



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:33 PM UTC

PDB ID : 5DXH / pdb_00005dxh
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	: 4-5-2 with Phenix2.0
Mogul	: 2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	: 2.0
EDS	: 3.0
Buster-report	: wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	: 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	: 9.0.010 (Gargrove)
Density-Fitness	: 1.0.12
Ideal geometry (proteins)	: Engh & Huber (2001)

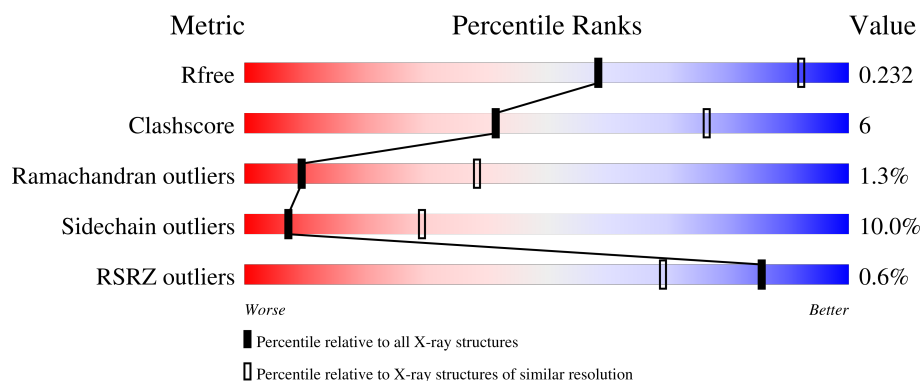
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1067	 70% 19% • 7%
1	D	1067	 68% 20% • 8%
2	B	169	 54% 14% • 28%

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
2	E	169	% 55% 15% • 26%

2 Entry composition [i](#)

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.

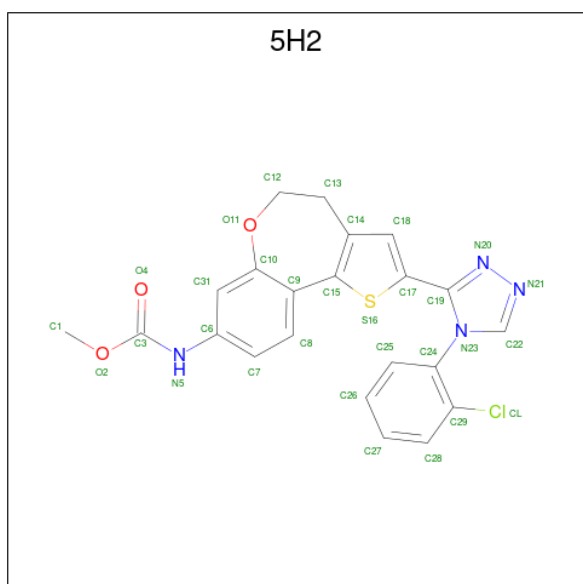
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit alpha isoform.

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 (CCD ID: 5H2) (formula: C₂₂H₁₇ClN₄O₃S).

