



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:48 AM UTC

PDB ID : 4ANU / pdb_00004anu
Title : Complexes of PI3Kgamma with isoform selective inhibitors.
Authors : Foster, P.G.; Lougheed, J.C.
Deposited on : 2012-03-22
Resolution : 2.81 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)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

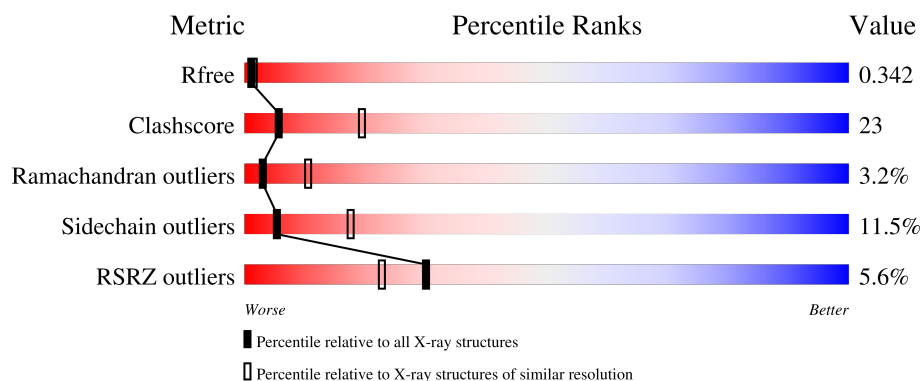
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	980	5% 45% 32% 7% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6810 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 GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	833	Total	C	N	O	S	0	0	0
			6757	4334	1153	1235	35			

There are 21 discrepancies between the modelled and reference sequences:

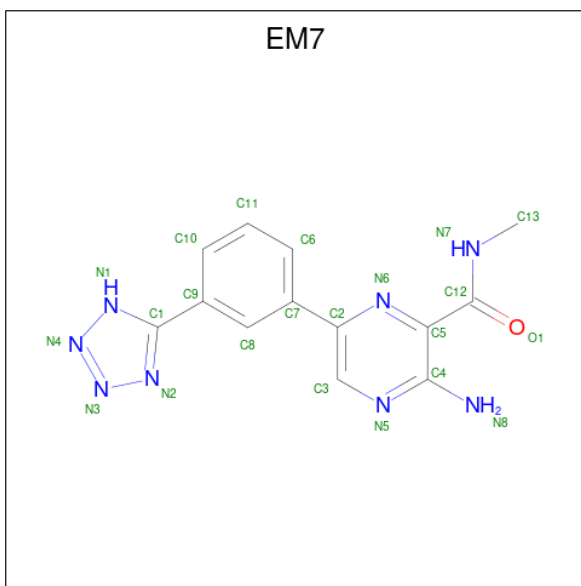
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	expression tag	UNP P48736
A	140	LEU	-	expression tag	UNP P48736
A	141	LEU	-	expression tag	UNP P48736
A	142	GLY	-	expression tag	UNP P48736
A	143	SER	-	expression tag	UNP P48736
A	1103	GLU	-	expression tag	UNP P48736
A	1104	PHE	-	expression tag	UNP P48736
A	1105	GLY	-	expression tag	UNP P48736
A	1106	LEU	-	expression tag	UNP P48736
A	1107	VAL	-	expression tag	UNP P48736
A	1108	PRO	-	expression tag	UNP P48736
A	1109	ARG	-	expression tag	UNP P48736
A	1110	GLY	-	expression tag	UNP P48736
A	1111	SER	-	expression tag	UNP P48736
A	1112	GLY	-	expression tag	UNP P48736
A	1113	HIS	-	expression tag	UNP P48736
A	1114	HIS	-	expression tag	UNP P48736
A	1115	HIS	-	expression tag	UNP P48736
A	1116	HIS	-	expression tag	UNP P48736
A	1117	HIS	-	expression tag	UNP P48736
A	1118	HIS	-	expression tag	UNP P48736

