41
1:A:1032:ILE:CD1	1:A:1078:ILE:HG22	2.51	0.41
1:A:1086:ASP:OD1	1:A:1089:SER:HB2	2.21	0.41
1:B:1124:ALA:HB2	1:B:1259:PHE:HB3	2.02	0.41
1:D:1010:PHE:N	1:D:1010:PHE:CD1	2.89	0.41
1:A:1177:ARG:NH1	1:A:1212:PRO:O	2.54	0.40
1:A:1041:MET:C	1:A:1043:GLU:N	2.73	0.40
1:B:1104:LEU:O	1:B:1105:ALA:HB2	2.21	0.40
1:B:1195:VAL:O	1:B:1248:CYS:HB3	2.21	0.40
1:C:995:ALA:C	1:C:997:GLU:N	2.74	0.40
1:C:1242:PHE:O	1:C:1245:MET:HB2	2.22	0.40
1:B:1044:ARG:CZ	1:B:1073:GLN:NE2	2.85	0.40
1:A:1045:ILE:H	1:A:1045:ILE:CD1	2.24	0.40
1:A:1221:VAL:O	1:A:1222:LEU:C	2.60	0.40
1:B:996:ARG:HH21	1:B:1069:VAL:CG1	2.35	0.40
1:B:1041:MET:O	1:B:1045:ILE:HG13	2.22	0.40
1:D:1017:VAL:HA	1:D:1028:THR:O	2.21	0.40
1:D:1111:LYS:O	1:D:1115:MET:HG3	2.20	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	283/336 (84%)	230 (81%)	46 (16%)	7 (2%)	5 28
1	B	291/336 (87%)	247 (85%)	40 (14%)	4 (1%)	11 43
1	C	287/336 (85%)	245 (85%)	33 (12%)	9 (3%)	4 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	274/336 (82%)	230 (84%)	39 (14%)	5 (2%)	8	37
All	All	1135/1344 (84%)	952 (84%)	158 (14%)	25 (2%)	6	31

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	GLN
1	B	1165	TYR
1	B	1171	LYS
1	C	1173	LEU
1	D	1153	ASP
1	A	1097	GLU
1	B	1209	ALA
1	C	1162	GLU
1	A	1070	SER
1	A	1285	ASN
1	C	989	PRO
1	A	1038	ALA
1	C	996	ARG
1	C	1026	PRO
1	C	1073	GLN
1	D	992	TRP
1	D	1282	SER
1	C	1129	ASN
1	D	1254	LYS
1	A	1043	GLU
1	B	1063	VAL
1	C	1072	GLY
1	D	1063	VAL
1	C	1262	ILE
1	A	1272	PRO

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	252/294 (86%)	235 (93%)	17 (7%)	16	49
1	B	258/294 (88%)	242 (94%)	16 (6%)	18	52
1	C	258/294 (88%)	250 (97%)	8 (3%)	40	75
1	D	248/294 (84%)	239 (96%)	9 (4%)	35	70
All	All	1016/1176 (86%)	966 (95%)	50 (5%)	25	61

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1019	LYS
1	A	1056	GLU
1	A	1058	ASN
1	A	1064	ARG
1	A	1065	LEU
1	A	1081	LEU
1	A	1099	GLU
1	A	1127	ASN
1	A	1146	ASP
1	A	1160	ILE
1	A	1219	GLU
1	A	1244	LEU
1	A	1246	ARG
1	A	1261	GLU
1	A	1268	GLU
1	A	1272	PRO
1	A	1283	GLU
1	B	997	GLU
1	B	1048	LEU
1	B	1064	ARG
1	B	1068	VAL
1	B	1081	LEU
1	B	1110	SER
1	B	1129	ASN
1	B	1186	ASP
1	B	1223	ARG
1	B	1235	ASP
1	B	1240	MET
1	B	1252	ASN
1	B	1268	GLU
1	B	1272	PRO
1	B	1276	GLU
1	B	1277	VAL