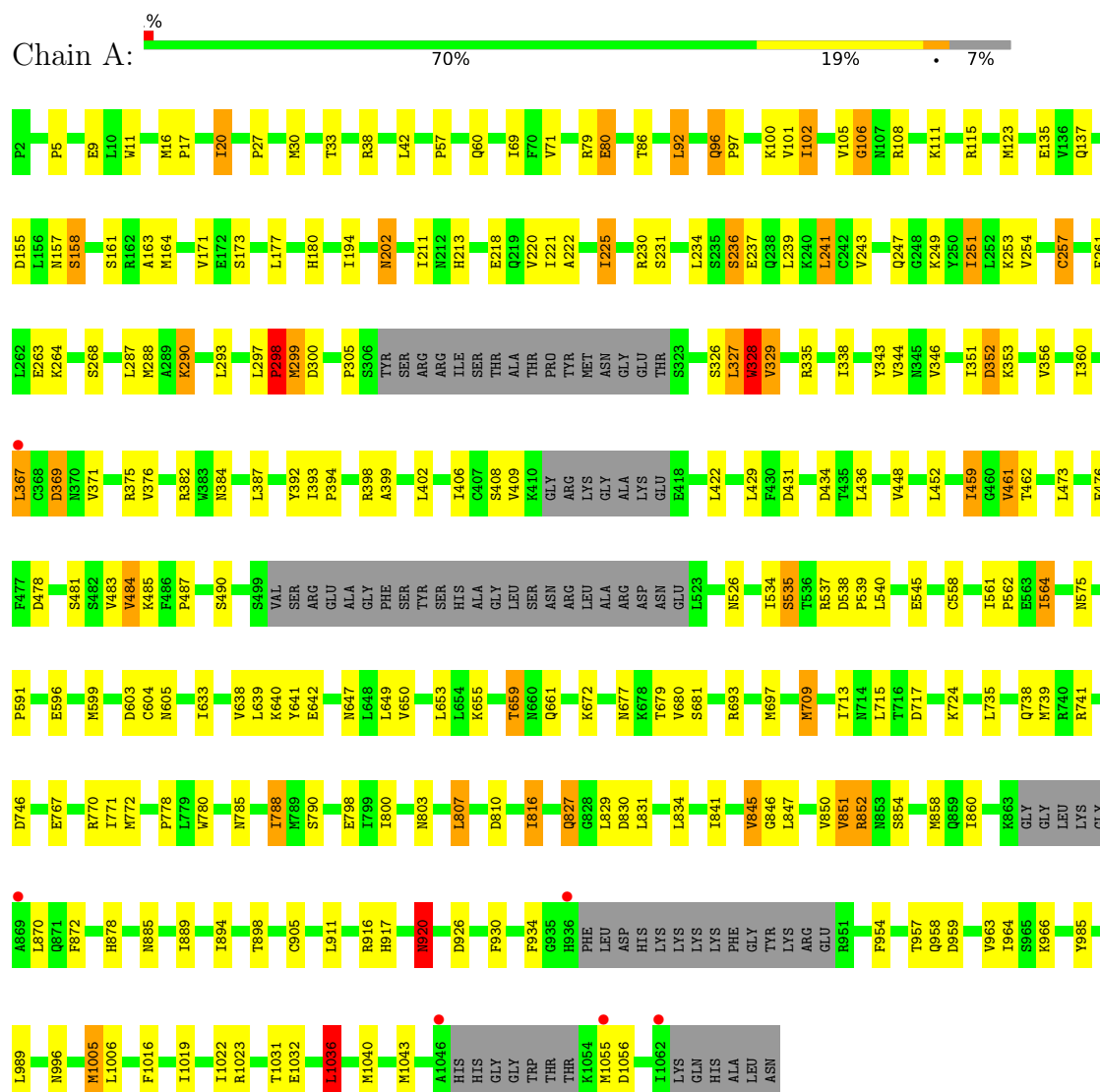


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			31	22	1	4	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			31	22	1	4	3	1		

3 Residue-property plots

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



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



4 Data and refinement statistics

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 49.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.50-3.00) 97.4 (49.50-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.218 0.198 , 0.232	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 , 72.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.86	6/8273 (0.1%)	1.39	45/11184 (0.4%)
1	D	0.85	2/8214 (0.0%)	1.39	49/11104 (0.4%)
2	B	0.83	0/1064	1.53	3/1414 (0.2%)
2	E	0.80	0/1106	1.50	4/1473 (0.3%)
All	All	0.85	8/18657 (0.0%)	1.40	101/25175 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	ILE	CA-CB	6.80	1.57	1.54
1	D	393	ILE	CA-CB	6.79	1.57	1.54
1	D	325	LYS	CA-C	5.83	1.60	1.52
1	A	561	ILE	CA-C	5.58	1.58	1.52
1	A	1055	MET	CA-C	5.54	1.59	1.52
1	A	709	MET	SD-CE	-5.28	1.66	1.79
1	A	211	ILE	CG1-CD1	5.10	1.71	1.51
1	A	1043	MET	SD-CE	-5.09	1.66	1.79

