Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 12:39 pm BST

PDB ID	:	5DXH
Title	:	p110alpha/p85alpha with compound 5
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Deposited on	:	2015-09-23
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 ⓘ symbol.

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

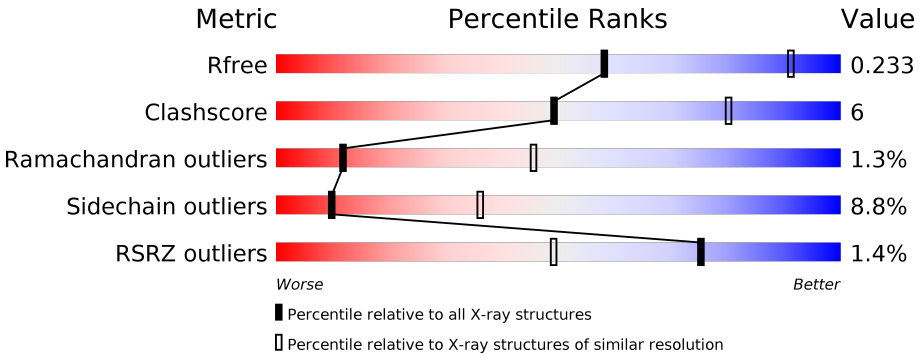
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 on 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	1067	% 73% 18% • 7%
1	D	1067	% 72% 18% • 8%
2	B	169	% 56% 14% • 28%
2	E	169	9% 57% 14% • 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18333 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.

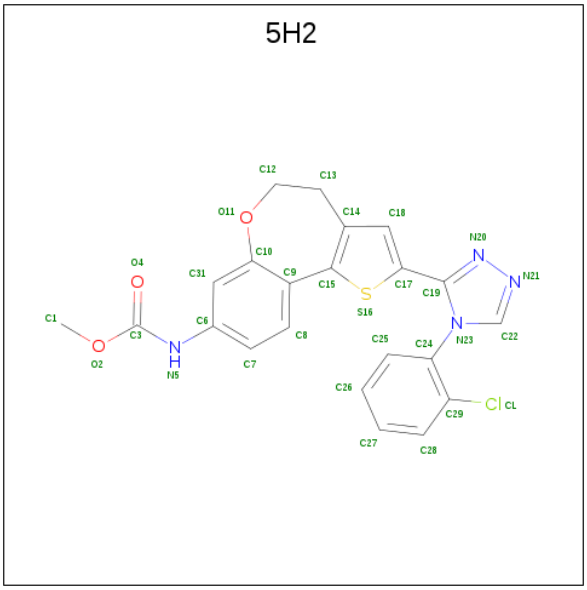
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	989	Total	C	N	O	S	0	0	0
			8093	5185	1375	1464	69			
1	D	981	Total	C	N	O	S	0	0	0
			8033	5153	1361	1450	69			

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			1053	648	194	207	4			
2	E	125	Total	C	N	O	S	0	0	0
			1092	674	198	216	4			

- Molecule 3 is methyl {2-[4-(2-chlorophenyl)-4H-1,2,4-triazol-3-yl]-4,5-dihydrothieno[3,2-d][1]benzoxepin-8-yl}carbamate (three-letter code: 5H2) (formula: $C_{22}H_{17}ClN_4O_3S$).



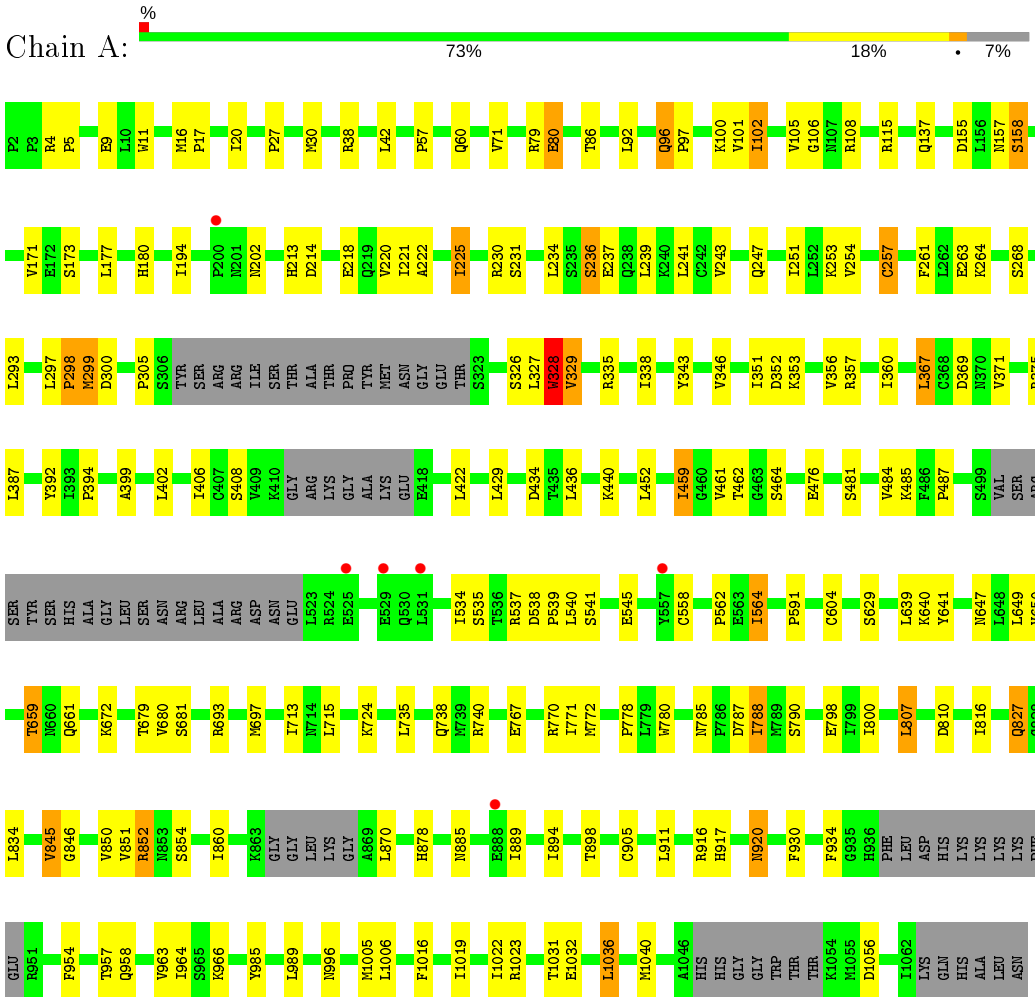
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			31	22	1	4	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			31	22	1	4	3	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

