Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 06:03 pm GMT

PDB ID	:	4A55
Title	:	Crystal structure of p110alpha in complex with iSH2 of p85alpha and the inhibitor PIK-108
Authors	:	Hon, W.-C.; Berndt, A.; Williams, R.L.
Deposited on	:	2011-10-24
Resolution	:	3.50 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
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:

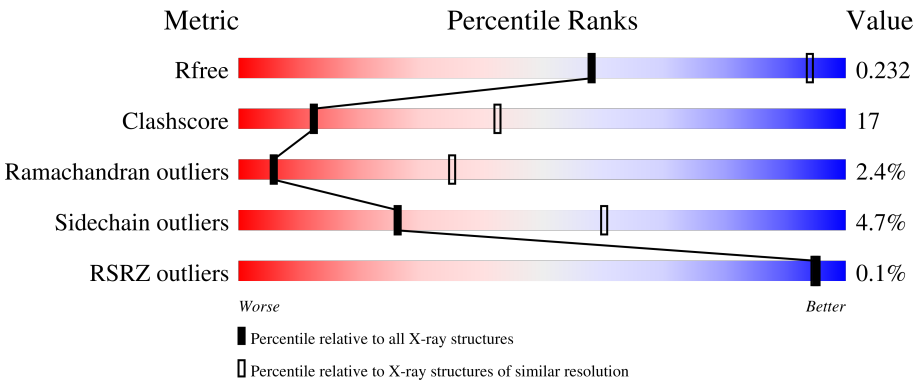
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	1096	62% 26% • 9%
2	B	279	38% 11% • 49%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9508 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 PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT ALPHA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1001	8214	5266	1397	1485	66	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP P42337
A	-26	SER	-	expression tag	UNP P42337
A	-25	TYR	-	expression tag	UNP P42337
A	-24	TYR	-	expression tag	UNP P42337
A	-23	HIS	-	expression tag	UNP P42337
A	-22	HIS	-	expression tag	UNP P42337
A	-21	HIS	-	expression tag	UNP P42337
A	-20	HIS	-	expression tag	UNP P42337
A	-19	HIS	-	expression tag	UNP P42337
A	-18	HIS	-	expression tag	UNP P42337
A	-17	ASP	-	expression tag	UNP P42337
A	-16	TYR	-	expression tag	UNP P42337
A	-15	ASP	-	expression tag	UNP P42337
A	-14	ILE	-	expression tag	UNP P42337
A	-13	PRO	-	expression tag	UNP P42337
A	-12	THR	-	expression tag	UNP P42337
A	-11	THR	-	expression tag	UNP P42337
A	-10	GLU	-	expression tag	UNP P42337
A	-9	ASN	-	expression tag	UNP P42337
A	-8	LEU	-	expression tag	UNP P42337
A	-7	TYR	-	expression tag	UNP P42337
A	-6	PHE	-	expression tag	UNP P42337
A	-5	GLN	-	expression tag	UNP P42337
A	-4	GLY	-	expression tag	UNP P42337
A	-3	ALA	-	expression tag	UNP P42337
A	-2	MET	-	expression tag	UNP P42337

Continued on next page...

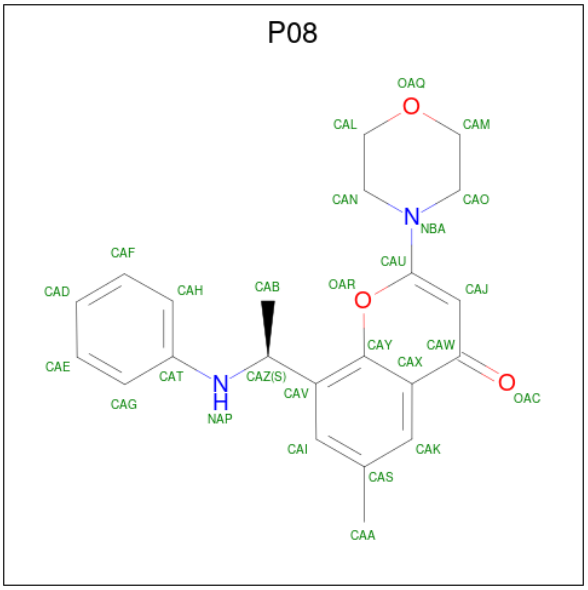
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP P42337
A	0	PRO	-	expression tag	UNP P42337

- Molecule 2 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE REGULATORY SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	141	1240	772	224	239	5	0	0	0

- Molecule 3 is PIK-108 (three-letter code: P08) (formula: $C_{22}H_{24}N_2O_3$).



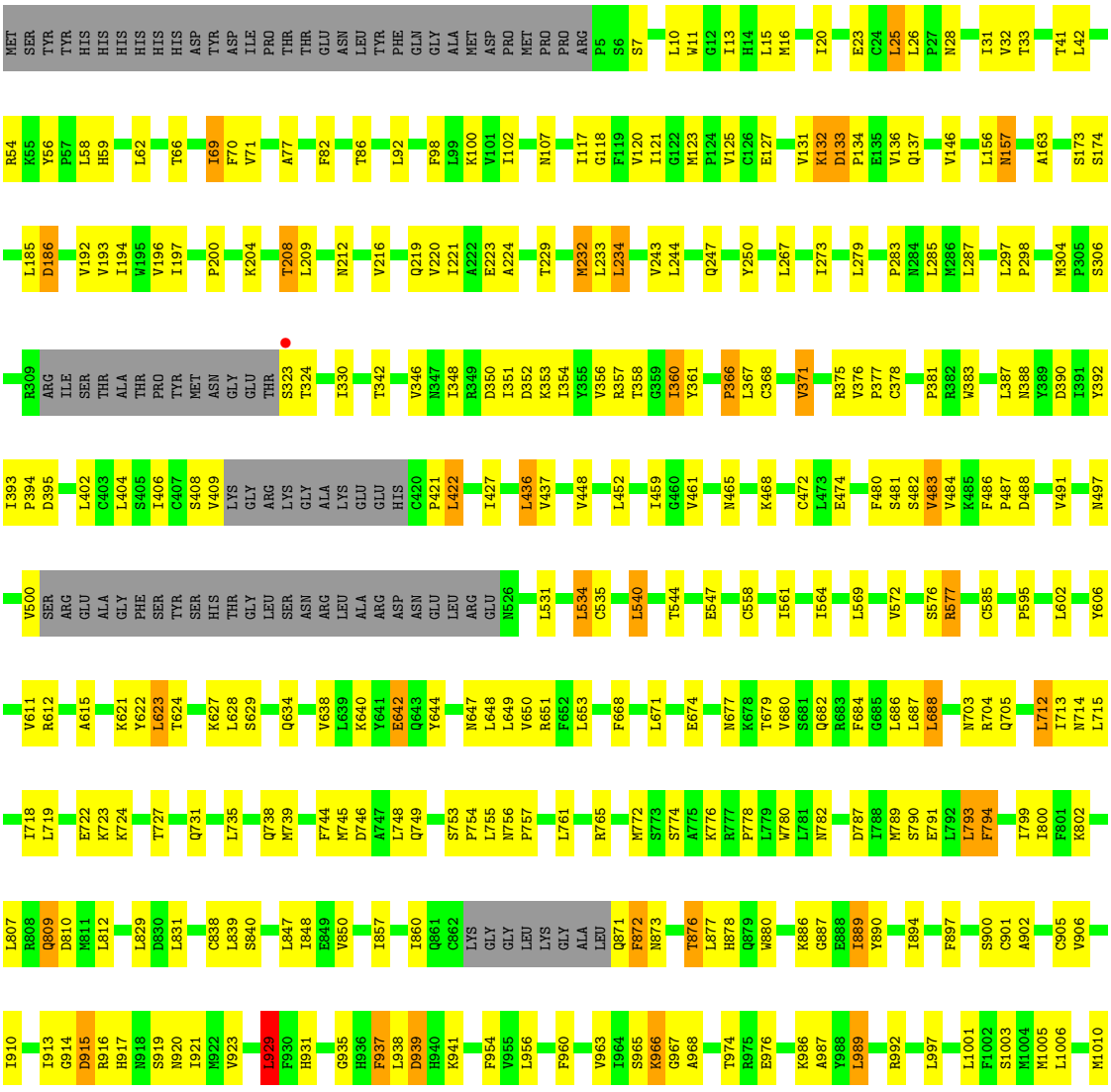
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	22	2	3	0	0
3	A	1	27	22	2	3	0	0