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 3-AMINO-N-METHYL-6-[3-(1H-TETRAZOL-5-YL)PHENYL]PYRAZINE-2-CARBOXAMIDE (CCD ID: EM7) (formula: $C_{13}H_{12}N_8O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	13	8	1		

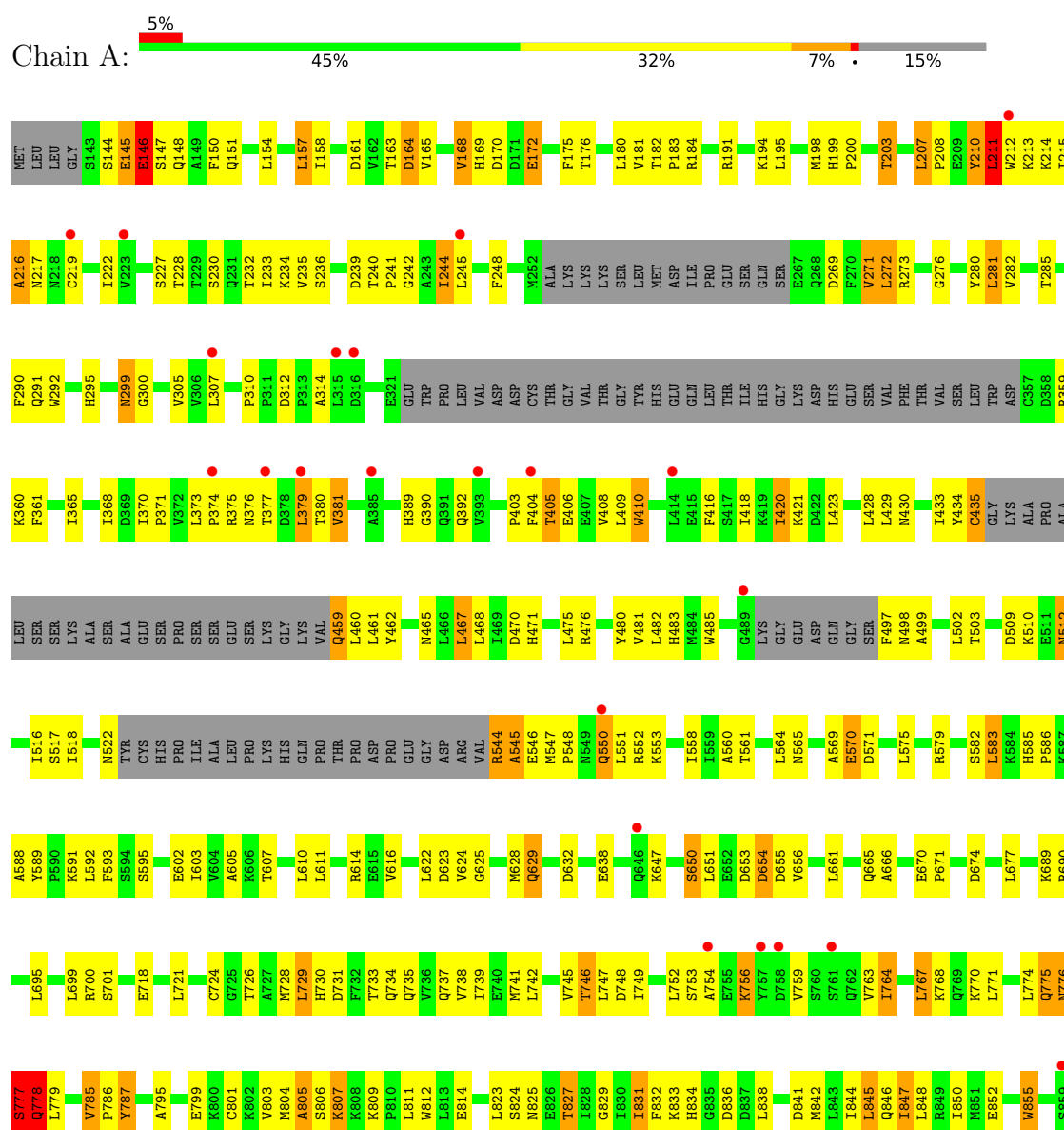
- Molecule 4 is water.