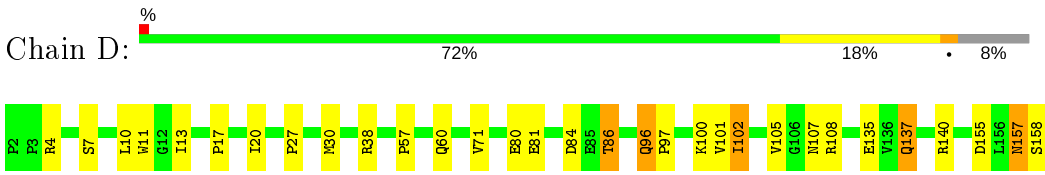
• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

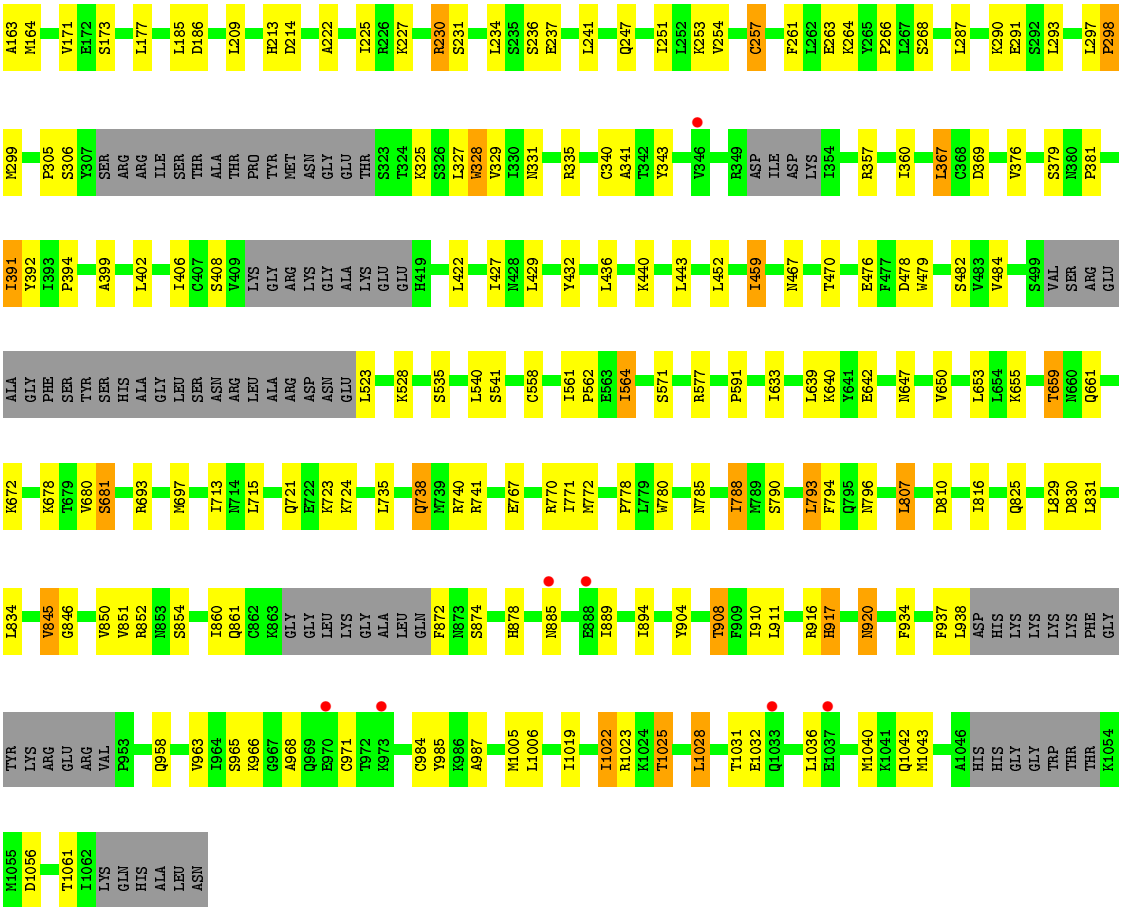
Chain A:



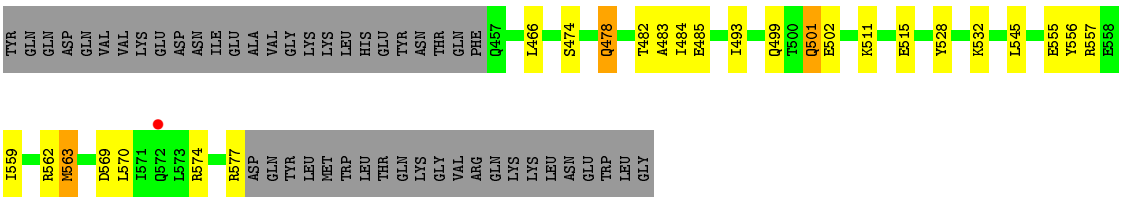
• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

Chain D:

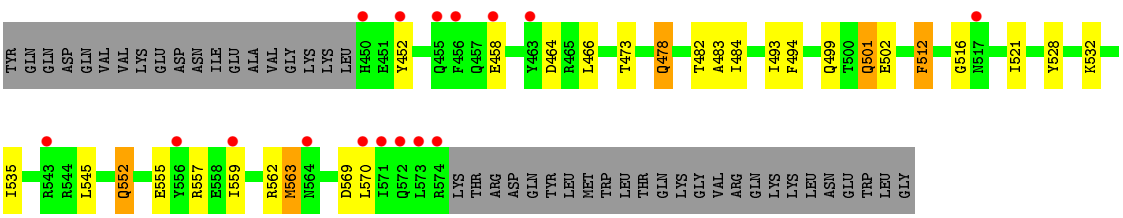




- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	92.66Å 121.83Å 166.36Å 90.00° 102.33° 90.00°	Depositor
Resolution (Å)	49.50 – 3.00 48.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.50-3.00) 97.5 (48.74-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.218 0.198 , 0.233	Depositor DCC
R_{free} test set	3490 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	88.8	Xtriage
Anisotropy	0.438	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 73.1	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	0.95	EDS
Total number of atoms	18333	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5H2