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.

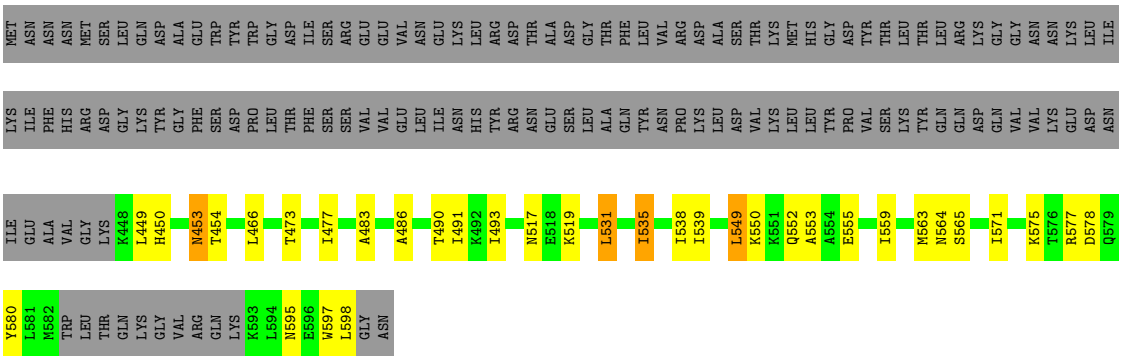
• Molecule 1: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT ALPHA ISOFORM

Chain A: 62% 26% • 9%



• Molecule 2: PHOSPHATIDYLINOSITOL 3-KINASE REGULATORY SUBUNIT ALPHA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	136.09Å 147.18Å 226.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.41 – 3.50 68.05 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (123.41-3.50) 100.0 (68.05-3.50)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 3.49Å)	Xtriage
Refinement program	REFMAC 5.7.0002	Depositor
R, R_{free}	0.183 , 0.228 0.188 , 0.232	Depositor DCC
R_{free} test set	1484 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	124.3	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 94.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9508	wwPDB-VP
Average B, all atoms (Å^2)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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: P08