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	325	LYS	N-CA-C	-9.73	96.07	110.48
1	D	633	ILE	N-CA-CB	8.46	120.44	110.55
1	A	603	ASP	CA-CB-CG	7.43	120.03	112.60
1	D	448	VAL	N-CA-CB	7.35	116.92	110.08
1	A	448	VAL	N-CA-CB	6.91	116.51	110.08
1	A	202	ASN	CA-C-N	6.68	131.43	120.94
1	A	202	ASN	C-N-CA	6.68	131.43	120.94
1	A	327	LEU	N-CA-C	-6.53	101.29	110.50
1	D	298	PRO	CA-C-N	6.51	133.97	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	298	PRO	C-N-CA	6.51	133.97	121.54
1	A	92	LEU	N-CA-C	-6.49	99.44	109.76
1	D	92	LEU	N-CA-C	-6.45	99.50	109.76
1	A	329	VAL	N-CA-C	-6.36	96.11	109.34
1	D	717	ASP	CA-CB-CG	6.35	118.95	112.60
1	A	717	ASP	CA-CB-CG	6.22	118.82	112.60
1	A	431	ASP	CA-CB-CG	6.19	118.79	112.60
1	D	369	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	298	PRO	CA-C-N	6.12	133.23	121.54
1	A	298	PRO	C-N-CA	6.12	133.23	121.54
1	D	329	VAL	N-CA-C	-6.05	96.75	109.34
1	D	920	ASN	CA-CB-CG	5.94	118.54	112.60
1	D	157	ASN	CA-C-N	5.91	136.22	121.80
1	D	157	ASN	C-N-CA	5.91	136.22	121.80
1	D	926	ASP	CA-CB-CG	5.89	118.49	112.60
2	E	559	ILE	N-CA-C	-5.84	104.82	110.72
1	A	605	ASN	CA-CB-CG	5.80	118.41	112.60
2	B	509	ILE	CA-C-N	5.77	127.94	120.44
2	B	509	ILE	C-N-CA	5.77	127.94	120.44
1	A	369	ASP	CA-CB-CG	5.76	118.36	112.60
2	E	509	ILE	CA-C-N	5.75	127.91	120.44
2	E	509	ILE	C-N-CA	5.75	127.91	120.44
1	A	926	ASP	CA-CB-CG	5.72	118.33	112.60
2	B	559	ILE	N-CA-C	-5.72	104.94	110.72
1	D	153	LEU	CA-C-N	5.70	128.48	120.28
1	D	153	LEU	C-N-CA	5.70	128.48	120.28
1	A	959	ASP	CA-CB-CG	5.69	118.29	112.60
1	A	328	TRP	CA-CB-CG	5.67	124.36	113.60
1	D	377	PRO	CA-C-N	5.59	128.09	120.54
1	D	377	PRO	C-N-CA	5.59	128.09	120.54
1	D	1024	LYS	CA-C-N	5.54	128.47	120.38
1	D	1024	LYS	C-N-CA	5.54	128.47	120.38
1	A	575	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	249	LYS	N-CA-C	-5.48	106.27	113.17
1	D	959	ASP	CA-CB-CG	5.47	118.08	112.60
1	A	920	ASN	CA-CB-CG	5.46	118.06	112.60
1	D	773	SER	CA-C-N	5.41	128.78	120.82
1	D	773	SER	C-N-CA	5.41	128.78	120.82
1	A	803	ASN	CA-CB-CG	5.39	118.00	112.60
1	D	739	MET	CA-C-N	5.38	128.49	120.31
1	D	739	MET	C-N-CA	5.38	128.49	120.31
1	A	398	ARG	N-CA-C	-5.38	101.40	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	ASN	CA-CB-CG	5.37	117.97	112.60
1	A	535	SER	CA-C-N	5.36	128.46	120.31
1	A	535	SER	C-N-CA	5.36	128.46	120.31
1	D	51	LYS	CA-C-N	5.36	127.47	120.28
1	D	51	LYS	C-N-CA	5.36	127.47	120.28
1	A	739	MET	CA-C-N	5.35	128.44	120.31
1	A	739	MET	C-N-CA	5.35	128.44	120.31
1	D	13	ILE	CA-C-N	5.33	127.42	120.28
1	D	13	ILE	C-N-CA	5.33	127.42	120.28
1	A	135	GLU	CB-CG-CD	5.28	121.58	112.60
1	A	33	THR	CB-CA-C	5.27	118.44	109.80
1	D	33	THR	CB-CA-C	5.27	118.44	109.80
1	D	803	ASN	CA-CB-CG	5.26	117.86	112.60
1	D	398	ARG	N-CA-C	-5.26	101.57	109.15
1	D	907	ALA	CA-C-N	5.26	128.31	120.31
1	D	907	ALA	C-N-CA	5.26	128.31	120.31
1	D	163	ALA	CA-C-N	5.24	127.30	120.28
1	D	163	ALA	C-N-CA	5.24	127.30	120.28
1	D	742	PRO	CA-C-N	5.24	127.56	120.38
1	D	742	PRO	C-N-CA	5.24	127.56	120.38
1	D	1055	MET	CA-C-N	5.24	131.54	121.54
1	D	1055	MET	C-N-CA	5.24	131.54	121.54
1	A	851	VAL	CB-CA-C	5.23	116.88	111.23
1	A	328	TRP	CA-C-N	5.22	131.36	121.97
1	A	328	TRP	C-N-CA	5.22	131.36	121.97
1	A	478	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	329	VAL	CA-C-N	5.20	128.20	122.22
1	A	329	VAL	C-N-CA	5.20	128.20	122.22
1	D	478	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	526	ASN	CA-C-N	5.18	127.22	120.28
1	A	526	ASN	C-N-CA	5.18	127.22	120.28
1	A	1036	LEU	CA-C-N	5.16	127.51	120.54
1	A	1036	LEU	C-N-CA	5.16	127.51	120.54
2	E	509	ILE	N-CA-C	-5.14	105.40	111.00
1	D	431	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	352	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	465	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	490	SER	CA-C-N	5.06	127.04	120.56
1	A	490	SER	C-N-CA	5.06	127.04	120.56
1	D	3	PRO	CA-C-N	5.04	127.82	120.51
1	D	3	PRO	C-N-CA	5.04	127.82	120.51
1	D	490	SER	CA-C-N	5.04	127.00	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	490	SER	C-N-CA	5.04	127.00	120.56
1	A	746	ASP	CA-C-N	5.03	126.97	120.44
1	A	746	ASP	C-N-CA	5.03	126.97	120.44
1	D	535	SER	CA-C-N	5.02	127.50	120.28
1	D	535	SER	C-N-CA	5.02	127.50	120.28
1	A	241	LEU	CA-C-N	5.00	126.94	120.44
1	A	241	LEU	C-N-CA	5.00	126.94	120.44
1	D	605	ASN	CA-CB-CG	5.00	117.60	112.60