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Mol	Chain	Res	Type
1	C	987	TYR
1	C	991	GLU
1	C	1083	THR
1	C	1164	ASP
1	C	1219	GLU
1	C	1223	ARG
1	C	1244	LEU
1	C	1268	GLU
1	D	991	GLU
1	D	1076	LEU
1	D	1104	LEU
1	D	1130	LYS
1	D	1159	ASP
1	D	1162	GLU
1	D	1240	MET
1	D	1260	LEU
1	D	1277	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1058	ASN
1	B	1049	ASN
1	B	1060	HIS
1	B	1061	HIS
1	B	1218	ASN
1	B	1236	ASN
1	B	1252	ASN
1	C	1007	GLN
1	C	1049	ASN
1	C	1060	HIS
1	C	1236	ASN
1	C	1252	ASN
1	D	1007	GLN
1	D	1049	ASN
1	D	1114	GLN
1	D	1214	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)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EPE	A	1287	-	12,12,15	1.51	2 (16%)	14,16,20	2.04	5 (35%)
2	PDR	B	2	-	23,27,27	1.84	7 (30%)	19,40,40	3.19	5 (26%)
4	SO4	A	3	-	4,4,4	1.94	2 (50%)	6,6,6	0.89	0
2	PDR	C	3	-	23,27,27	2.11	9 (39%)	19,40,40	2.98	5 (26%)
2	PDR	D	4	-	23,27,27	2.06	9 (39%)	19,40,40	3.01	4 (21%)
4	SO4	B	1287	-	4,4,4	1.86	2 (50%)	6,6,6	0.97	0
2	PDR	A	1	-	23,27,27	2.03	9 (39%)	19,40,40	2.93	5 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EPE	A	1287	-	-	2/6/14/19	0/1/1/1
2	PDR	B	2	-	-	2/4/8/8	0/4/4/4
2	PDR	C	3	-	-	4/4/8/8	0/4/4/4
2	PDR	D	4	-	-	4/4/8/8	0/4/4/4
2	PDR	A	1	-	-	2/4/8/8	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	PDR	C3-C4	4.45	1.44	1.36
2	A	1	PDR	O21-C5	4.21	1.41	1.35
2	D	4	PDR	C18-C10	4.07	1.49	1.42
2	D	4	PDR	C3-C4	4.06	1.43	1.36
2	B	2	PDR	C3-C4	4.03	1.43	1.36
2	A	1	PDR	C3-C4	3.81	1.43	1.36
2	C	3	PDR	C15-C18	3.67	1.44	1.36
2	C	3	PDR	O21-C5	3.44	1.40	1.35
2	C	3	PDR	O23-C4	3.42	1.42	1.37
2	D	4	PDR	O21-C5	3.34	1.40	1.35
2	B	2	PDR	O21-C5	3.31	1.40	1.35
4	A	3	SO4	O2-S	3.20	1.63	1.46
2	A	1	PDR	C1-N6	3.19	1.41	1.36
2	A	1	PDR	C5-N6	3.19	1.38	1.30
2	A	1	PDR	C15-C18	3.14	1.43	1.36
2	D	4	PDR	C15-C18	3.13	1.43	1.36
4	B	1287	SO4	O2-S	3.12	1.62	1.46