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	0.63	1/8403 (0.0%)	0.79	3/11365 (0.0%)
2	B	0.53	0/1256	0.67	0/1670
All	All	0.62	1/9659 (0.0%)	0.78	3/13035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	915	ASP	CB-CG	5.63	1.63	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1028	LEU	CA-CB-CG	6.51	130.26	115.30
1	A	938	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	929	LEU	CA-CB-CG	5.02	126.84	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	8214	0	8219	292	0
2	B	1240	0	1234	36	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	54	0	48	7	0
All	All	9508	0	9501	322	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 (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ILE:HA	1:A:1025:THR:HG21	1.22	1.18
1:A:535:CYS:HB3	1:A:564:ILE:HG22	1.38	1.06
1:A:279:LEU:HD13	1:A:279:LEU:O	1.62	0.99
1:A:23:GLU:OE1	1:A:33:THR:HG22	1.63	0.99
1:A:992:ARG:NH1	1:A:1027:ALA:HB3	1.81	0.96
1:A:715:LEU:HD21	1:A:735:LEU:HD13	1.46	0.96
1:A:461:VAL:HG11	1:A:679:THR:HG23	1.46	0.95
1:A:913:ILE:HG22	1:A:916:ARG:HD3	1.48	0.95
1:A:461:VAL:HG11	1:A:679:THR:CG2	1.99	0.93
1:A:913:ILE:CG2	1:A:916:ARG:HD3	2.00	0.92
1:A:1027:ALA:HB1	1:A:1030:LYS:HB2	1.51	0.90
1:A:679:THR:HG22	1:A:680:VAL:HG13	1.55	0.89
1:A:121:ILE:HG13	1:A:688:LEU:HD12	1.56	0.85
1:A:712:LEU:CD1	1:A:748:LEU:HD11	2.08	0.84
1:A:376:VAL:O	1:A:376:VAL:HG13	1.77	0.84
1:A:722:GLU:O	1:A:724:LYS:N	2.13	0.82
1:A:910:ILE:CA	1:A:1025:THR:HG21	2.08	0.82
1:A:569:LEU:O	1:A:572:VAL:HG12	1.80	0.81
1:A:910:ILE:HA	1:A:1025:THR:CG2	2.07	0.81
1:A:297:LEU:HD12	1:A:297:LEU:O	1.81	0.80
1:A:422:LEU:HD22	2:B:564:ASN:ND2	1.97	0.80
1:A:1003:SER:HA	1:A:1006:LEU:HD13	1.65	0.78
1:A:367:LEU:HD21	1:A:390:ASP:OD1	1.82	0.78
1:A:793:LEU:HD12	1:A:794:PHE:CZ	2.19	0.78
1:A:544:THR:HG22	1:A:547:GLU:OE2	1.84	0.78
1:A:448:VAL:HG13	1:A:452:LEU:HD23	1.67	0.76
1:A:860:ILE:HD11	1:A:880:TRP:CZ3	2.20	0.76
1:A:193:VAL:HG22	1:A:208:THR:HG22	1.68	0.76
1:A:966:LYS:O	1:A:968:ALA:N	2.15	0.75
1:A:886:LYS:O	1:A:889:ILE:HD12	1.86	0.75
1:A:744:PHE:CE1	1:A:748:LEU:HD12	2.21	0.75
1:A:712:LEU:HD11	1:A:748:LEU:CD1	2.17	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:ILE:HD11	1:A:880:TRP:CE3	2.21	0.75
1:A:535:CYS:CB	1:A:564:ILE:HG22	2.17	0.74
1:A:353:LYS:HA	1:A:376:VAL:HG21	1.69	0.73
1:A:409:VAL:HG12	1:A:409:VAL:O	1.90	0.72
1:A:921:ILE:HD12	1:A:931:HIS:CE1	2.26	0.71
1:A:234:LEU:HD12	1:A:234:LEU:O	1.90	0.71
2:B:535:ILE:HD12	2:B:535:ILE:C	2.11	0.71
1:A:916:ARG:HA	1:A:920:ASN:HD22	1.56	0.70
1:A:1027:ALA:HB2	1:A:1035:ALA:HB2	1.72	0.70
1:A:488:ASP:O	1:A:491:VAL:HG12	1.92	0.70
1:A:624:THR:HG23	1:A:627:LYS:H	1.54	0.69
1:A:640:LYS:HG2	1:A:680:VAL:HG11	1.75	0.69
1:A:1006:LEU:HD11	1:A:1019:ILE:HD11	1.74	0.69
1:A:361:TYR:HA	1:A:366:PRO:HD3	1.75	0.68
1:A:873:ASN:O	1:A:876:THR:HG22	1.92	0.67
1:A:793:LEU:HD12	1:A:794:PHE:CE2	2.30	0.67
1:A:860:ILE:HG21	1:A:877:LEU:HD23	1.76	0.66
1:A:1027:ALA:HB2	1:A:1035:ALA:CB	2.24	0.66
2:B:535:ILE:HD12	2:B:535:ILE:O	1.95	0.66
1:A:558:CYS:SG	1:A:564:ILE:HD11	2.36	0.65
1:A:682:GLN:O	1:A:686:LEU:HD13	1.97	0.65
1:A:193:VAL:HG22	1:A:208:THR:CG2	2.25	0.65
1:A:712:LEU:HD11	1:A:748:LEU:HD11	1.78	0.64
1:A:26:LEU:HD12	1:A:32:VAL:HG21	1.80	0.64
1:A:26:LEU:CD1	1:A:32:VAL:HG21	2.28	0.64
1:A:871:GLN:O	1:A:872:PHE:HB3	1.98	0.64
1:A:497:ASN:HA	1:A:500:VAL:HG12	1.80	0.64
3:A:2062:P08:HAB3	3:A:2062:P08:OAR	1.99	0.63
1:A:860:ILE:HD11	1:A:880:TRP:CD2	2.32	0.63
1:A:860:ILE:HD11	1:A:880:TRP:CH2	2.33	0.63
1:A:360:ILE:HD11	1:A:366:PRO:HG2	1.79	0.63
1:A:544:THR:HG22	1:A:547:GLU:CD	2.19	0.63
1:A:712:LEU:CD1	1:A:748:LEU:CD1	2.77	0.62
1:A:780:TRP:CE3	1:A:800:ILE:HD11	2.35	0.62
1:A:857:ILE:O	1:A:860:ILE:HG22	2.00	0.62
2:B:473:THR:HG22	2:B:477:ILE:CD1	2.29	0.62
1:A:650:VAL:HG13	1:A:687:LEU:HD13	1.81	0.62
1:A:712:LEU:HD11	1:A:748:LEU:HD13	1.81	0.62
1:A:989:LEU:HD21	1:A:1032:GLU:HG2	1.81	0.61
1:A:26:LEU:HD12	1:A:32:VAL:CG2	2.31	0.61
1:A:267:LEU:CD1	1:A:273:ILE:HG12	2.30	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HG23	1:A:123:MET:H	1.66	0.61
1:A:23:GLU:OE1	1:A:33:THR:CG2	2.44	0.60
1:A:992:ARG:HH11	1:A:1027:ALA:HB3	1.60	0.60
1:A:358:THR:HG21	1:A:387:LEU:HD12	1.82	0.60
1:A:69:ILE:HD11	1:A:82:PHE:O	2.03	0.59
1:A:1005:MET:CE	1:A:1010:MET:HE2	2.32	0.59
1:A:267:LEU:HD13	1:A:273:ILE:HG12	1.83	0.59
1:A:376:VAL:O	1:A:376:VAL:CG1	2.48	0.59
1:A:684:PHE:O	1:A:688:LEU:HB2	2.02	0.59
1:A:42:LEU:HD11	1:A:92:LEU:HD11	1.85	0.59
1:A:602:LEU:O	1:A:638:VAL:HG22	2.03	0.59
1:A:360:ILE:CD1	1:A:366:PRO:HG2	2.32	0.59
1:A:900:SER:OG	1:A:929:LEU:HD12	2.02	0.59
1:A:916:ARG:HA	1:A:920:ASN:ND2	2.16	0.59
1:A:197:ILE:C	1:A:197:ILE:HD12	2.23	0.59
1:A:459:ILE:HG22	1:A:459:ILE:O	2.03	0.59
2:B:450:HIS:O	2:B:454:THR:HG23	2.03	0.59
1:A:69:ILE:HD12	1:A:70:PHE:H	1.66	0.58
2:B:473:THR:HG22	2:B:477:ILE:HD13	1.85	0.58
1:A:802:LYS:HD2	1:A:807:LEU:HD21	1.85	0.58
1:A:436:LEU:HD22	1:A:437:VAL:N	2.18	0.58
1:A:1027:ALA:CB	1:A:1035:ALA:HB2	2.32	0.58
1:A:71:VAL:HG21	1:A:102:ILE:HD11	1.86	0.58
1:A:350:ASP:OD2	2:B:565:SER:OG	2.22	0.58
1:A:216:VAL:HG22	1:A:219:GLN:OE1	2.03	0.58