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	0.50	0/8273	0.71	2/11184 (0.0%)
1	D	0.49	0/8214	0.72	3/11104 (0.0%)
2	B	0.48	0/1064	0.66	0/1414
2	E	0.45	0/1106	0.63	0/1473
All	All	0.49	0/18657	0.71	5/25175 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ASN	C-N-CA	5.81	136.22	121.70
1	A	328	TRP	CA-CB-CG	5.61	124.36	113.70
1	D	325	LYS	N-CA-C	-5.53	96.07	111.00
1	A	329	VAL	N-CA-C	-5.51	96.11	111.00
1	D	329	VAL	N-CA-C	-5.28	96.75	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8093	0	8119	106	0
1	D	8033	0	8051	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1053	0	1053	13	0
2	E	1092	0	1072	13	0
3	A	31	0	17	4	0
3	D	31	0	17	0	0
All	All	18333	0	18329	217	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 6.

All (217) 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:851:VAL:HG11	1:A:930:PHE:CZ	2.01	0.93
1:D:328:TRP:HB2	1:D:394:PRO:HB3	1.58	0.82
1:D:721:GLN:O	1:D:724:LYS:HG2	1.87	0.73
1:D:558:CYS:SG	1:D:564:ILE:HD11	2.28	0.73
1:A:558:CYS:SG	1:A:564:ILE:HD11	2.30	0.72
1:A:298:PRO:HG2	1:A:697:MET:HG3	1.72	0.71
1:D:910:ILE:O	1:D:1025:THR:HG21	1.91	0.70
1:A:392:TYR:HB3	1:A:394:PRO:HD2	1.73	0.69
1:D:904:TYR:O	1:D:908:THR:HB	1.92	0.68
1:A:305:PRO:HG3	1:A:693:ARG:HD3	1.76	0.68
1:A:328:TRP:HB2	1:A:394:PRO:HB3	1.76	0.68
1:A:243:VAL:O	1:A:247:GLN:HB2	1.93	0.67
1:D:1023:ARG:HA	1:D:1028:LEU:HD22	1.76	0.67
1:D:305:PRO:HG3	1:D:693:ARG:HD3	1.76	0.66
1:D:298:PRO:HG2	1:D:697:MET:HG3	1.77	0.66
1:A:851:VAL:HG13	1:A:854:SER:OG	1.96	0.65
1:A:851:VAL:HG12	3:A:1101:5H2:H7	1.79	0.65
1:A:851:VAL:HG11	1:A:930:PHE:HZ	1.62	0.65
1:A:328:TRP:HA	1:A:394:PRO:HG3	1.80	0.64
1:A:788:ILE:H	1:A:788:ILE:HD12	1.63	0.64
1:D:878:HIS:HD2	1:D:963:VAL:HA	1.64	0.62
1:A:851:VAL:HG12	3:A:1101:5H2:C12	2.29	0.62
1:A:299:MET:HB3	1:A:697:MET:HG2	1.80	0.62
1:A:434:ASP:HB2	1:A:485:LYS:HE3	1.82	0.61
2:E:484:ILE:HG13	2:E:545:LEU:HD23	1.83	0.61
2:B:484:ILE:HG13	2:B:545:LEU:HD23	1.83	0.60
1:D:639:LEU:HD22	1:D:650:VAL:HG22	1.82	0.60
1:D:965:SER:HB3	1:D:968:ALA:HB3	1.82	0.60
1:A:916:ARG:HA	1:A:920:ASN:HD21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.84	0.60
1:D:788:ILE:H	1:D:788:ILE:HD12	1.65	0.60
1:D:1022:ILE:HA	1:D:1025:THR:HG22	1.83	0.59
1:A:985:TYR:CZ	1:A:1040:MET:HG2	2.39	0.58
1:D:327:LEU:HG	1:D:328:TRP:N	2.19	0.57
1:A:251:ILE:HG21	1:A:293:LEU:HD12	1.87	0.57
1:D:985:TYR:CZ	1:D:1040:MET:HG2	2.39	0.57
1:D:640:LYS:HG2	1:D:680:VAL:HG11	1.87	0.57
1:D:793:LEU:HD13	1:D:794:PHE:CE1	2.40	0.57
1:D:831:LEU:HD11	1:D:987:ALA:HB2	1.87	0.56
1:A:894:ILE:HG21	1:A:966:LYS:HG3	1.86	0.56
1:A:27:PRO:HD3	1:A:101:VAL:HB	1.88	0.56
2:B:466:LEU:HD21	2:B:562:ARG:HB3	1.87	0.56
1:D:816:ILE:HG21	1:D:911:LEU:HD21	1.87	0.56
1:A:604:CYS:HB3	1:A:641:TYR:CE1	2.41	0.55
1:A:798:GLU:HB2	1:A:852:ARG:HH12	1.72	0.55
1:D:535:SER:OG	1:D:564:ILE:HG22	2.06	0.55
1:D:427:ILE:HD11	1:D:443:LEU:HD22	1.88	0.55
1:A:251:ILE:HD12	1:A:290:LYS:HA	1.89	0.55
1:D:540:LEU:HB3	1:D:1023:ARG:HD2	1.89	0.55
2:E:466:LEU:HD21	2:E:562:ARG:HB3	1.89	0.55
1:A:816:ILE:HG21	1:A:911:LEU:HD21	1.89	0.55
1:D:713:ILE:HG12	1:D:845:VAL:HG11	1.89	0.55
1:D:937:PHE:HD1	1:D:938:LEU:HG	1.72	0.55
1:D:640:LYS:HE2	1:D:680:VAL:HG11	1.88	0.54
1:D:251:ILE:HD13	1:D:293:LEU:HD23	1.88	0.54
1:D:27:PRO:HD3	1:D:101:VAL:HB	1.88	0.54
1:D:655:LYS:O	1:D:659:THR:HB	2.08	0.54
1:A:406:ILE:HG22	1:A:422:LEU:HD12	1.89	0.54
1:D:100:LYS:HD2	2:E:493:ILE:HG23	1.90	0.54
1:A:71:VAL:CG2	1:A:102:ILE:HG12	2.39	0.53
1:A:715:LEU:HD21	1:A:735:LEU:HD12	1.90	0.53
1:D:715:LEU:HD21	1:D:735:LEU:HD12	1.90	0.53
1:A:328:TRP:HB3	1:A:394:PRO:HA	1.91	0.53