3	A	1287	EPE	C6-N1	3.01	1.55	1.46
2	B	2	PDR	C18-C10	2.92	1.47	1.42
2	C	3	PDR	C18-C10	2.90	1.47	1.42
2	B	2	PDR	C1-N6	2.84	1.41	1.36
2	D	4	PDR	O23-C4	2.81	1.41	1.37
2	B	2	PDR	C15-C18	2.76	1.42	1.36
2	C	3	PDR	C5-N6	2.76	1.37	1.30
2	A	1	PDR	C18-C10	2.69	1.46	1.42
2	D	4	PDR	C16-N17	2.64	1.37	1.32
2	D	4	PDR	C5-N6	2.63	1.36	1.30
2	D	4	PDR	C1-N6	2.63	1.40	1.36
2	C	3	PDR	C1-N6	2.61	1.40	1.36
2	A	1	PDR	C15-C16	2.60	1.43	1.38
2	B	2	PDR	C5-N6	2.55	1.36	1.30
2	B	2	PDR	O23-C4	2.51	1.41	1.37
2	C	3	PDR	C15-C16	2.34	1.43	1.38
2	C	3	PDR	C16-N17	2.32	1.37	1.32
3	A	1287	EPE	C6-C5	2.19	1.56	1.51
4	A	3	SO4	O4-S	-2.18	1.30	1.47
2	D	4	PDR	C15-C16	2.02	1.42	1.38
2	A	1	PDR	C11-N17	2.02	1.39	1.37
4	B	1287	SO4	O4-S	-2.01	1.31	1.47
2	A	1	PDR	O23-C4	2.00	1.40	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	PDR	C10-C14-C13	-11.97	98.34	107.13
2	C	3	PDR	C10-C14-C13	-11.38	98.77	107.13
2	A	1	PDR	C10-C14-C13	-11.08	99.00	107.13
2	D	4	PDR	C10-C14-C13	-10.87	99.15	107.13
2	D	4	PDR	C22-O21-C5	-4.63	112.62	117.21
2	B	2	PDR	C22-O21-C5	-4.40	112.85	117.21
3	A	1287	EPE	C3-C2-N1	-3.60	105.79	110.94
3	A	1287	EPE	C6-N1-C2	3.43	116.55	108.83
2	A	1	PDR	C22-O21-C5	-3.32	113.92	117.21
2	C	3	PDR	C22-O21-C5	-3.18	114.06	117.21
3	A	1287	EPE	O1S-S-C10	-3.07	103.22	106.92
3	A	1287	EPE	C9-N1-C6	-2.75	104.20	111.23
2	B	2	PDR	C3-C2-C1	-2.55	118.14	120.55
2	D	4	PDR	C16-N17-C11	2.49	119.67	116.60
2	C	3	PDR	C16-N17-C11	2.39	119.54	116.60
2	C	3	PDR	C3-C2-C1	-2.33	118.35	120.55
2	B	2	PDR	C16-N17-C11	2.30	119.44	116.60
2	D	4	PDR	C3-C2-C1	-2.23	118.44	120.55
2	A	1	PDR	C2-C1-N6	-2.23	122.30	125.12
2	C	3	PDR	C14-C10-C11	2.17	111.46	105.30
3	A	1287	EPE	O2S-S-C10	2.12	109.46	106.92
2	A	1	PDR	C14-C10-C11	2.10	111.25	105.30
2	B	2	PDR	C14-C10-C11	2.08	111.20	105.30
2	A	1	PDR	C3-C2-C1	-2.01	118.65	120.55