2:B:449:LEU:HD11	2:B:580:TYR:HB2	1.85	0.58
1:A:15:LEU:HD23	1:A:16:MET:O	2.04	0.58
1:A:602:LEU:O	1:A:638:VAL:CG2	2.52	0.57
1:A:540:LEU:HD12	1:A:540:LEU:O	2.04	0.57
1:A:913:ILE:HG21	1:A:916:ARG:HD3	1.81	0.57
1:A:194:ILE:HD11	1:A:220:VAL:CG1	2.34	0.57
1:A:353:LYS:HA	1:A:376:VAL:CG2	2.34	0.56
1:A:650:VAL:CG1	1:A:687:LEU:HD13	2.34	0.56
1:A:997:LEU:HD13	1:A:997:LEU:O	2.06	0.56
1:A:1005:MET:HE3	1:A:1010:MET:HE2	1.86	0.56
1:A:756:ASN:HD22	1:A:757:PRO:HD2	1.72	0.55
1:A:921:ILE:HD12	1:A:931:HIS:NE2	2.21	0.55
1:A:229:THR:HG23	1:A:232:MET:CE	2.36	0.55
1:A:204:LYS:HG2	1:A:789:MET:HE1	1.87	0.55
1:A:361:TYR:HA	1:A:366:PRO:CD	2.36	0.55
1:A:229:THR:HG21	1:A:234:LEU:HD21	1.87	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:744:PHE:HE1	1:A:748:LEU:HD12	1.72	0.54
2:B:549:LEU:HD23	2:B:550:LYS:N	2.22	0.54
1:A:32:VAL:HG13	1:A:56:TYR:CE2	2.42	0.54
1:A:234:LEU:CD1	1:A:234:LEU:C	2.76	0.54
2:B:491:ILE:HG22	2:B:538:ILE:CG2	2.38	0.54
1:A:829:LEU:HD21	1:A:986:LYS:HB2	1.90	0.54
1:A:873:ASN:O	1:A:876:THR:CG2	2.56	0.54
1:A:800:ILE:HD13	1:A:850:VAL:HG22	1.88	0.54
1:A:357:ARG:HG3	1:A:371:VAL:HG12	1.90	0.54
1:A:243:VAL:HG23	1:A:244:LEU:N	2.23	0.53
1:A:279:LEU:O	1:A:279:LEU:CD1	2.47	0.53
1:A:421:PRO:HG2	1:A:448:VAL:HG21	1.90	0.53
1:A:860:ILE:HD11	1:A:880:TRP:CE2	2.42	0.53
1:A:939:ASP:O	1:A:941:LYS:N	2.41	0.53
1:A:831:LEU:CD1	1:A:987:ALA:HB2	2.39	0.53
1:A:234:LEU:HD12	1:A:234:LEU:C	2.28	0.53
1:A:902:ALA:O	1:A:906:VAL:HG12	2.07	0.53
1:A:897:PHE:CZ	1:A:963:VAL:HG11	2.44	0.53
1:A:185:LEU:O	1:A:186:ASP:HB3	2.08	0.53
2:B:559:ILE:O	2:B:563:MET:HB2	2.09	0.53
1:A:346:VAL:CG2	2:B:564:ASN:HD22	2.22	0.52
1:A:561:ILE:N	1:A:561:ILE:HD12	2.24	0.52
1:A:196:VAL:HG22	1:A:287:LEU:HB3	1.90	0.52
1:A:229:THR:CG2	1:A:234:LEU:HD21	2.40	0.52
1:A:712:LEU:HD13	1:A:748:LEU:HD11	1.87	0.52
1:A:960:PHE:O	1:A:963:VAL:HG12	2.09	0.52
1:A:98:PHE:CE2	2:B:490:THR:HG23	2.45	0.52
2:B:517:ASN:O	2:B:519:LYS:N	2.38	0.52
1:A:209:LEU:HD23	1:A:223:GLU:HB3	1.91	0.51
1:A:772:MET:HB2	3:A:2062:P08:CAD	2.40	0.51
1:A:10:LEU:HD23	1:A:13:ILE:HD12	1.91	0.51
1:A:367:LEU:HD13	1:A:368:CYS:C	2.31	0.51
1:A:221:ILE:O	1:A:224:ALA:HB3	2.10	0.51
1:A:367:LEU:HD13	1:A:368:CYS:O	2.11	0.51
1:A:677:ASN:OD1	1:A:677:ASN:C	2.49	0.51
1:A:739:MET:HG2	1:A:744:PHE:CE1	2.46	0.51
1:A:250:TYR:CD1	1:A:287:LEU:HD21	2.45	0.51
1:A:357:ARG:NH1	1:A:371:VAL:CG1	2.74	0.51
1:A:623:LEU:HD23	1:A:628:LEU:HB2	1.93	0.51
1:A:358:THR:HG21	1:A:387:LEU:CD1	2.40	0.51
1:A:954:PHE:CE2	3:A:2063:P08:CAW	2.94	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:HD12	1:A:209:LEU:HD13	1.93	0.50
1:A:221:ILE:HD12	1:A:250:TYR:HB2	1.94	0.50
1:A:461:VAL:HG11	1:A:679:THR:HG21	1.87	0.50
1:A:32:VAL:HG13	1:A:56:TYR:HE2	1.76	0.50
1:A:77:ALA:HB2	2:B:486:ALA:HB2	1.94	0.50
1:A:917:HIS:HD2	1:A:919:SER:H	1.60	0.50
2:B:449:LEU:HD21	2:B:580:TYR:HB3	1.93	0.50
2:B:550:LYS:O	2:B:553:ALA:HB3	2.12	0.50
2:B:571:ILE:HG23	2:B:575:LYS:HZ3	1.75	0.50
1:A:612:ARG:NH1	1:A:642:GLU:OE1	2.44	0.50
1:A:352:ASP:O	1:A:376:VAL:HG21	2.11	0.50
1:A:713:ILE:HG22	1:A:714:ASN:N	2.27	0.50
2:B:491:ILE:CG2	2:B:538:ILE:HG22	2.42	0.50
2:B:598:LEU:N	2:B:598:LEU:HD22	2.27	0.49
1:A:860:ILE:HD11	1:A:880:TRP:CZ2	2.47	0.49
1:A:346:VAL:HG22	2:B:564:ASN:HB2	1.95	0.49
1:A:876:THR:HG23	1:A:877:LEU:N	2.26	0.49
1:A:671:LEU:CB	1:A:688:LEU:HD23	2.41	0.49
1:A:197:ILE:HD12	1:A:197:ILE:O	2.12	0.49
1:A:15:LEU:HB2	1:A:718:ILE:HD11	1.93	0.49
1:A:1056:ASP:C	1:A:1057:TRP:O	2.49	0.49
1:A:243:VAL:O	1:A:244:LEU:C	2.51	0.49
2:B:466:LEU:CD1	2:B:559:ILE:HG23	2.42	0.49
1:A:367:LEU:CD2	1:A:390:ASP:OD1	2.57	0.48
1:A:704:ARG:NH2	1:A:746:ASP:O	2.46	0.48
1:A:623:LEU:HD21	1:A:628:LEU:HA	1.96	0.48
1:A:1005:MET:CE	1:A:1010:MET:CE	2.91	0.48
2:B:491:ILE:CG2	2:B:538:ILE:CG2	2.91	0.48
1:A:354:ILE:HB	1:A:376:VAL:HG23	1.95	0.48
1:A:360:ILE:O	1:A:366:PRO:HD2	2.13	0.48
1:A:602:LEU:HD13	1:A:649:LEU:HD22	1.95	0.48
1:A:642:GLU:O	1:A:644:TYR:N	2.39	0.48
1:A:719:LEU:HD22	1:A:731:GLN:NE2	2.28	0.48
1:A:342:THR:HG23	1:A:472:CYS:O	2.13	0.48
1:A:409:VAL:O	1:A:409:VAL:CG1	2.61	0.48
1:A:602:LEU:HD21	1:A:615:ALA:HB3	1.96	0.48
1:A:1003:SER:HA	1:A:1006:LEU:CD1	2.38	0.48
1:A:146:VAL:HG21	1:A:651:ARG:HD3	1.95	0.48
1:A:348:ILE:O	1:A:352:ASP:HB3	2.14	0.47
1:A:375:ARG:HG3	1:A:377:PRO:HD3	1.96	0.47
1:A:487:PRO:HB2	1:A:491:VAL:CG1	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:O	1:A:186:ASP:CB	2.62	0.47
1:A:905:CYS:SG	1:A:1043:MET:CE	3.02	0.47
2:B:473:THR:O	2:B:477:ILE:HD13	2.14	0.47
1:A:323:SER:O	1:A:482:SER:HB2	2.14	0.47
1:A:606:TYR:HB3	1:A:611:VAL:HG11	1.96	0.47
1:A:324:THR:HG22	1:A:483:VAL:HG12	1.97	0.47
1:A:133:ASP:HB3	1:A:136:VAL:HG22	1.97	0.47
1:A:897:PHE:CE1	1:A:963:VAL:HG11	2.50	0.47
1:A:871:GLN:O	1:A:872:PHE:CB	2.62	0.47
1:A:323:SER:O	1:A:323:SER:OG	2.25	0.47
1:A:342:THR:HG21	1:A:472:CYS:HB3	1.97	0.47
1:A:480:PHE:O	1:A:481:SER:C	2.52	0.47
1:A:1006:LEU:HD11	1:A:1019:ILE:CD1	2.44	0.47
1:A:901:CYS:HA	1:A:929:LEU:HD11	1.97	0.46
1:A:531:LEU:HD23	1:A:534:LEU:HD21	1.97	0.46
1:A:1031:THR:O	1:A:1032:GLU:C	2.54	0.46
1:A:146:VAL:HG23	1:A:651:ARG:HH11	1.80	0.46