1:A:30:MET:CE	1:A:57:PRO:HD2	2.39	0.53
1:A:100:LYS:HD2	2:B:493:ILE:HG23	1.90	0.53
1:A:785:ASN:HB3	1:A:790:SER:HB2	1.91	0.53
2:B:466:LEU:HD23	2:B:563:MET:HG3	1.91	0.53
1:A:253:LYS:HE2	1:A:257:CYS:O	2.09	0.52
1:D:406:ILE:HG22	1:D:422:LEU:HD12	1.90	0.52
1:A:540:LEU:HD11	1:A:1016:PHE:HD2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:466:LEU:HD23	2:E:563:MET:HG3	1.91	0.52
1:A:655:LYS:O	1:A:659:THR:HB	2.10	0.52
1:D:71:VAL:HG23	1:D:102:ILE:HG12	1.92	0.52
1:D:251:ILE:HD12	1:D:290:LYS:HA	1.91	0.52
1:A:96:GLN:HG3	1:A:97:PRO:HD2	1.90	0.52
1:D:793:LEU:HD13	1:D:794:PHE:HE1	1.74	0.52
1:A:71:VAL:HG23	1:A:102:ILE:HG12	1.93	0.51
2:B:501:GLN:HG2	2:B:528:TYR:CD1	2.45	0.51
1:D:254:VAL:HG23	1:D:261:PHE:HE1	1.76	0.51
1:D:71:VAL:CG2	1:D:102:ILE:HG12	2.39	0.51
1:D:253:LYS:HE2	1:D:257:CYS:O	2.10	0.51
1:D:30:MET:HE1	1:D:57:PRO:HD2	1.92	0.51
1:D:642:GLU:HG2	1:D:647:ASN:CG	2.31	0.51
1:D:408:SER:HB3	1:D:422:LEU:HD21	1.92	0.51
1:D:96:GLN:HG3	1:D:97:PRO:HD2	1.92	0.51
1:A:221:ILE:O	1:A:225:ILE:HG23	2.11	0.50
1:D:916:ARG:HA	1:D:920:ASN:HD21	1.77	0.50
2:E:512:PHE:HB3	2:E:521:ILE:HG12	1.94	0.50
1:A:894:ILE:O	1:A:898:THR:HG23	2.11	0.50
1:A:851:VAL:HG12	3:A:1101:5H2:O11	2.12	0.50
2:E:483:ALA:HB3	2:E:545:LEU:HD21	1.94	0.50
1:A:80:GLU:OE2	1:A:115:ARG:HD3	2.12	0.49
1:A:878:HIS:HD2	1:A:963:VAL:HA	1.75	0.49
1:A:535:SER:OG	1:A:564:ILE:HG22	2.13	0.49
1:D:984:CYS:HB3	1:D:1043:MET:HE1	1.95	0.49
1:D:328:TRP:HA	1:D:394:PRO:HG3	1.94	0.49
1:D:213:HIS:HB2	1:D:268:SER:HB3	1.94	0.49
1:A:225:ILE:HD11	1:A:243:VAL:HA	1.94	0.48
1:A:408:SER:HB3	1:A:422:LEU:HD21	1.94	0.48
1:D:459:ILE:O	1:D:459:ILE:HG22	2.13	0.48
1:D:11:TRP:CZ2	2:E:483:ALA:HB2	2.49	0.48
1:A:1006:LEU:HD21	1:A:1019:ILE:HD11	1.96	0.48
1:A:351:ILE:HG21	1:A:408:SER:HB2	1.96	0.48
1:A:800:ILE:HG21	3:A:1101:5H2:CL	2.51	0.48
1:A:213:HIS:HB2	1:A:268:SER:HB3	1.96	0.48
1:D:436:LEU:HB3	1:D:484:VAL:HB	1.96	0.48
1:A:713:ILE:HG12	1:A:845:VAL:HG11	1.94	0.47
2:B:555:GLU:O	2:B:559:ILE:HG12	2.14	0.47
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.95	0.47
1:A:807:LEU:HD13	1:A:846:GLY:HA3	1.95	0.47
1:A:254:VAL:HG23	1:A:261:PHE:HE1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:483:ALA:HB3	2:B:545:LEU:HD21	1.95	0.47
1:A:180:HIS:CD2	1:A:830:ASP:HB2	2.50	0.47
1:D:1006:LEU:HD21	1:D:1019:ILE:HD11	1.95	0.47
1:A:780:TRP:CH2	1:A:850:VAL:HG11	2.49	0.47
1:D:222:ALA:HA	1:D:225:ILE:HD12	1.97	0.47
1:D:861:GLN:O	1:D:872:PHE:HB3	2.15	0.47
1:D:137:GLN:NE2	1:D:140:ARG:HH11	2.12	0.47
2:E:473:THR:HG23	2:E:552:GLN:NE2	2.30	0.47
1:A:30:MET:HE1	1:A:57:PRO:HD2	1.97	0.47
1:D:535:SER:CB	1:D:564:ILE:HG22	2.45	0.47
1:A:17:PRO:HD2	1:A:20:ILE:HG22	1.97	0.47
1:A:436:LEU:HB3	1:A:484:VAL:HB	1.96	0.47
1:D:851:VAL:HG12	1:D:854:SER:OG	2.15	0.47
1:D:30:MET:CE	1:D:57:PRO:HD2	2.45	0.47
1:A:346:VAL:HG13	1:A:351:ILE:HB	1.97	0.46
1:D:17:PRO:HD2	1:D:20:ILE:HG22	1.96	0.46
1:A:640:LYS:HG2	1:A:680:VAL:HG11	1.97	0.46
1:D:825:GLN:HE22	1:D:830:ASP:HA	1.80	0.46
1:A:164:MET:CE	1:A:263:GLU:HB2	2.44	0.46
1:A:327:LEU:HB3	1:A:487:PRO:HD3	1.98	0.46
1:A:639:LEU:HD21	1:A:653:LEU:HD12	1.97	0.46
1:A:772:MET:HB2	1:A:778:PRO:HD2	1.98	0.46
1:D:780:TRP:CH2	1:D:850:VAL:HG11	2.51	0.45
1:A:562:PRO:HB3	1:A:591:PRO:HG2	1.98	0.45
1:A:79:ARG:HG3	2:B:493:ILE:HD11	1.98	0.45
2:E:555:GLU:O	2:E:559:ILE:HG12	2.16	0.45
1:A:985:TYR:CE1	1:A:1040:MET:HG2	2.52	0.45
1:A:299:MET:HB2	1:A:300:ASP:H	1.43	0.45
1:A:851:VAL:CG1	1:A:930:PHE:HZ	2.28	0.45
1:D:639:LEU:HD21	1:D:653:LEU:HD12	1.99	0.45
1:D:807:LEU:HD13	1:D:846:GLY:HA3	1.98	0.45
1:A:236:SER:HA	1:A:239:LEU:HD12	1.98	0.45