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2	PDR	C4-C5-O21-C22
2	B	2	PDR	N6-C5-O21-C22
2	D	4	PDR	C4-C5-O21-C22
2	D	4	PDR	N6-C5-O21-C22
2	C	3	PDR	C5-C4-O23-C24
2	A	1	PDR	C5-C4-O23-C24
2	D	4	PDR	C5-C4-O23-C24
2	D	4	PDR	C3-C4-O23-C24
2	C	3	PDR	C3-C4-O23-C24
2	A	1	PDR	C3-C4-O23-C24
2	C	3	PDR	C4-C5-O21-C22
2	C	3	PDR	N6-C5-O21-C22
3	A	1287	EPE	C10-C9-N1-C2
3	A	1287	EPE	C10-C9-N1-C6

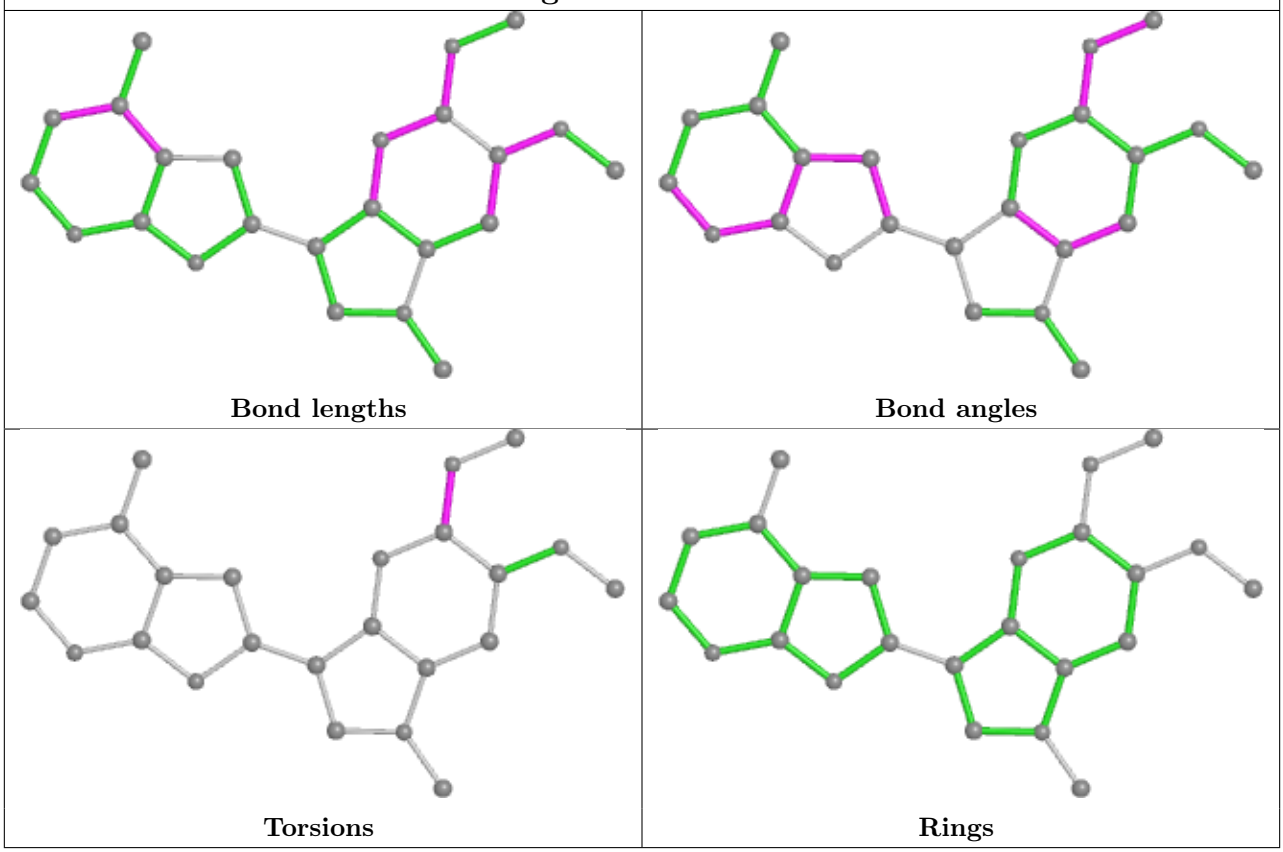
There are no ring outliers.

3 monomers are involved in 3 short contacts:

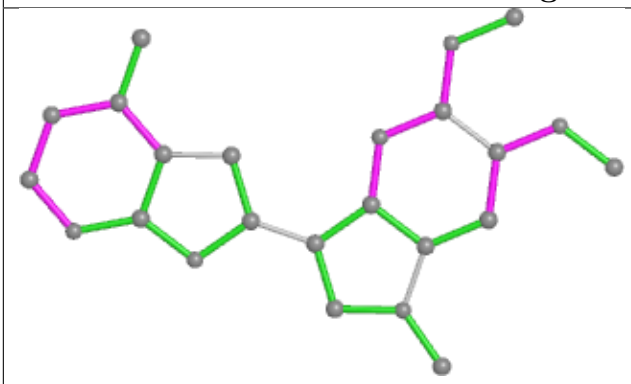
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	PDR	1	0
2	C	3	PDR	1	0
2	A	1	PDR	1	0

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 then 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.