1:A:921:ILE:HD12	1:A:931:HIS:CD2	2.49	0.46
1:A:954:PHE:HE2	3:A:2063:P08:CAW	2.28	0.46
1:A:558:CYS:CB	1:A:564:ILE:HD11	2.45	0.46
1:A:353:LYS:CA	1:A:376:VAL:HG21	2.40	0.46
1:A:448:VAL:CG1	1:A:452:LEU:HD23	2.42	0.46
1:A:921:ILE:HG21	1:A:929:LEU:HD22	1.97	0.46
1:A:640:LYS:HZ3	1:A:674:GLU:HG2	1.80	0.46
1:A:208:THR:C	1:A:209:LEU:HD12	2.36	0.46
1:A:393:ILE:N	1:A:394:PRO:CD	2.78	0.46
1:A:671:LEU:HB2	1:A:688:LEU:HD23	1.98	0.46
1:A:900:SER:OG	1:A:929:LEU:O	2.34	0.46
1:A:1043:MET:HB3	3:A:2063:P08:CAG	2.45	0.46
3:A:2062:P08:OAR	3:A:2062:P08:CAB	2.64	0.46
2:B:531:LEU:O	2:B:535:ILE:HG23	2.15	0.46
1:A:163:ALA:HB2	1:A:297:LEU:HD21	1.98	0.45
1:A:921:ILE:CD1	1:A:931:HIS:CD2	2.99	0.45
1:A:719:LEU:HD22	1:A:731:GLN:HE21	1.81	0.45
1:A:905:CYS:SG	1:A:1043:MET:HE3	2.56	0.45
2:B:453:ASN:ND2	2:B:577:ARG:HD2	2.32	0.45
1:A:595:PRO:HB3	1:A:623:LEU:HD12	1.98	0.45
1:A:1005:MET:HE3	1:A:1010:MET:CE	2.46	0.45
1:A:146:VAL:CG2	1:A:651:ARG:HD3	2.45	0.45
1:A:812:LEU:HD23	1:A:937:PHE:HZ	1.81	0.45
1:A:860:ILE:CG2	1:A:877:LEU:HD23	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:ILE:HG21	2:B:539:ILE:HD13	1.99	0.45
2:B:595:ASN:O	2:B:598:LEU:HD23	2.16	0.45
1:A:544:THR:HG22	1:A:547:GLU:CG	2.47	0.44
1:A:787:ASP:O	1:A:790:SER:OG	2.35	0.44
1:A:26:LEU:HD11	1:A:32:VAL:HG21	2.00	0.44
1:A:376:VAL:O	1:A:376:VAL:HG22	2.18	0.44
1:A:376:VAL:HG22	1:A:378:CYS:SG	2.58	0.44
2:B:535:ILE:C	2:B:535:ILE:CD1	2.79	0.44
1:A:58:LEU:HD12	1:A:58:LEU:N	2.32	0.44
1:A:356:VAL:HG22	1:A:406:ILE:HG12	1.99	0.44
1:A:395:ASP:HA	1:A:577:ARG:HB2	1.99	0.44
1:A:634:GLN:HG2	1:A:1001:LEU:HD22	1.98	0.44
1:A:229:THR:HG23	1:A:232:MET:HE1	2.00	0.44
1:A:402:LEU:HD21	1:A:404:LEU:HD23	1.99	0.44
1:A:923:VAL:HG22	1:A:929:LEU:HB3	2.00	0.44
1:A:427:ILE:O	1:A:427:ILE:HG22	2.17	0.43
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.39	0.43
1:A:812:LEU:HD23	1:A:937:PHE:CZ	2.53	0.43
1:A:829:LEU:HD21	1:A:986:LYS:CB	2.48	0.43
1:A:965:SER:C	1:A:966:LYS:O	2.57	0.43
1:A:71:VAL:HG21	1:A:102:ILE:CD1	2.48	0.43
1:A:878:HIS:CD2	1:A:963:VAL:HA	2.53	0.43
1:A:120:VAL:HG22	1:A:703:ASN:HA	2.01	0.43
1:A:194:ILE:HD12	1:A:209:LEU:CD1	2.48	0.43
1:A:244:LEU:HD12	1:A:244:LEU:O	2.19	0.43
1:A:913:ILE:HG22	1:A:916:ARG:CD	2.34	0.43
1:A:25:LEU:HD12	1:A:31:ILE:HG13	1.99	0.43
1:A:297:LEU:O	1:A:297:LEU:CD1	2.62	0.43
1:A:839:LEU:HD12	1:A:840:SER:N	2.33	0.43
2:B:491:ILE:HG22	2:B:538:ILE:HG21	2.00	0.43
2:B:535:ILE:O	2:B:539:ILE:HG12	2.19	0.43
1:A:28:ASN:HB3	1:A:62:LEU:HD21	2.01	0.43
1:A:897:PHE:CE1	1:A:963:VAL:CG1	3.02	0.43
1:A:544:THR:HG23	1:A:547:GLU:H	1.84	0.43
1:A:486:PHE:CG	1:A:487:PRO:HD2	2.54	0.42
1:A:753:SER:HB2	1:A:761:LEU:HD21	2.01	0.42
2:B:571:ILE:HG23	2:B:575:LYS:NZ	2.34	0.42
1:A:648:LEU:H	1:A:648:LEU:HD12	1.83	0.42
1:A:41:THR:HG22	1:A:86:THR:O	2.20	0.42
1:A:287:LEU:HD23	1:A:287:LEU:C	2.40	0.42
1:A:623:LEU:CD2	1:A:628:LEU:HB2	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:PHE:CE1	1:A:688:LEU:HD11	2.55	0.42
2:B:466:LEU:HD12	2:B:559:ILE:HG23	2.01	0.42
1:A:82:PHE:CE1	1:A:92:LEU:HD22	2.54	0.42
1:A:765:ARG:HB2	1:A:782:ASN:HB3	2.02	0.42
1:A:279:LEU:HD13	1:A:279:LEU:C	2.36	0.42
1:A:243:VAL:O	1:A:247:GLN:HB2	2.20	0.42
1:A:360:ILE:C	1:A:360:ILE:HD12	2.40	0.42
1:A:376:VAL:CG2	1:A:378:CYS:SG	3.08	0.42
1:A:679:THR:HG22	1:A:680:VAL:CG1	2.36	0.42
1:A:576:SER:O	1:A:577:ARG:CB	2.68	0.41
1:A:954:PHE:CE2	3:A:2063:P08:CAJ	3.02	0.41
1:A:15:LEU:HD11	1:A:738:GLN:OE1	2.20	0.41
1:A:131:VAL:HG12	1:A:137:GLN:HE22	1.85	0.41
1:A:192:VAL:HG22	1:A:283:PRO:HG2	2.02	0.41
1:A:229:THR:CG2	1:A:232:MET:HE3	2.50	0.41
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.55	0.41
1:A:800:ILE:HD13	1:A:850:VAL:CG2	2.50	0.41
1:A:131:VAL:O	1:A:132:LYS:O	2.38	0.41
1:A:755:LEU:HD12	1:A:799:ILE:HD13	2.02	0.41
1:A:809:GLN:HE21	1:A:809:GLN:HB2	1.65	0.41
1:A:11:TRP:CH2	2:B:483:ALA:HB2	2.56	0.41
1:A:330:ILE:HD11	1:A:484:VAL:HG22	2.03	0.41
1:A:974:THR:CG2	1:A:976:GLU:HG2	2.51	0.41
1:A:408:SER:HB3	1:A:422:LEU:HD11	2.03	0.41
1:A:234:LEU:O	1:A:234:LEU:CD1	2.66	0.41
1:A:465:ASN:O	1:A:468:LYS:NZ	2.54	0.41
1:A:649:LEU:HD12	1:A:653:LEU:HD23	2.03	0.41
1:A:772:MET:HG3	1:A:774:SER:H	1.85	0.41
1:A:54:ARG:HA	1:A:59:HIS:HB2	2.03	0.41
1:A:754:PRO:HB2	1:A:847:LEU:HD12	2.03	0.41
1:A:800:ILE:HB	1:A:848:ILE:HB	2.02	0.41
1:A:914:GLY:O	1:A:915:ASP:C	2.59	0.41
1:A:997:LEU:HD13	1:A:997:LEU:C	2.41	0.41
1:A:621:LYS:HG2	1:A:622:TYR:CE1	2.57	0.40
1:A:778:PRO:HB3	1:A:802:LYS:HG3	2.03	0.40
1:A:118:GLY:HA2	1:A:121:ILE:HG22	2.04	0.40
1:A:156:LEU:O	1:A:157:ASN:CB	2.69	0.40
1:A:745:MET:O	1:A:749:GLN:HB2	2.21	0.40
2:B:552:GLN:HA	2:B:555:GLU:HG2	2.03	0.40
1:A:100:LYS:HB2	2:B:493:ILE:HD11	2.03	0.40
1:A:117:ILE:O	1:A:121:ILE:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:HD22	1:A:285:LEU:N	2.36	0.40
1:A:544:THR:CG2	1:A:547:GLU:OE2	2.62	0.40
1:A:890:TYR:CE1	1:A:894:ILE:HD12	2.57	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	991/1096 (90%)	855 (86%)	109 (11%)	27 (3%)	5 33
2	B	137/279 (49%)	130 (95%)	7 (5%)	0	100 100
All	All	1128/1375 (82%)	985 (87%)	116 (10%)	27 (2%)	6 35