1:A:770:ARG:HG3	1:A:780:TRP:HB3	1.99	0.45
1:D:227:LYS:O	1:D:230:ARG:HB2	2.18	0.44
1:D:885:ASN:HB3	1:D:889:ILE:HG22	1.98	0.44
1:D:1022:ILE:HA	1:D:1025:THR:CG2	2.47	0.44
1:A:827:GLN:HE22	1:D:528:LYS:NZ	2.16	0.44
1:D:163:ALA:HB2	1:D:297:LEU:HD11	1.99	0.44
1:A:9:GLU:HB3	1:A:16:MET:HG2	2.00	0.43
1:D:214:ASP:HA	1:D:266:PRO:HB3	1.99	0.43
1:D:772:MET:HB2	1:D:778:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:HB2	1:A:247:GLN:HG3	2.01	0.43
1:D:894:ILE:HG21	1:D:966:LYS:HG2	2.01	0.43
2:E:501:GLN:HG2	2:E:528:TYR:CE1	2.54	0.43
1:D:562:PRO:HB3	1:D:591:PRO:HG2	2.00	0.43
1:D:738:GLN:NE2	1:D:741:ARG:HE	2.17	0.43
1:D:917:HIS:H	1:D:920:ASN:ND2	2.17	0.43
1:A:163:ALA:HB2	1:A:297:LEU:HD11	2.01	0.43
1:A:459:ILE:HG22	1:A:459:ILE:O	2.18	0.43
1:A:534:ILE:HA	1:A:537:ARG:HD3	2.01	0.43
1:D:164:MET:CE	1:D:263:GLU:HB2	2.48	0.43
1:A:298:PRO:HD2	1:A:299:MET:HG2	2.01	0.43
1:A:810:ASP:HA	1:A:934:PHE:HB2	2.01	0.43
1:A:647:ASN:ND2	1:A:650:VAL:H	2.15	0.43
1:D:770:ARG:HG3	1:D:780:TRP:HB3	2.00	0.43
1:D:360:ILE:HG22	1:D:367:LEU:HD23	2.00	0.43
1:A:989:LEU:HD11	1:A:1036:LEU:HG	2.01	0.42
1:A:371:VAL:HG12	1:A:387:LEU:HD22	2.00	0.42
1:D:810:ASP:HA	1:D:934:PHE:HB2	2.01	0.42
1:D:985:TYR:CE1	1:D:1040:MET:HG2	2.55	0.42
1:D:878:HIS:CD2	1:D:963:VAL:HA	2.51	0.42
1:D:137:GLN:HE22	1:D:140:ARG:HH11	1.66	0.42
2:B:556:TYR:HD1	2:B:556:TYR:O	2.02	0.42
1:D:164:MET:HE3	1:D:263:GLU:HB2	2.01	0.42
1:D:785:ASN:HB3	1:D:790:SER:HB2	2.01	0.42
1:A:218:GLU:HG2	1:A:247:GLN:HG2	2.01	0.42
1:A:402:LEU:HB2	1:A:429:LEU:HD21	2.02	0.42
1:A:829:LEU:HB3	1:A:831:LEU:HD12	2.01	0.42
1:D:17:PRO:HD2	1:D:20:ILE:CG2	2.50	0.42
1:D:341:ALA:HB3	1:D:381:PRO:HB2	2.01	0.42
1:D:788:ILE:H	1:D:788:ILE:CD1	2.32	0.42
1:A:360:ILE:HG22	1:A:367:LEU:HB2	2.02	0.41
2:B:474:SER:HB2	2:B:556:TYR:HE2	1.84	0.41
1:A:538:ASP:HA	1:A:996:ASN:ND2	2.35	0.41
1:A:338:ILE:HD12	1:A:356:VAL:HG11	2.01	0.41
1:A:788:ILE:H	1:A:788:ILE:CD1	2.31	0.41
1:A:5:PRO:HG3	1:A:11:TRP:CH2	2.55	0.41
2:B:501:GLN:HG2	2:B:528:TYR:CE1	2.55	0.41
1:A:905:CYS:HB3	1:A:954:PHE:CZ	2.56	0.41
2:B:574:ARG:HD3	2:B:577:ARG:HH21	1.85	0.41
1:D:402:LEU:HB2	1:D:429:LEU:HD21	2.03	0.41
2:B:478:GLN:O	2:B:482:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:TRP:CE2	1:A:487:PRO:HG2	2.56	0.41
1:A:647:ASN:HD22	1:A:649:LEU:H	1.69	0.41
1:A:898:THR:HG22	1:A:964:ILE:HA	2.03	0.41
1:D:678:LYS:HA	1:D:681:SER:HB2	2.03	0.41
1:A:328:TRP:HD1	1:A:328:TRP:O	2.04	0.41
1:A:326:SER:O	1:A:329:VAL:HB	2.21	0.41
1:A:539:PRO:HD3	1:A:996:ASN:HD22	1.85	0.41
1:A:461:VAL:HG21	1:A:679:THR:HB	2.02	0.41
1:A:989:LEU:HA	1:A:989:LEU:HD23	1.98	0.41
1:D:367:LEU:HB3	1:D:391:ILE:HD13	2.03	0.41
1:A:17:PRO:HD2	1:A:20:ILE:CG2	2.50	0.40
1:A:353:LYS:HD3	1:A:375:ARG:HB3	2.02	0.40
1:D:735:LEU:HD22	1:D:771:ILE:HG13	2.03	0.40
1:D:71:VAL:HG22	1:D:81:GLU:HG2	2.02	0.40
1:D:84:ASP:OD1	1:D:86:THR:HB	2.21	0.40
1:A:42:LEU:HD11	1:A:92:LEU:HD21	2.02	0.40
1:A:885:ASN:HB3	1:A:889:ILE:HG22	2.03	0.40
1:A:297:LEU:HA	1:A:298:PRO:HD3	1.89	0.40
1:D:678:LYS:NZ	2:E:478:GLN:HG2	2.37	0.40
1:A:194:ILE:HD11	1:A:220:VAL:HG12	2.04	0.40
1:A:735:LEU:HD22	1:A:771:ILE:HG13	2.03	0.40
1:D:135:GLU:HG3	1:D:432:TYR:CG	2.56	0.40
2:E:478:GLN:O	2:E:482:THR:HG23	2.22	0.40
2:E:494:PHE:HB3	2:E:535:ILE:HG12	2.04	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	975/1067 (91%)	914 (94%)	49 (5%)	12 (1%)	13 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	965/1067 (90%)	903 (94%)	49 (5%)	13 (1%)	12	45
2	B	119/169 (70%)	116 (98%)	1 (1%)	2 (2%)	9	39
2	E	123/169 (73%)	119 (97%)	2 (2%)	2 (2%)	9	40
All	All	2182/2472 (88%)	2052 (94%)	101 (5%)	29 (1%)	12	45