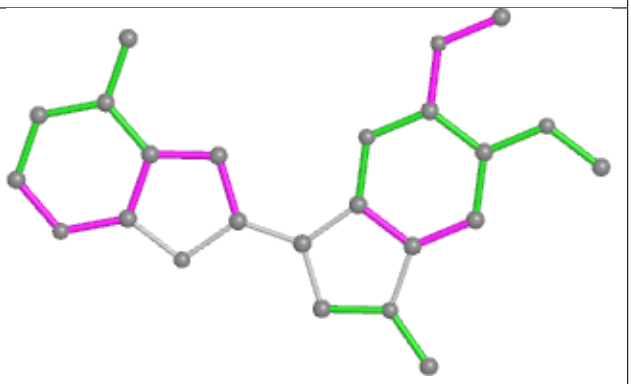
Ligand PDR B 2



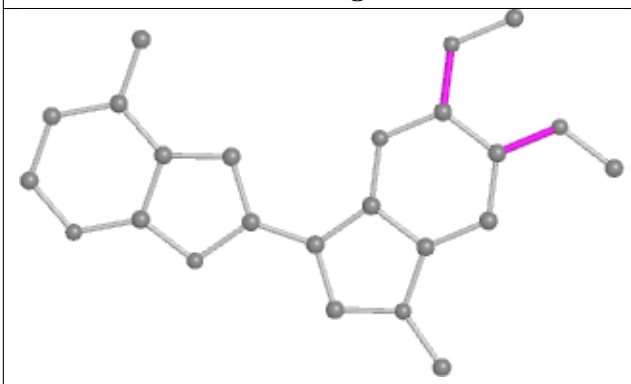
Ligand PDR C 3



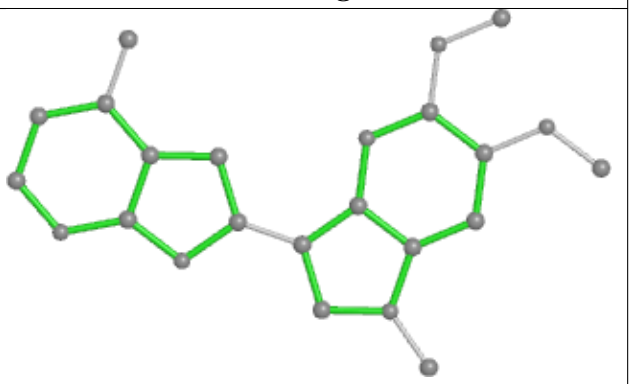
Bond lengths



Bond angles

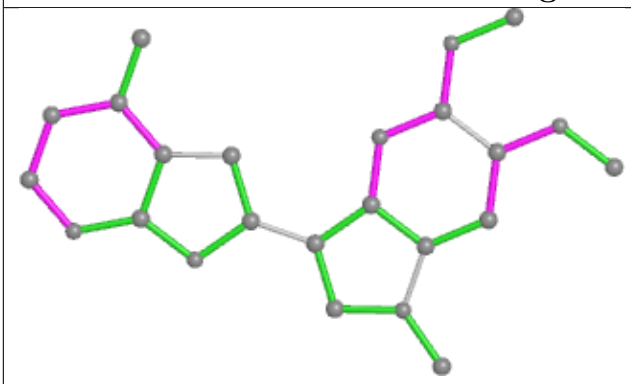


Torsions

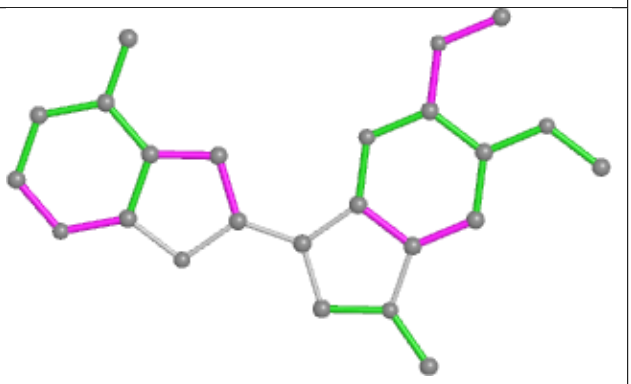


Rings

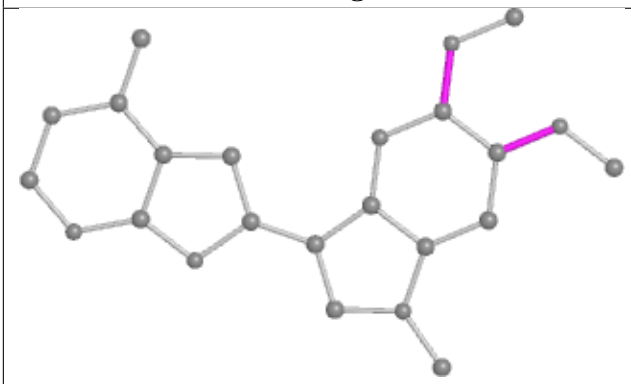
Ligand PDR D 4



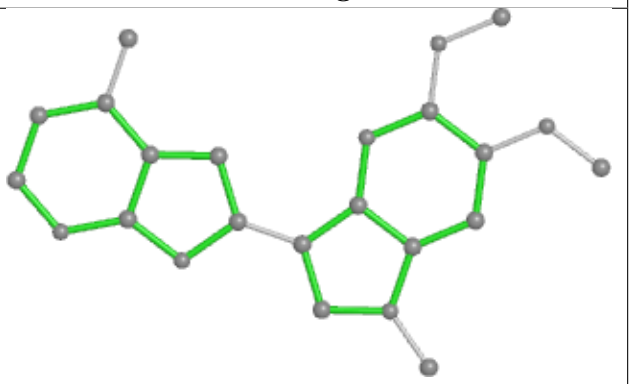
Bond lengths



Bond angles

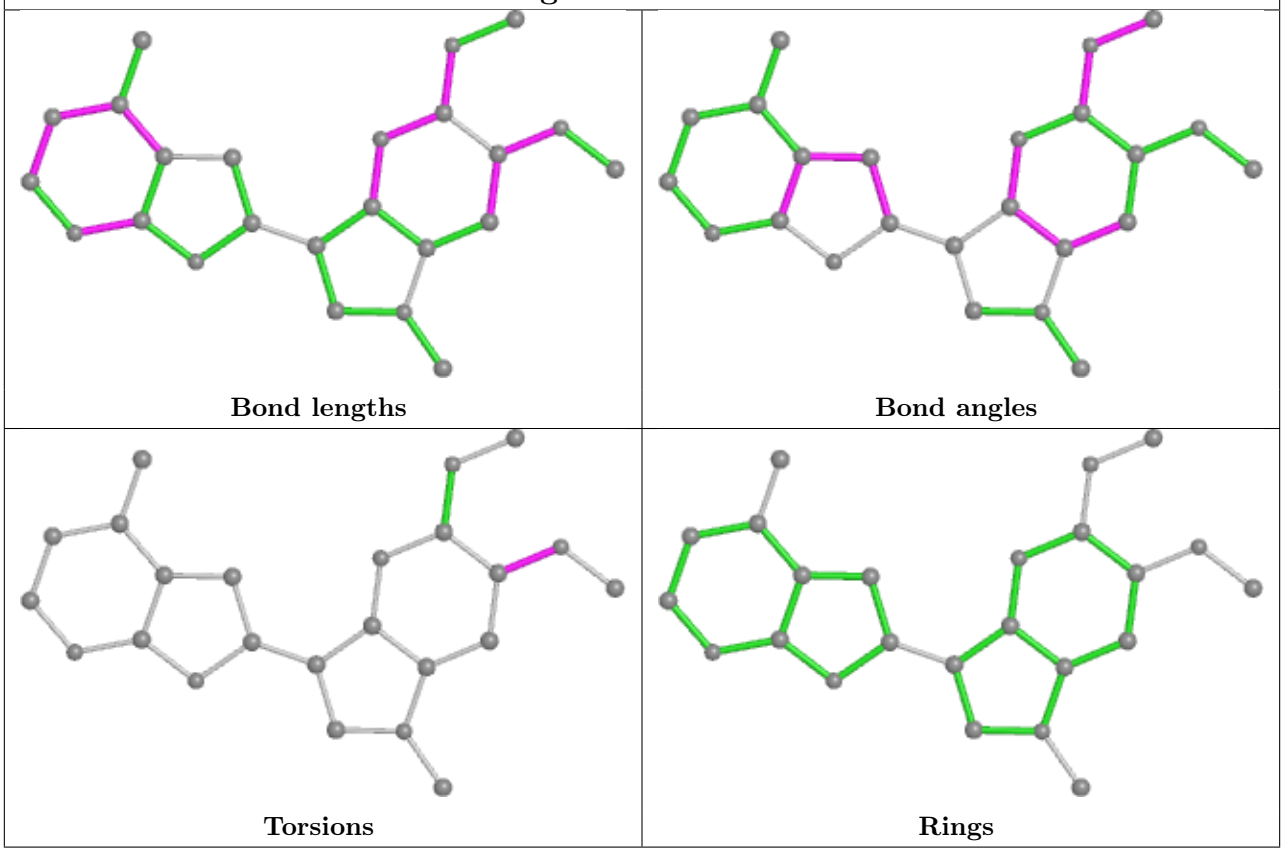


Torsions



Rings

Ligand PDR A 1