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	116	0
1	D	8033	0	8051	95	0
2	B	1053	0	1053	14	0
2	E	1092	0	1072	14	0
3	A	31	0	17	4	0
3	D	31	0	17	0	0
All	All	18333	0	18329	233	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 (233) 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:A:164:MET:HE1	1:A:263:GLU:HB2	1.51	0.92
1:D:164:MET:HE1	1:D:263:GLU:HB2	1.54	0.88
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:298:PRO:HG2	1:D:697:MET:HG3	1.77	0.66
1:D:305:PRO:HG3	1:D:693:ARG:HD3	1.76	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
1:A:639:LEU:HD22	1:A:650:VAL:HG22	1.84	0.60
1:D:788:ILE:HD12	1:D:788:ILE:H	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:A:30:MET:HE1	1:A:57:PRO:HD2	1.86	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:642:GLU:HG2	1:D:647:ASN:CG	2.31	0.56
1:A:633:ILE:CG2	1:A:1005:MET:HE1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:GLY:H	1:D:111:LYS:HZ2	1.53	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:A:709:MET:HE1	1:A:847:LEU:HD21	1.90	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
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:D:709:MET:HE1	1:D:847:LEU:HD21	1.92	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:71:VAL:CG2	1:D:102:ILE:HG12	2.39	0.51
1:D:254:VAL:HG23	1:D:261:PHE:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LYS:HE2	1:D:257:CYS:O	2.10	0.51
1:D:408:SER:HB3	1:D:422:LEU:HD21	1.92	0.51
1:D:596:GLU:HA	1:D:599:MET:HE2	1.93	0.51
1:A:106:GLY:H	1:A:111:LYS:HZ2	1.57	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:30:MET:HE1	1:D:57:PRO:HD2	1.93	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:328:TRP:HA	1:D:394:PRO:HG3	1.94	0.49
2:E:476:GLU:HA	2:E:479:MET:HE2	1.94	0.49
1:D:213:HIS:HB2	1:D:268:SER:HB3	1.94	0.49
2:B:476:GLU:HA	2:B:479:MET:HE2	1.94	0.48
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:HG22	1:D:459:ILE:O	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:D:984:CYS:HB3	1:D:1043:MET:HE1	1.96	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
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:596:GLU:HA	1:A:599:MET:HE2	1.96	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:137:GLN:NE2	1:D:140:ARG:HH11	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:861:GLN:O	1:D:872:PHE:HB3	2.15	0.47
2:E:473:THR:HG23	2:E:552:GLN:NE2	2.30	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:A:858:MET:HE1	1:A:872:PHE:CZ	2.50	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:A:123:MET:HE3	1:A:123:MET:HB2	1.85	0.46
1:D:825:GLN:HE22	1:D:830:ASP:HA	1.80	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:299:MET:HB2	1:A:300:ASP:H	1.43	0.45
1:A:985:TYR:CE1	1:A:1040:MET:HG2	2.52	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:A:633:ILE:HG22	1:A:1005:MET:HE1	1.98	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
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:A:253:LYS:HD3	1:A:288:MET:HE1	2.00	0.43
1:D:562:PRO:HB3	1:D:591:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:920:ASN:C	1:A:920:ASN:HD22	2.26	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:253:LYS:HD3	1:D:288:MET:HE1	2.00	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:878:HIS:CD2	1:D:963:VAL:HA	2.51	0.42
1:D:985:TYR:CE1	1:D:1040:MET:HG2	2.55	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: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
1:D:1012:GLU:H	1:D:1012:GLU:CD	2.29	0.41
2:B:478:GLN:O	2:B:482:THR:HG23	2.20	0.41
1:A:328:TRP:CE2	1:A:487:PRO:HG2	2.56	0.41
1:A:328:TRP:HD1	1:A:328:TRP:O	2.04	0.41
1:A:647:ASN:HD22	1:A:649:LEU:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:288:MET:HE3	1:A:288:MET:HB2	1.88	0.41
1:A:326:SER:O	1:A:329:VAL:HB	2.21	0.41
1:A:461:VAL:HG21	1:A:679:THR:HB	2.02	0.41
1:A:539:PRO:HD3	1:A:996:ASN:HD22	1.85	0.41
1:A:989:LEU:HD23	1:A:989:LEU:HA	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: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:D:735:LEU:HD22	1:D:771:ILE:HG13	2.03	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%)	10	40
1	D	965/1067 (90%)	903 (94%)	49 (5%)	13 (1%)	9	38
2	B	119/169 (70%)	116 (98%)	1 (1%)	2 (2%)	7	32

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	123/169 (73%)	119 (97%)	2 (2%)	2 (2%)	7	34
All	All	2182/2472 (88%)	2052 (94%)	101 (5%)	29 (1%)	9	38