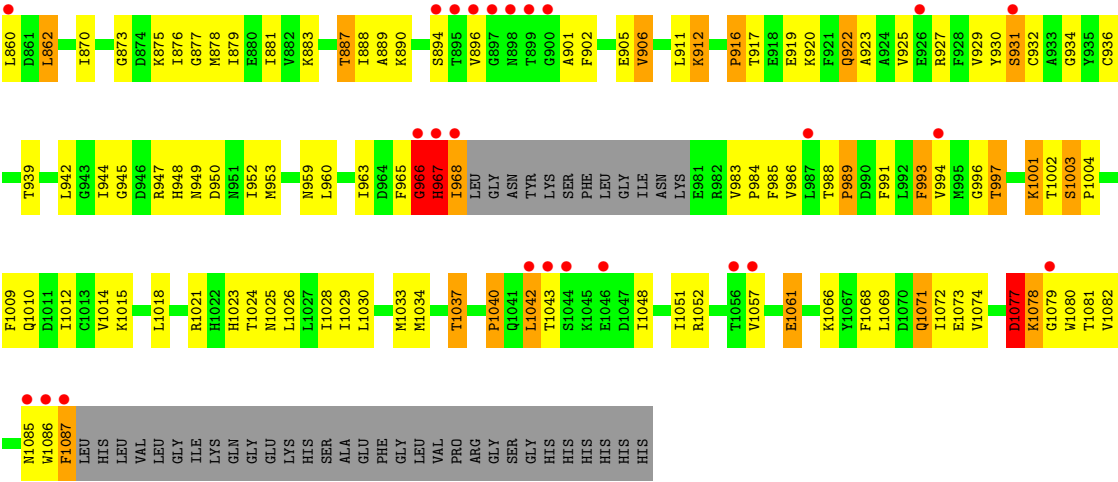
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		

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 GAMMA ISOFORM





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.25Å 68.53Å 106.86Å 90.00° 95.29° 90.00°	Depositor
Resolution (Å)	28.70 – 2.81 28.70 – 2.81	Depositor EDS
% Data completeness (in resolution range)	93.9 (28.70-2.81) 93.8 (28.70-2.81)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.254 , 0.338 0.260 , 0.342	Depositor DCC
R_{free} test set	1242 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.9	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6810	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, EM7

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	1.26	2/6901 (0.0%)	1.13	28/9334 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	HIS	C-N	-78.81	0.23	1.33
1	A	777	SER	CA-C	5.22	1.57	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	967	HIS	CA-C-N	-29.00	69.49	121.70
1	A	967	HIS	C-N-CA	-29.00	69.49	121.70
1	A	967	HIS	O-C-N	26.06	164.70	123.00
1	A	210	TYR	N-CA-C	10.34	126.22	113.50
1	A	775	GLN	N-CA-C	8.85	121.73	111.11
1	A	410	TRP	N-CA-C	7.45	122.11	112.12
1	A	210	TYR	CA-C-N	7.32	134.88	121.70
1	A	210	TYR	C-N-CA	7.32	134.88	121.70
1	A	1077	ASP	CA-C-N	7.14	134.55	121.70
1	A	1077	ASP	C-N-CA	7.14	134.55	121.70
1	A	172	GLU	N-CA-C	6.31	117.82	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	GLN	CA-C-N	6.14	132.75	121.70
1	A	775	GLN	C-N-CA	6.14	132.75	121.70
1	A	785	VAL	CA-C-N	-6.03	113.46	119.92
1	A	785	VAL	C-N-CA	-6.03	113.46	119.92
1	A	966	GLY	CA-C-N	5.84	132.21	121.70
1	A	966	GLY	C-N-CA	5.84	132.21	121.70
1	A	831	ILE	CB-CA-C	-5.64	104.20	111.53
1	A	381	VAL	N-CA-C	5.63	115.78	108.35
1	A	993	PHE	N-CA-C	-5.57	103.14	110.33
1	A	777	SER	CA-C-N	5.46	131.96	121.54
1	A	777	SER	C-N-CA	5.46	131.96	121.54
1	A	1003	SER	N-CA-C	5.45	113.03	108.13
1	A	775	GLN	CA-C-O	-5.39	115.13	120.90
1	A	670	GLU	CA-C-N	5.28	124.79	119.19
1	A	670	GLU	C-N-CA	5.28	124.79	119.19
1	A	145	GLU	CA-C-N	5.26	131.17	121.70
1	A	145	GLU	C-N-CA	5.26	131.17	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	777	SER	Peptide
1	A	967	HIS	Mainchain