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	289/336 (86%)	-0.27	0	100	100	21, 45, 81, 95	18 (6%)
1	B	295/336 (87%)	-0.39	0	100	100	18, 38, 63, 83	11 (3%)
1	C	292/336 (86%)	-0.19	4 (1%)	75	49	19, 46, 79, 88	13 (4%)
1	D	282/336 (83%)	-0.02	6 (2%)	63	34	21, 53, 94, 102	17 (6%)
All	All	1158/1344 (86%)	-0.22	10 (0%)	84	63	18, 45, 84, 102	59 (5%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1001	MET	3.6
1	D	1002	SER	2.9
1	D	1017	VAL	2.8
1	C	1159	ASP	2.3
1	D	999	ILE	2.3
1	D	1029	ARG	2.3
1	C	997	GLU	2.2
1	D	1169	GLY	2.2
1	C	1002	SER	2.1
1	C	1161	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

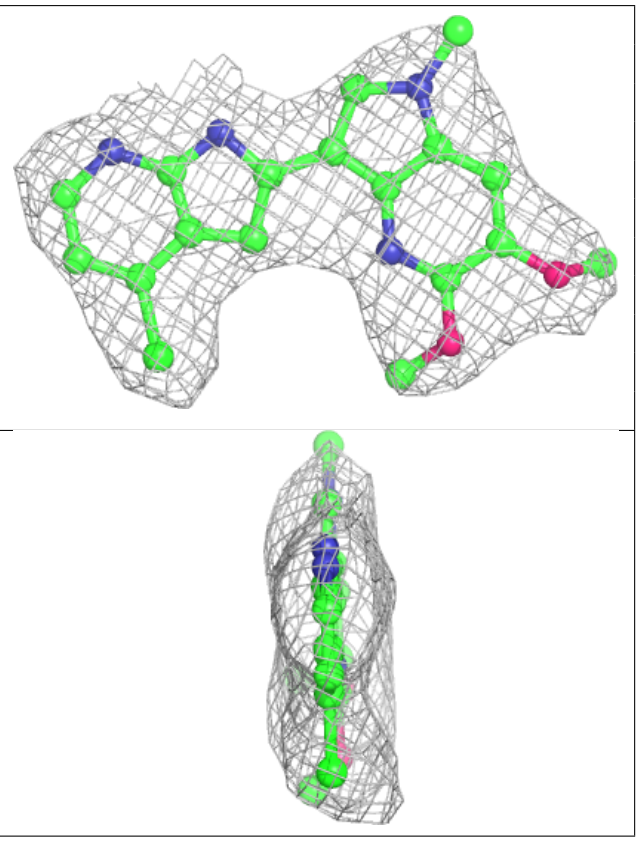
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PDR	C	3	24/24	0.93	0.29	43,44,47,51	0
2	PDR	A	1	24/24	0.94	0.23	29,33,39,48	0
2	PDR	B	2	24/24	0.95	0.19	22,26,31,42	0
2	PDR	D	4	24/24	0.95	0.35	56,57,60,60	0
4	SO4	B	1287	5/5	0.96	0.22	47,48,48,48	0
3	EPE	A	1287	12/15	0.97	0.19	33,34,35,36	0
4	SO4	A	3	5/5	0.98	0.18	44,44,44,44	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.

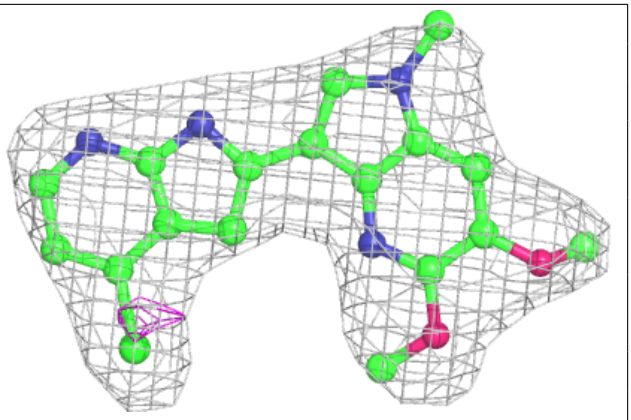
Electron density around PDR C 3:

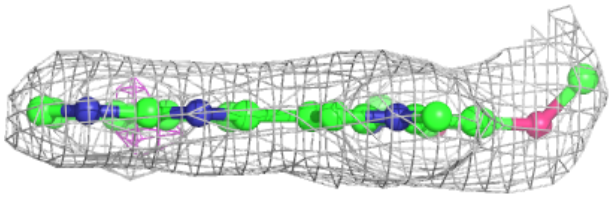
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

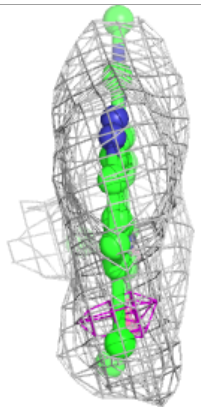


Electron density around PDR A 1:

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

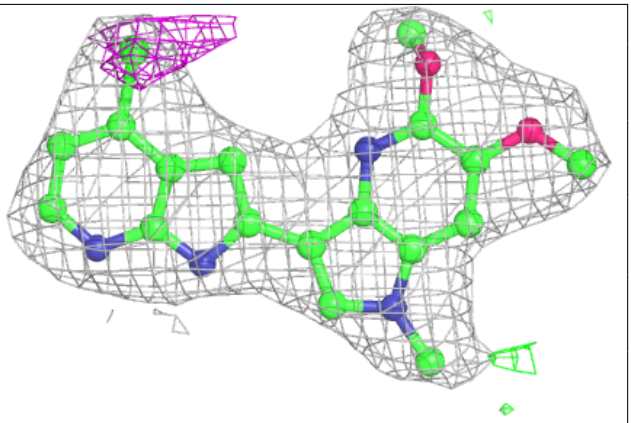


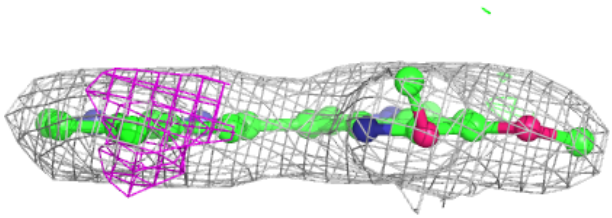


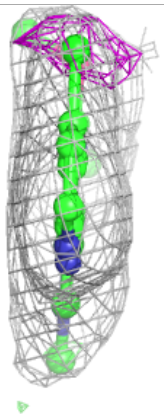


Electron density around PDR B 2:

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

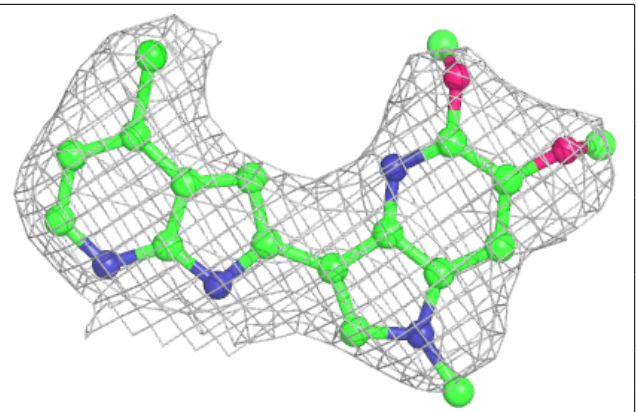


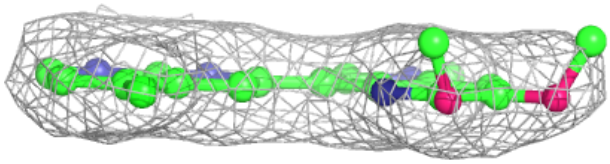


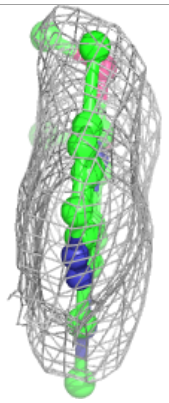


Electron density around PDR D 4:

$2mF_o$-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.