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	LYS
1	A	200	PRO
1	A	366	PRO
1	A	577	ARG
1	A	723	LYS
1	A	935	GLY
1	A	1047	HIS
1	A	173	SER
1	A	186	ASP
1	A	939	ASP
1	A	967	GLY
1	A	157	ASN
1	A	351	ILE
1	A	966	LYS
1	A	1032	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	174	SER
1	A	422	LEU
1	A	872	PHE
1	A	887	GLY
1	A	1057	TRP
1	A	107	ASN
1	A	133	ASP
1	A	298	PRO
1	A	134	PRO
1	A	876	THR
1	A	381	PRO
1	A	371	VAL

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	924/1003 (92%)	880 (95%)	44 (5%)	25	60
2	B	136/259 (52%)	130 (96%)	6 (4%)	28	62
All	All	1060/1262 (84%)	1010 (95%)	50 (5%)	26	60

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

Mol	Chain	Res	Type
1	A	7	SER
1	A	20	ILE
1	A	25	LEU
1	A	66	THR
1	A	69	ILE
1	A	125	VAL
1	A	127	GLU
1	A	208	THR
1	A	212	ASN
1	A	232	MET
1	A	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	234	LEU
1	A	304	MET
1	A	306	SER
1	A	360	ILE
1	A	388	ASN
1	A	392	TYR
1	A	436	LEU
1	A	474	GLU
1	A	483	VAL
1	A	534	LEU
1	A	540	LEU
1	A	585	CYS
1	A	623	LEU
1	A	629	SER
1	A	642	GLU
1	A	688	LEU
1	A	705	GLN
1	A	712	LEU
1	A	727	THR
1	A	776	LYS
1	A	791	GLU
1	A	793	LEU
1	A	794	PHE
1	A	809	GLN
1	A	810	ASP
1	A	838	CYS
1	A	889	ILE
1	A	929	LEU
1	A	937	PHE
1	A	956	LEU
1	A	989	LEU
1	A	1052	THR
1	A	1061	THR
2	B	453	ASN
2	B	531	LEU
2	B	535	ILE
2	B	549	LEU
2	B	578	ASP
2	B	597	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	63	GLN
1	A	114	ASN
1	A	160	HIS
1	A	205	GLN
1	A	212	ASN
1	A	238	GLN
1	A	269	GLN
1	A	374	GLN
1	A	384	ASN
1	A	467	ASN
1	A	605	ASN
1	A	630	GLN
1	A	705	GLN
1	A	731	GLN
1	A	756	ASN
1	A	760	GLN
1	A	809	GLN
1	A	917	HIS
1	A	920	ASN
1	A	981	GLN
1	A	1014	GLN
1	A	1044	ASN
2	B	478	GLN
2	B	564	ASN

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)

2 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	P08	A	2062	-	29,30,30	2.00	7 (24%)	34,42,42	1.31	5 (14%)
3	P08	A	2063	-	29,30,30	2.35	7 (24%)	34,42,42	1.43	4 (11%)