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	PRO
1	A	299	MET
1	A	399	ALA
1	D	298	PRO
1	D	399	ALA
1	A	264	LYS
2	B	557	ARG
1	D	7	SER
1	D	157	ASN
1	D	247	GLN
1	D	264	LYS
1	D	299	MET
2	E	557	ARG
1	A	157	ASN
1	A	481	SER
1	A	1056	ASP
2	B	515	GLU
1	A	724	LYS
1	D	158	SER
1	D	159	PRO
1	D	306	SER
1	A	384	ASN
1	D	874	SER
1	D	1056	ASP
1	A	459	ILE
1	D	459	ILE
1	A	106	GLY
2	E	516	GLY
1	A	158	SER

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	912/973 (94%)	842 (92%)	70 (8%)	13 42
1	D	905/973 (93%)	817 (90%)	88 (10%)	8 31
2	B	116/160 (72%)	106 (91%)	10 (9%)	10 37
2	E	120/160 (75%)	107 (89%)	13 (11%)	6 26
All	All	2053/2266 (91%)	1872 (91%)	181 (9%)	10 36

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	38	ARG
1	A	60	GLN
1	A	80	GLU
1	A	86	THR
1	A	96	GLN
1	A	102	ILE
1	A	105	VAL
1	A	108	ARG
1	A	137	GLN
1	A	155	ASP
1	A	158	SER
1	A	161	SER
1	A	171	VAL
1	A	173	SER
1	A	177	LEU
1	A	202	ASN
1	A	214	ASP
1	A	225	ILE
1	A	230	ARG
1	A	231	SER
1	A	234	LEU
1	A	236	SER
1	A	237	GLU

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Mol	Chain	Res	Type
1	A	241	LEU
1	A	257	CYS
1	A	287	LEU
1	A	328	TRP
1	A	335	ARG
1	A	343	TYR
1	A	352	ASP
1	A	357	ARG
1	A	367	LEU
1	A	369	ASP
1	A	376	VAL
1	A	440	LYS
1	A	452	LEU
1	A	462	THR
1	A	464	SER
1	A	476	GLU
1	A	541	SER
1	A	545	GLU
1	A	564	ILE
1	A	629	SER
1	A	659	THR
1	A	661	GLN
1	A	672	LYS
1	A	681	SER
1	A	738	GLN
1	A	740	ARG
1	A	767	GLU
1	A	787	ASP
1	A	788	ILE
1	A	807	LEU
1	A	827	GLN
1	A	834	LEU
1	A	845	VAL
1	A	852	ARG
1	A	860	ILE
1	A	870	LEU
1	A	917	HIS
1	A	920	ASN
1	A	957	THR
1	A	958	GLN
1	A	1005	MET
1	A	1022	ILE

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Mol	Chain	Res	Type
1	A	1023	ARG
1	A	1031	THR
1	A	1032	GLU
1	A	1036	LEU
2	B	478	GLN
2	B	485	GLU
2	B	499	GLN
2	B	501	GLN
2	B	502	GLU
2	B	511	LYS
2	B	532	LYS
2	B	563	MET
2	B	569	ASP
2	B	570	LEU
1	D	4	ARG
1	D	10	LEU
1	D	13	ILE
1	D	38	ARG
1	D	60	GLN
1	D	80	GLU
1	D	86	THR
1	D	96	GLN
1	D	102	ILE
1	D	105	VAL
1	D	107	ASN
1	D	108	ARG
1	D	137	GLN
1	D	155	ASP
1	D	161	SER
1	D	171	VAL
1	D	173	SER
1	D	177	LEU
1	D	185	LEU
1	D	186	ASP
1	D	209	LEU
1	D	230	ARG
1	D	231	SER
1	D	234	LEU
1	D	236	SER
1	D	237	GLU
1	D	241	LEU
1	D	257	CYS

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Mol	Chain	Res	Type
1	D	287	LEU
1	D	291	GLU
1	D	328	TRP
1	D	331	ASN
1	D	335	ARG
1	D	340	CYS
1	D	343	TYR
1	D	357	ARG
1	D	367	LEU
1	D	369	ASP
1	D	376	VAL
1	D	379	SER
1	D	391	ILE
1	D	392	TYR
1	D	440	LYS
1	D	452	LEU
1	D	467	ASN
1	D	470	THR
1	D	476	GLU
1	D	478	ASP
1	D	479	TRP
1	D	482	SER
1	D	523	LEU
1	D	541	SER
1	D	561	ILE
1	D	564	ILE
1	D	571	SER
1	D	577	ARG
1	D	633	ILE
1	D	659	THR
1	D	661	GLN
1	D	672	LYS
1	D	681	SER
1	D	723	LYS
1	D	738	GLN
1	D	740	ARG
1	D	767	GLU
1	D	788	ILE
1	D	793	LEU
1	D	796	ASN
1	D	807	LEU
1	D	829	LEU