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 ⓘ

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%)	835 (92%)	77 (8%)	10	37
1	D	905/973 (93%)	803 (89%)	102 (11%)	5	24
2	B	116/160 (72%)	103 (89%)	13 (11%)	6	24
2	E	120/160 (75%)	106 (88%)	14 (12%)	5	23
All	All	2053/2266 (91%)	1847 (90%)	206 (10%)	7	29

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	38	ARG
1	A	60	GLN
1	A	69	ILE
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	225	ILE
1	A	230	ARG
1	A	231	SER
1	A	234	LEU
1	A	236	SER
1	A	237	GLU
1	A	241	LEU
1	A	251	ILE
1	A	257	CYS
1	A	287	LEU
1	A	290	LYS
1	A	328	TRP

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Mol	Chain	Res	Type
1	A	335	ARG
1	A	343	TYR
1	A	344	VAL
1	A	352	ASP
1	A	367	LEU
1	A	369	ASP
1	A	376	VAL
1	A	382	ARG
1	A	409	VAL
1	A	452	LEU
1	A	461	VAL
1	A	462	THR
1	A	473	LEU
1	A	476	GLU
1	A	483	VAL
1	A	484	VAL
1	A	545	GLU
1	A	564	ILE
1	A	638	VAL
1	A	642	GLU
1	A	659	THR
1	A	661	GLN
1	A	672	LYS
1	A	681	SER
1	A	738	GLN
1	A	741	ARG
1	A	767	GLU
1	A	788	ILE
1	A	807	LEU
1	A	816	ILE
1	A	827	GLN
1	A	834	LEU
1	A	841	ILE
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

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Mol	Chain	Res	Type
1	A	1022	ILE
1	A	1023	ARG
1	A	1031	THR
1	A	1032	GLU
1	A	1036	LEU
2	B	478	GLN
2	B	484	ILE
2	B	485	GLU
2	B	499	GLN
2	B	501	GLN
2	B	502	GLU
2	B	510	GLU
2	B	511	LYS
2	B	532	LYS
2	B	557	ARG
2	B	563	MET
2	B	567	LYS
2	B	570	LEU
1	D	4	ARG
1	D	10	LEU
1	D	13	ILE
1	D	20	ILE
1	D	38	ARG
1	D	60	GLN
1	D	69	ILE
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	162	ARG
1	D	171	VAL
1	D	173	SER
1	D	177	LEU
1	D	185	LEU
1	D	186	ASP
1	D	209	LEU

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Mol	Chain	Res	Type
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	251	ILE
1	D	257	CYS
1	D	287	LEU
1	D	290	LYS
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	344	VAL
1	D	354	ILE
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	409	VAL
1	D	452	LEU
1	D	470	THR
1	D	474	GLU
1	D	476	GLU
1	D	479	TRP
1	D	482	SER
1	D	483	VAL
1	D	484	VAL
1	D	523	LEU
1	D	545	GLU
1	D	561	ILE
1	D	564	ILE
1	D	571	SER
1	D	633	ILE
1	D	636	VAL
1	D	638	VAL
1	D	659	THR

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Mol	Chain	Res	Type
1	D	661	GLN
1	D	672	LYS
1	D	681	SER
1	D	723	LYS
1	D	738	GLN
1	D	741	ARG
1	D	767	GLU
1	D	788	ILE
1	D	793	LEU
1	D	796	ASN
1	D	802	LYS
1	D	807	LEU
1	D	816	ILE
1	D	825	GLN
1	D	829	LEU
1	D	834	LEU
1	D	841	ILE
1	D	845	VAL
1	D	852	ARG
1	D	854	SER
1	D	860	ILE
1	D	863	LYS
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	484	ILE
2	E	499	GLN

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Mol	Chain	Res	Type
2	E	501	GLN
2	E	502	GLU
2	E	510	GLU
2	E	512	PHE
2	E	552	GLN
2	E	563	MET
2	E	567	LYS
2	E	570	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	189	GLN
1	A	201	ASN
1	A	219	GLN
1	A	238	GLN
1	A	345	ASN
1	A	370	ASN
1	A	384	ASN
1	A	450	HIS
1	A	495	HIS
1	A	530	GLN
1	A	575	ASN
1	A	630	GLN
1	A	647	ASN
1	A	782	ASN
1	A	825	GLN
1	A	827	GLN
1	A	861	GLN
1	A	917	HIS
1	A	920	ASN
1	A	993	GLN
2	B	526	HIS
2	B	564	ASN
2	B	572	GLN
1	D	137	GLN
1	D	213	HIS
1	D	219	GLN
1	D	347	ASN
1	D	370	ASN
1	D	380	ASN

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Mol	Chain	Res	Type
1	D	426	ASN
1	D	526	ASN
1	D	575	ASN
1	D	605	ASN
1	D	630	GLN
1	D	634	GLN
1	D	714	ASN
1	D	738	GLN
1	D	785	ASN
1	D	797	ASN
1	D	815	GLN
1	D	825	GLN
1	D	861	GLN
1	D	920	ASN
1	D	993	GLN
2	E	526	HIS
2	E	552	GLN
2	E	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 oligosaccharides 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	5H2	D	1101	-	35,35,35	1.08	1 (2%)	41,50,50	1.98	9 (21%)
3	5H2	A	1101	-	35,35,35	1.26	2 (5%)	41,50,50	2.20	13 (31%)