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	P08	A	2062	-	-	5/12/20/20	0/4/4/4
3	P08	A	2063	-	-	4/12/20/20	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2063	P08	CAV-CAZ	-8.20	1.42	1.52
3	A	2062	P08	CAV-CAZ	-7.46	1.42	1.52
3	A	2063	P08	CAT-NAP	-5.34	1.29	1.39
3	A	2063	P08	CAX-CAW	-4.76	1.40	1.48
3	A	2062	P08	CAX-CAW	-3.66	1.41	1.48
3	A	2063	P08	CAA-CAS	-3.49	1.38	1.51
3	A	2062	P08	CAJ-CAW	-3.06	1.38	1.44
3	A	2063	P08	CAJ-CAW	-2.64	1.39	1.44
3	A	2063	P08	CAZ-NAP	-2.46	1.43	1.46
3	A	2062	P08	CAA-CAS	-2.45	1.42	1.51
3	A	2063	P08	CAN-NBA	2.18	1.50	1.47
3	A	2062	P08	CAB-CAZ	2.13	1.57	1.52
3	A	2062	P08	CAT-NAP	-2.08	1.35	1.39
3	A	2062	P08	OAR-CAU	2.03	1.39	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2063	P08	OAR-CAY-CAV	5.22	120.88	115.22
3	A	2062	P08	OAC-CAW-CAJ	-3.37	116.16	121.79
3	A	2062	P08	CAT-NAP-CAZ	3.23	128.35	122.49
3	A	2062	P08	OAR-CAY-CAV	2.88	118.34	115.22
3	A	2063	P08	CAY-CAX-CAW	2.47	121.85	119.48
3	A	2062	P08	OAC-CAW-CAX	2.35	124.78	121.37
3	A	2062	P08	CAJ-CAU-NBA	-2.32	120.12	124.97
3	A	2063	P08	CAJ-CAU-NBA	-2.13	120.53	124.97
3	A	2063	P08	CAO-NBA-CAN	-2.05	108.67	112.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2062	P08	CAY-CAV-CAZ-CAB
3	A	2062	P08	CAY-CAV-CAZ-NAP
3	A	2062	P08	CAI-CAV-CAZ-CAB
3	A	2062	P08	CAG-CAT-NAP-CAZ
3	A	2062	P08	CAH-CAT-NAP-CAZ
3	A	2063	P08	OAR-CAU-NBA-CAO
3	A	2063	P08	CAV-CAZ-NAP-CAT
3	A	2063	P08	CAG-CAT-NAP-CAZ
3	A	2063	P08	CAH-CAT-NAP-CAZ

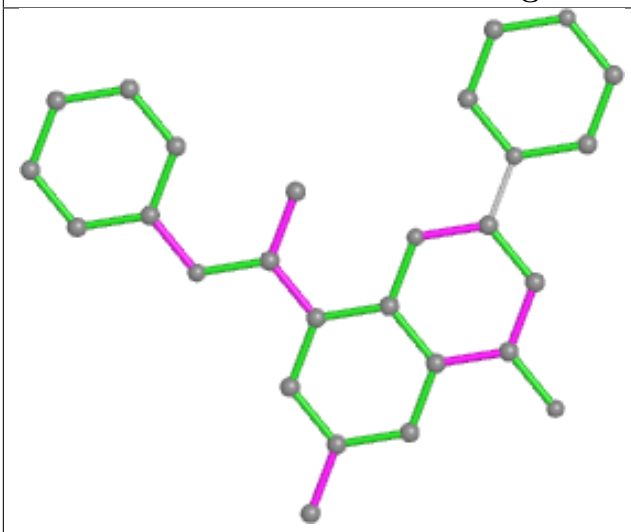
There are no ring outliers.

2 monomers are involved in 7 short contacts:

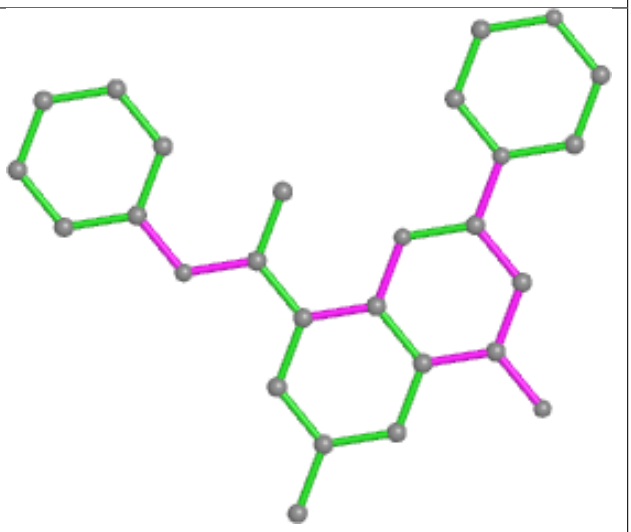
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2062	P08	3	0
3	A	2063	P08	4	0

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 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.