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Mol	Chain	Res	Type
1	D	834	LEU
1	D	845	VAL
1	D	852	ARG
1	D	860	ILE
1	D	908	THR
1	D	917	HIS
1	D	920	ASN
1	D	958	GLN
1	D	971	CYS
1	D	1005	MET
1	D	1022	ILE
1	D	1025	THR
1	D	1028	LEU
1	D	1031	THR
1	D	1032	GLU
1	D	1036	LEU
1	D	1042	GLN
1	D	1061	THR
2	E	452	TYR
2	E	458	GLU
2	E	464	ASP
2	E	478	GLN
2	E	499	GLN
2	E	501	GLN
2	E	502	GLU
2	E	512	PHE
2	E	532	LYS
2	E	552	GLN
2	E	563	MET
2	E	569	ASP
2	E	570	LEU

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

Mol	Chain	Res	Type
1	A	347	ASN
1	A	370	ASN
1	A	426	ASN
1	A	450	HIS
1	A	647	ASN
1	A	714	ASN
1	A	825	GLN

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Mol	Chain	Res	Type
1	A	827	GLN
1	A	917	HIS
1	A	920	ASN
1	D	137	GLN
1	D	213	HIS
1	D	347	ASN
1	D	467	ASN
1	D	634	GLN
1	D	738	GLN
1	D	815	GLN
1	D	825	GLN
1	D	885	ASN
1	D	920	ASN
1	D	993	GLN
2	E	501	GLN
2	E	522	GLN
2	E	564	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	5H2	A	1101	-	28,35,35	1.02	1 (3%)	30,50,50	2.50	10 (33%)
3	5H2	D	1101	-	28,35,35	0.98	1 (3%)	30,50,50	2.24	8 (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	5H2	A	1101	-	-	2/10/24/24	0/4/5/5
3	5H2	D	1101	-	-	3/10/24/24	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	5H2	N21-N20	-3.83	1.29	1.37
3	A	1101	5H2	N21-N20	-3.75	1.29	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	1101	5H2	O2-C3-N5	7.38	119.58	109.25
3	A	1101	5H2	C28-C29-C24	5.53	121.77	118.55
3	A	1101	5H2	O2-C3-N5	5.42	116.83	109.25
3	A	1101	5H2	C6-N5-C3	5.17	134.85	126.36
3	D	1101	5H2	C28-C29-C24	5.00	121.46	118.55
3	A	1101	5H2	C12-O11-C10	4.63	122.47	116.03
3	A	1101	5H2	C1-O2-C3	4.42	120.88	115.66
3	A	1101	5H2	O2-C3-O4	-3.97	118.75	124.58
3	D	1101	5H2	O2-C3-O4	-3.93	118.81	124.58
3	D	1101	5H2	C12-O11-C10	3.52	120.93	116.03
3	D	1101	5H2	C10-C9-C15	3.44	124.68	119.69
3	D	1101	5H2	O11-C10-C31	2.59	120.70	116.95
3	A	1101	5H2	O11-C10-C31	2.40	120.42	116.95
3	A	1101	5H2	C24-C29-CL	-2.39	120.09	123.21
3	D	1101	5H2	C19-N20-N21	2.25	110.25	104.86
3	A	1101	5H2	C31-C6-N5	-2.11	113.29	120.18
3	A	1101	5H2	C12-C13-C14	-2.10	108.94	114.47
3	D	1101	5H2	O4-C3-N5	-2.07	121.61	126.11

There are no chirality outliers.

All (5) torsion outliers are listed below:

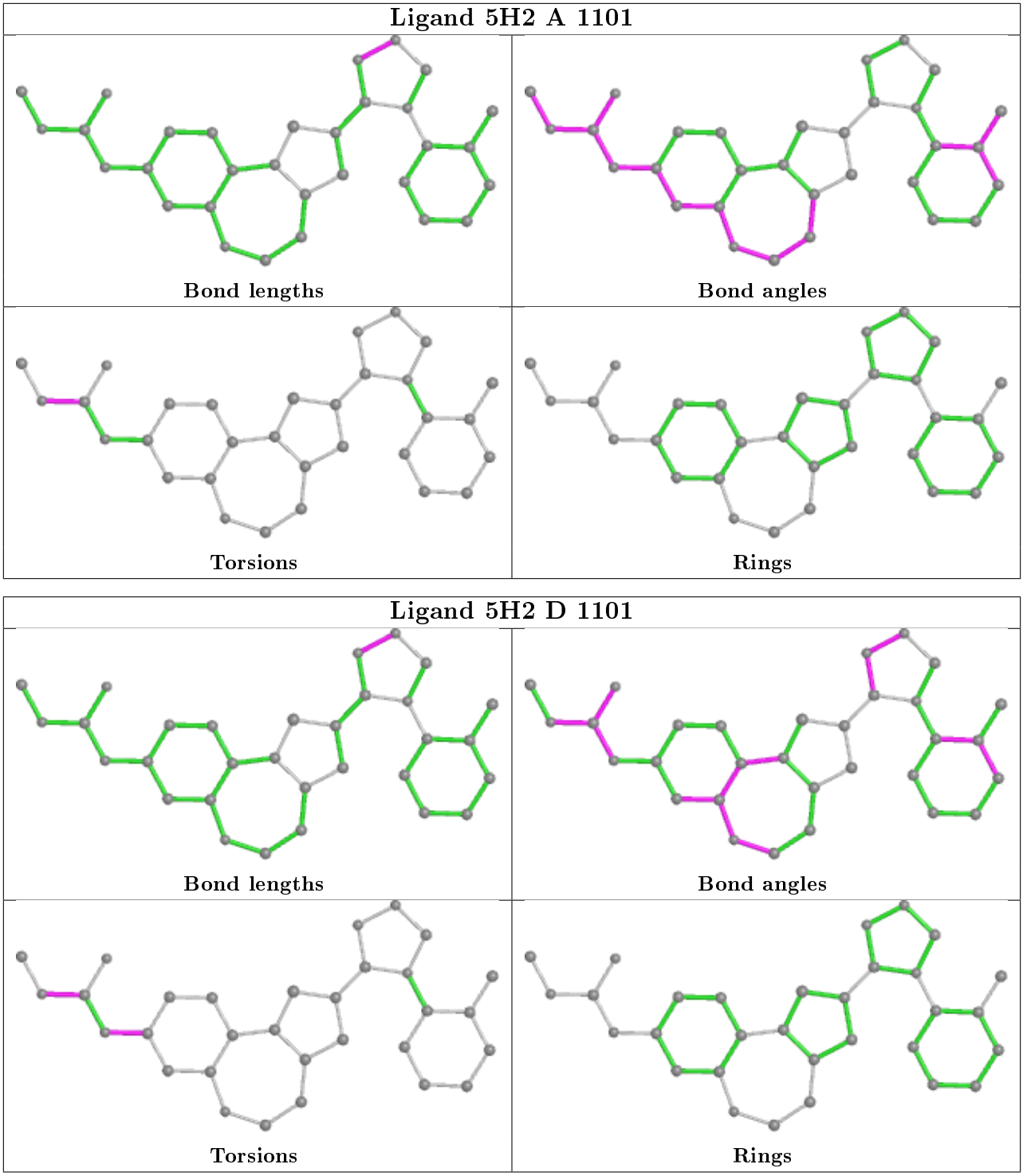
Mol	Chain	Res	Type	Atoms
3	A	1101	5H2	O4-C3-O2-C1
3	A	1101	5H2	N5-C3-O2-C1
3	D	1101	5H2	O4-C3-O2-C1
3	D	1101	5H2	N5-C3-O2-C1
3	D	1101	5H2	C7-C6-N5-C3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	5H2	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.