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	D	1101	-	-	3/14/24/24	0/5/5/5
3	5H2	A	1101	-	-	2/14/24/24	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	5H2	N21-N20	-4.85	1.29	1.39
3	A	1101	5H2	N21-N20	-4.76	1.29	1.39
3	A	1101	5H2	C24-N23	-2.17	1.40	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1101	5H2	O2-C3-N5	8.03	119.58	109.19
3	A	1101	5H2	O2-C3-N5	5.90	116.83	109.19
3	A	1101	5H2	C6-N5-C3	5.35	134.85	126.39
3	A	1101	5H2	C1-O2-C3	4.53	120.88	115.63
3	A	1101	5H2	O2-C3-O4	-4.03	118.75	124.62
3	D	1101	5H2	O2-C3-O4	-3.99	118.81	124.62
3	A	1101	5H2	C12-O11-C10	3.82	122.47	116.13
3	A	1101	5H2	C14-C15-S16	-3.54	108.65	111.36
3	A	1101	5H2	N23-C19-N20	-3.28	107.10	110.53
3	D	1101	5H2	N23-C19-N20	-3.22	107.15	110.53
3	D	1101	5H2	C12-O11-C10	2.89	120.93	116.13
3	D	1101	5H2	C19-C17-S16	2.70	125.70	117.24
3	D	1101	5H2	C14-C15-S16	-2.66	109.33	111.36
3	A	1101	5H2	C19-C17-S16	2.62	125.44	117.24
3	D	1101	5H2	C19-N20-N21	2.57	110.25	106.74
3	A	1101	5H2	C17-S16-C15	2.41	93.79	90.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1101	5H2	O11-C10-C31	2.38	120.70	116.83
3	A	1101	5H2	O11-C10-C31	2.21	120.42	116.83
3	D	1101	5H2	O4-C3-N5	-2.12	121.61	126.12
3	A	1101	5H2	C31-C6-N5	-2.10	113.29	120.13
3	A	1101	5H2	C18-C17-S16	-2.09	108.02	111.55
3	A	1101	5H2	C6-C31-C10	2.01	121.84	119.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

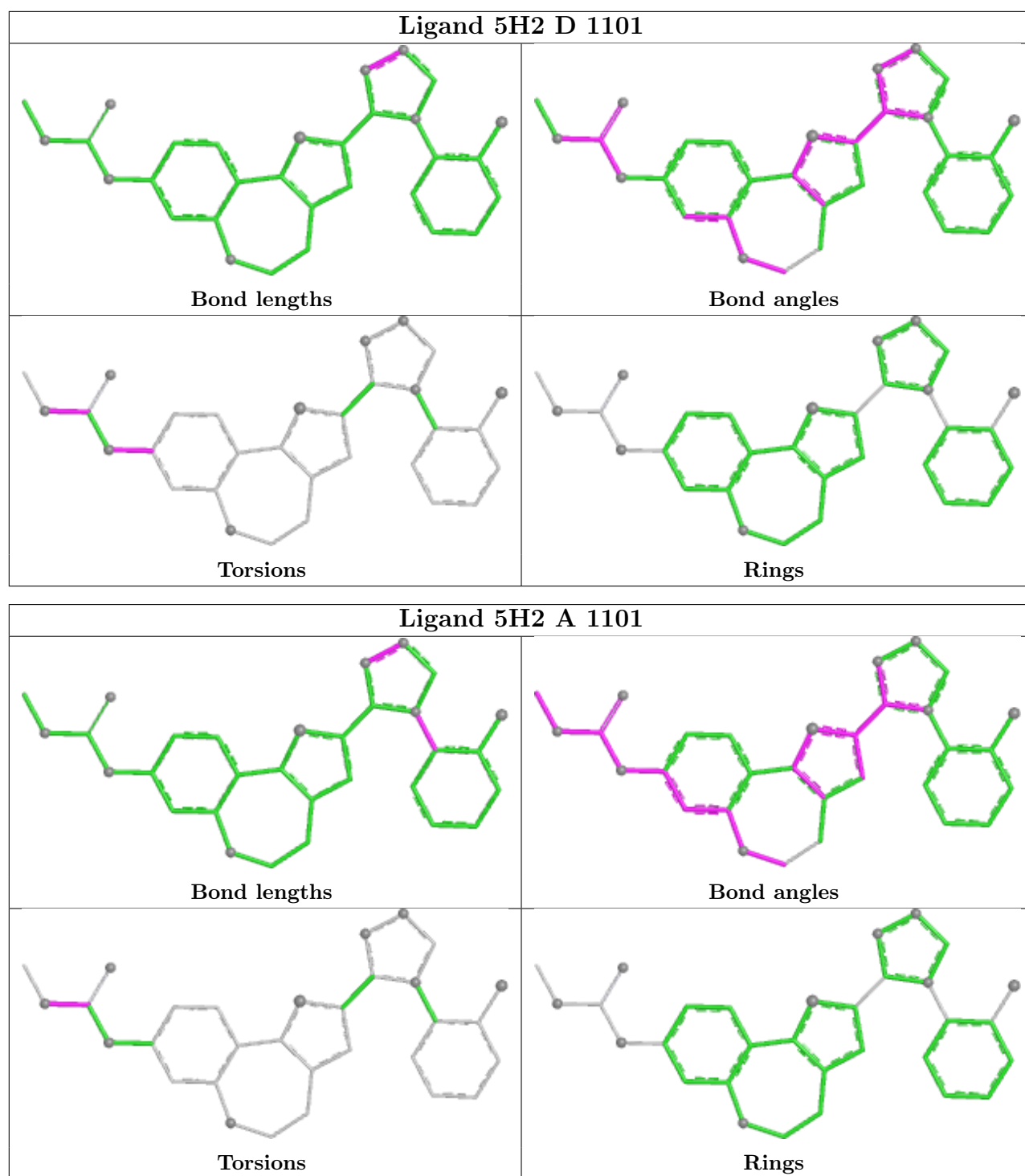
Mol	Chain	Res	Type	Atoms
3	A	1101	5H2	O4-C3-O2-C1
3	A	1101	5H2	N5-C3-O2-C1
3	D	1101	5H2	O4-C3-O2-C1
3	D	1101	5H2	N5-C3-O2-C1
3	D	1101	5H2	C7-C6-N5-C3