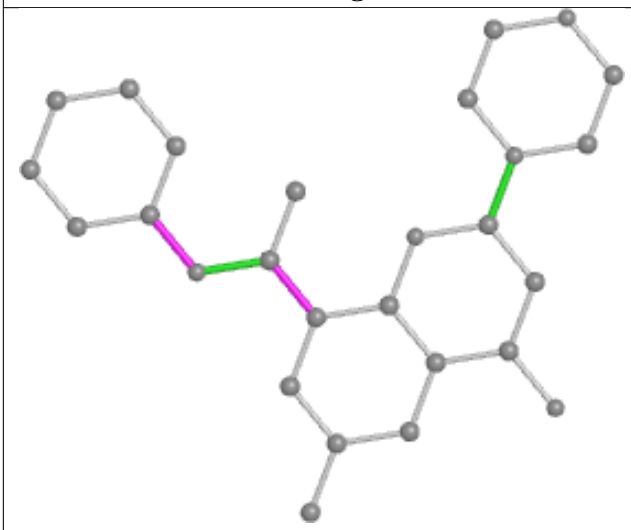
Ligand P08 A 2062



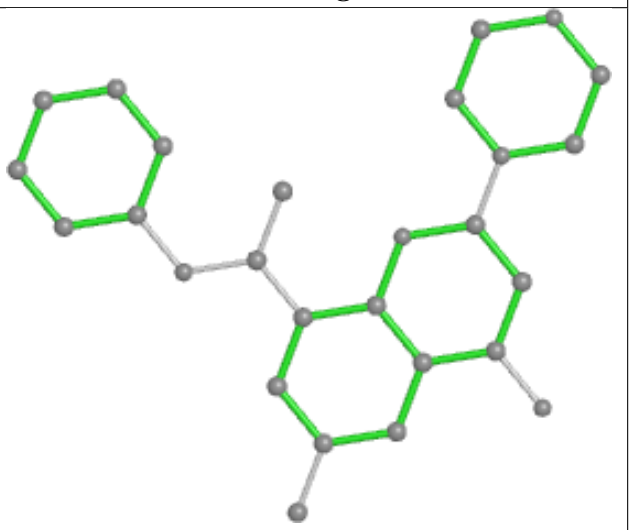
Bond lengths



Bond angles

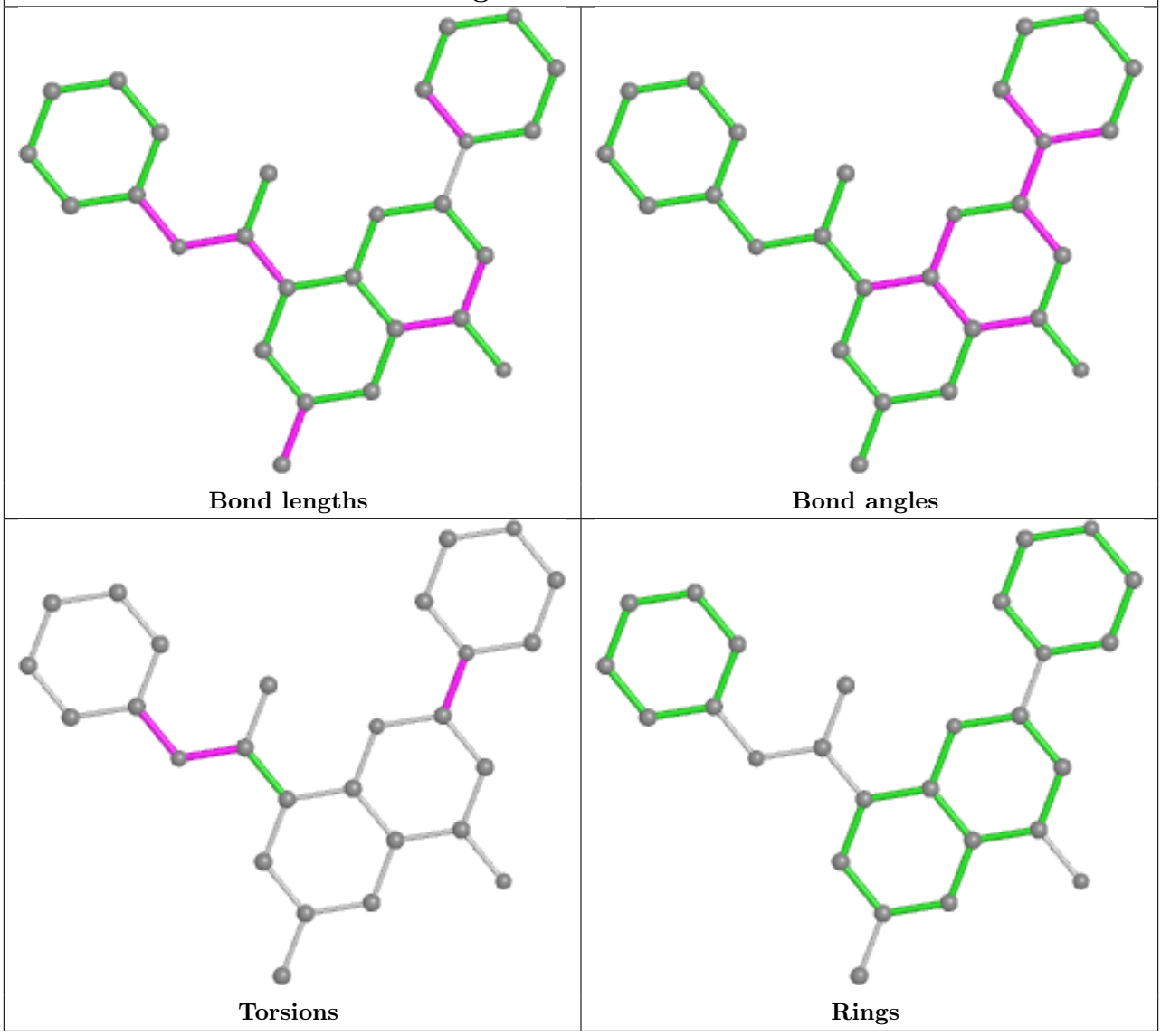


Torsions



Rings

Ligand P08 A 2063



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	1001/1096 (91%)	-0.21	1 (0%) 95 95	87, 134, 179, 231	0
2	B	141/279 (50%)	-0.31	0 100 100	116, 173, 226, 244	0
All	All	1142/1375 (83%)	-0.22	1 (0%) 95 95	87, 138, 191, 244	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	SER	2.3

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.

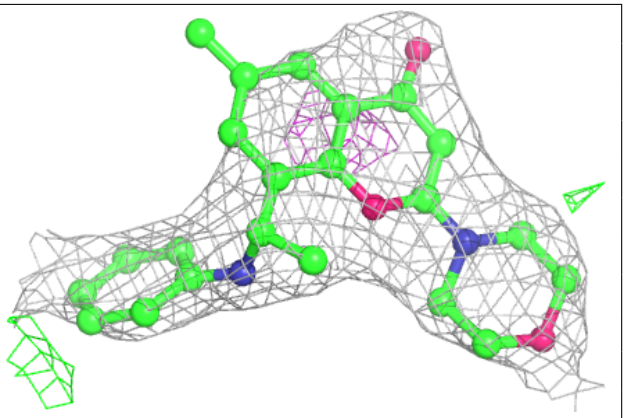
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	P08	A	2062	27/27	0.93	0.33	108,123,150,152	0
3	P08	A	2063	27/27	0.93	0.39	107,116,137,148	0

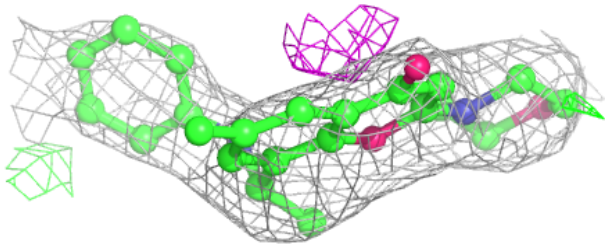
The following is a graphical depiction of the model fit to experimental electron density of all

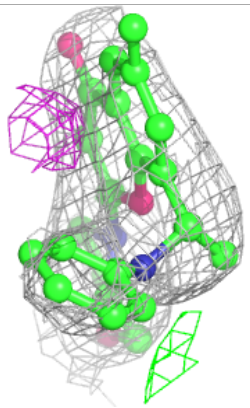
instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around P08 A 2062:

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

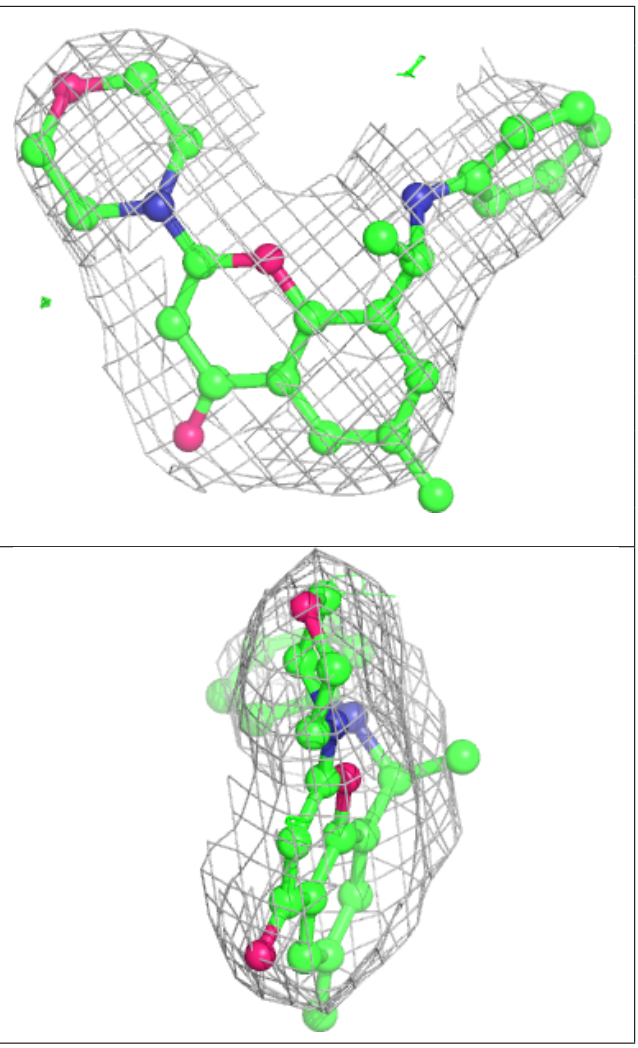






Electron density around P08 A 2063:

$2mF_o$-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.