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	989/1067 (92%)	-0.06	6 (0%) 89 72	54, 93, 136, 186	0
1	D	981/1067 (91%)	-0.03	7 (0%) 87 69	59, 98, 139, 186	0
2	B	121/169 (71%)	-0.00	1 (0%) 86 65	70, 103, 153, 182	0
2	E	125/169 (73%)	0.88	16 (12%) 3 1	95, 145, 195, 210	0
All	All	2216/2472 (89%)	0.01	30 (1%) 75 49	54, 98, 148, 210	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	571	ILE	4.4
1	D	973	LYS	4.3
2	E	458	GLU	4.2
2	E	452	TYR	4.1
2	E	455	GLN	4.0
1	A	200	PRO	3.9
2	B	572	GLN	3.4
1	A	888	GLU	3.2
2	E	570	LEU	3.0
1	D	970	GLU	3.0
2	E	572	GLN	2.9
2	E	456	PHE	2.7
2	E	574	ARG	2.6
1	A	531	LEU	2.5
2	E	543	ARG	2.5
1	D	885	ASN	2.4
1	A	557	TYR	2.4
1	D	1037	GLU	2.4
2	E	450	HIS	2.4
1	A	529	GLU	2.3
1	D	346	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	525	GLU	2.3
2	E	559	ILE	2.2
1	D	888	GLU	2.2
2	E	556	TYR	2.2
2	E	463	TYR	2.1
2	E	517	ASN	2.1
2	E	564	ASN	2.1
2	E	573	LEU	2.1
1	D	1033	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

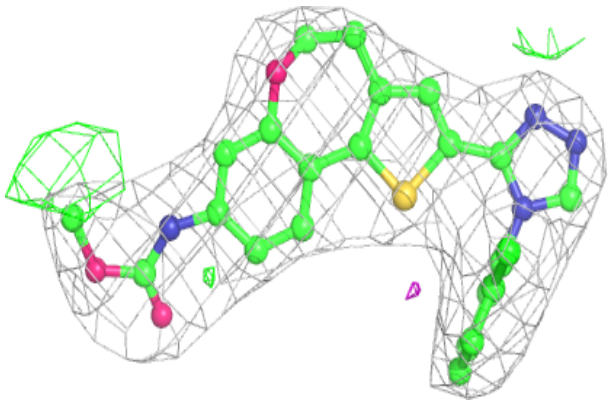
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

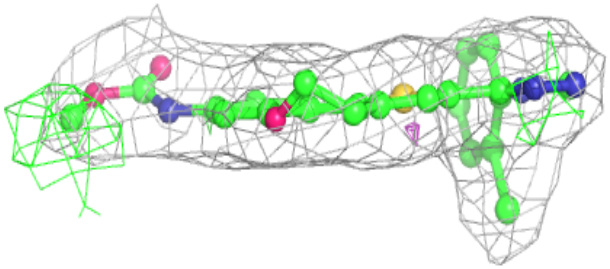
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	5H2	A	1101	31/31	0.97	0.23	60,68,76,81	0
3	5H2	D	1101	31/31	0.97	0.25	70,85,96,99	0

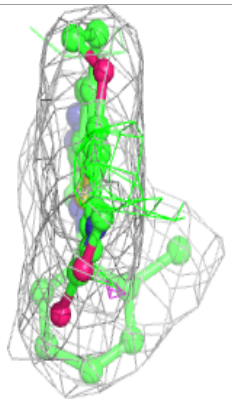
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5H2 A 1101:

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

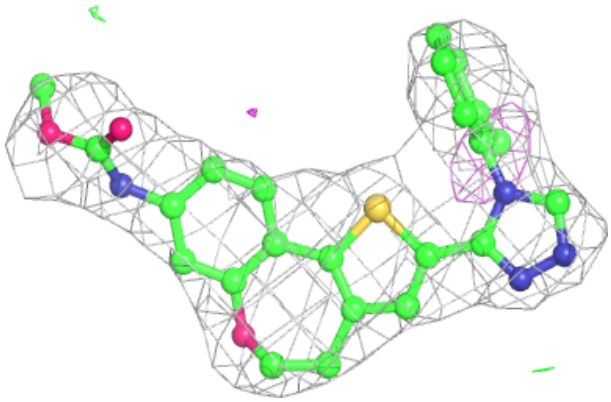


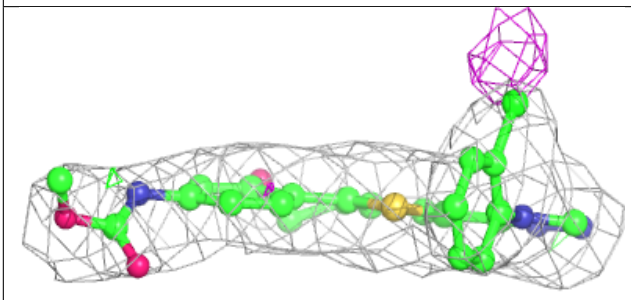


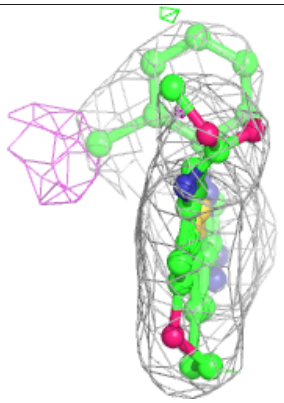


Electron density around 5H2 D 1101:

$2mF_o$-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.