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	989/1067 (92%)	-0.27	6 (0%) 85 69	54, 93, 136, 186	0
1	D	981/1067 (91%)	-0.25	7 (0%) 84 66	59, 98, 139, 186	0
2	B	121/169 (71%)	-0.27	0 100 100	70, 103, 153, 182	0
2	E	125/169 (73%)	0.09	1 (0%) 82 64	95, 145, 195, 210	0
All	All	2216/2472 (89%)	-0.24	14 (0%) 85 69	54, 98, 148, 210	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1046	ALA	4.6
1	D	1062	ILE	3.8
1	A	1062	ILE	3.1
1	A	869	ALA	2.8
1	D	7	SER	2.5
1	D	1061	THR	2.3
1	A	936	HIS	2.3
1	D	953	PRO	2.3
1	D	874	SER	2.2
1	A	1055	MET	2.2
1	A	367	LEU	2.1
1	D	1054	LYS	2.1
2	E	564	ASN	2.1
1	D	328	TRP	2.1

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](#)

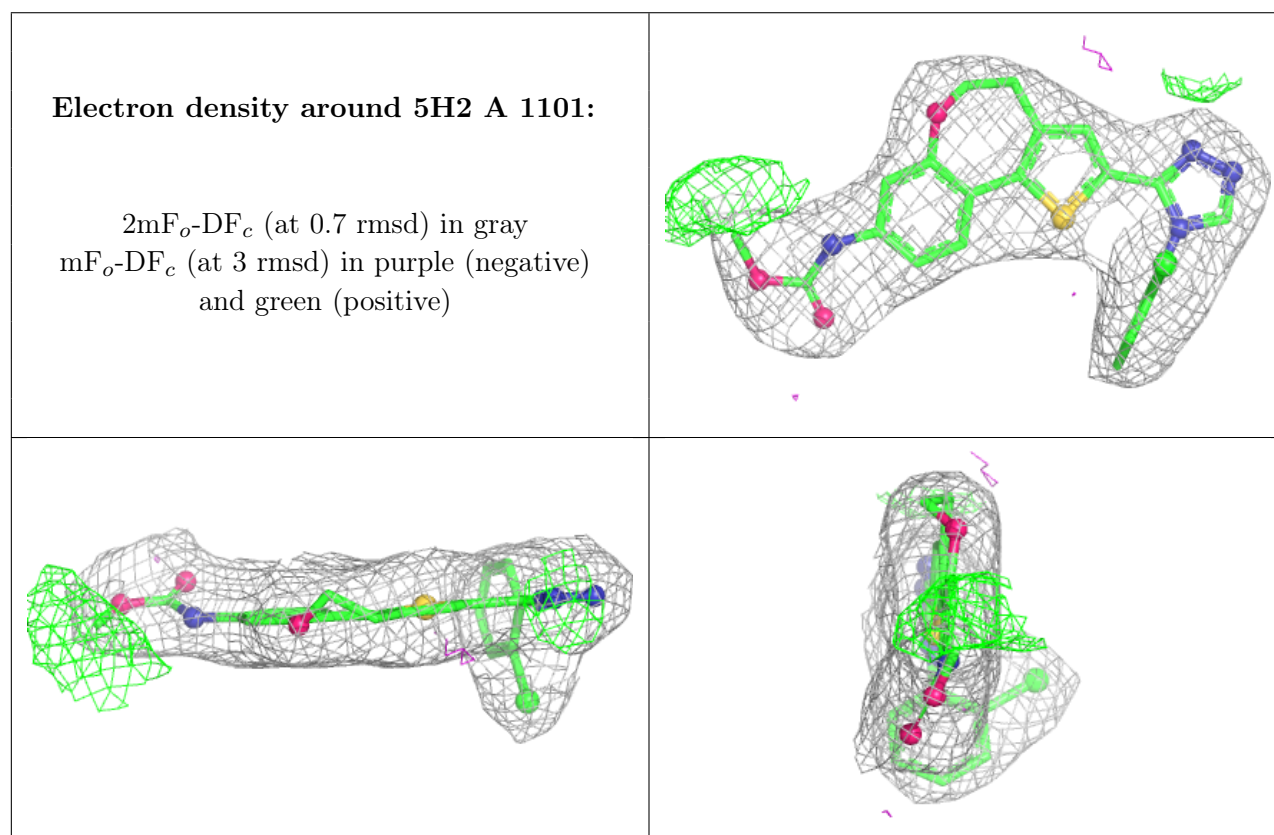
There are no oligosaccharides in this entry.

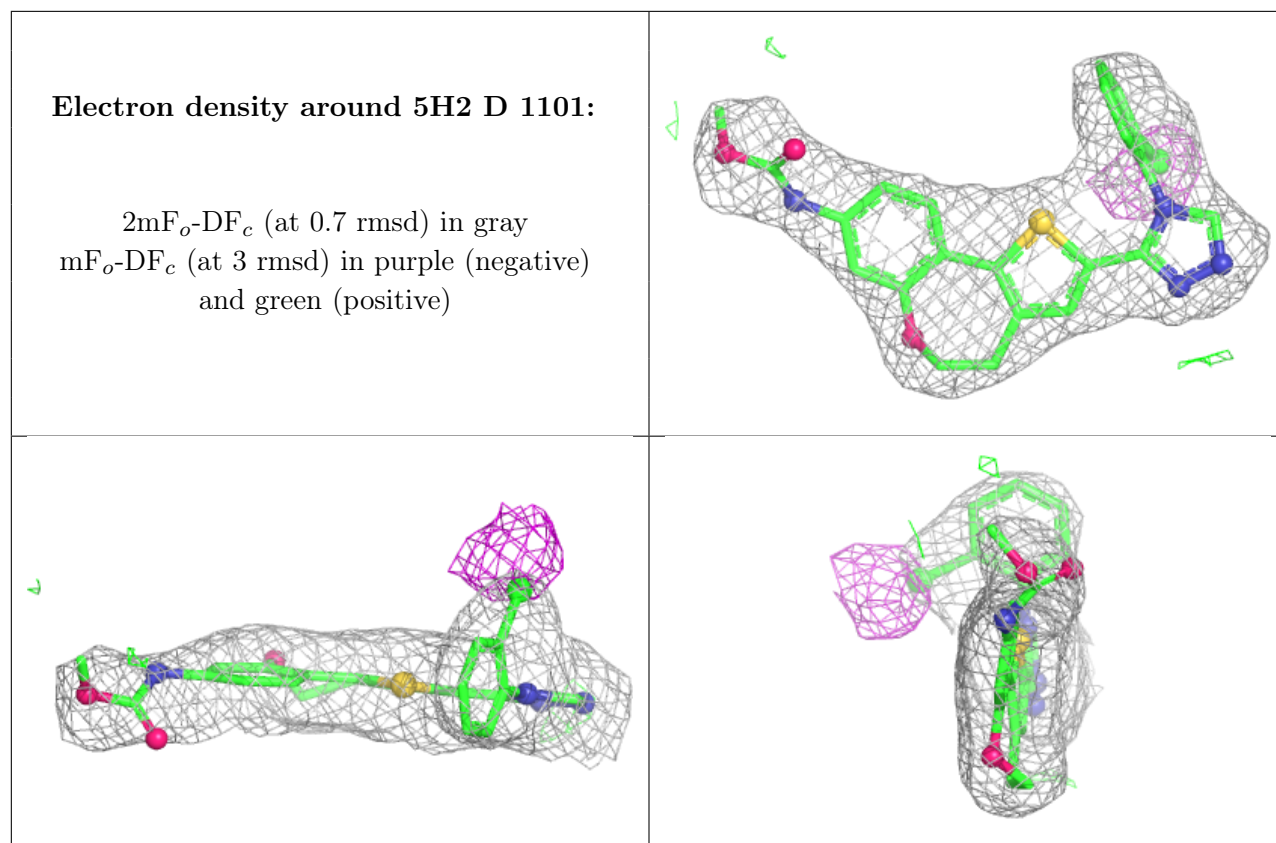
6.4 Ligands [i](#)

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($\text{\AA}^2$)	Q<0.9
3	5H2	A	1101	31/31	0.94	0.09	60,68,76,81	0
3	5H2	D	1101	31/31	0.95	0.10	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.