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	6757	0	6788	318	0
2	A	5	0	0	0	0
3	A	22	0	12	1	0
4	A	26	0	0	4	0
All	All	6810	0	6800	318	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 23.

All (318) 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:210:TYR:CE1	1:A:211:LEU:HD22	1.86	1.10
1:A:814:GLU:OE1	1:A:827:THR:HG21	1.59	1.03
1:A:628:MET:CE	1:A:1030:LEU:HD21	1.89	1.01
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.38	1.01
1:A:628:MET:HE3	1:A:1030:LEU:CD2	1.91	1.00
1:A:628:MET:HE3	1:A:1030:LEU:HD21	1.44	1.00
1:A:925:VAL:O	1:A:929:VAL:HG23	1.65	0.96
1:A:240:THR:HG22	1:A:242:GLY:H	1.34	0.92
1:A:742:LEU:O	1:A:746:THR:HG23	1.75	0.86
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.06	0.84
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.41	0.83
1:A:966:GLY:HA3	1:A:967:HIS:HB2	1.63	0.81
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.64	0.80
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.11	0.80
1:A:428:LEU:HD23	1:A:467:LEU:HD12	1.63	0.80
1:A:1077:ASP:HB2	1:A:1078:LYS:CG	2.13	0.79
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.64	0.79
1:A:235:VAL:HG11	1:A:244:ILE:HD11	1.63	0.78
1:A:947:ARG:NH2	1:A:963:ILE:O	2.16	0.78
1:A:207:LEU:HD23	1:A:208:PRO:HD2	1.67	0.76
1:A:671:PRO:HD2	4:A:2018:HOH:O	1.85	0.75
1:A:628:MET:HE2	1:A:1030:LEU:HD21	1.70	0.74
1:A:887:THR:HG22	1:A:890:LYS:H	1.53	0.74
1:A:1033:MET:O	1:A:1037:THR:HG23	1.87	0.73
1:A:145:GLU:HA	1:A:146:GLU:O	1.89	0.73
1:A:561:THR:HG22	1:A:591:LYS:HE2	1.71	0.73
1:A:607:THR:O	1:A:610:LEU:HD23	1.88	0.72
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.20	0.72
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.72	0.72
1:A:746:THR:HG22	1:A:811:LEU:CD1	2.19	0.71
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.73	0.71
1:A:777:SER:CB	1:A:778:GLN:HB2	2.21	0.71
1:A:896:VAL:HG12	1:A:896:VAL:O	1.90	0.71
1:A:827:THR:HG22	1:A:883:LYS:HZ2	1.55	0.71
1:A:920:LYS:O	1:A:923:ALA:HB3	1.89	0.70
1:A:208:PRO:HG2	1:A:211:LEU:HD23	1.74	0.70
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.74	0.69
1:A:405:THR:HG23	1:A:408:VAL:HG22	1.72	0.69
1:A:245:LEU:HD11	1:A:272:LEU:HD13	1.73	0.69
1:A:827:THR:HG22	1:A:883:LYS:NZ	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.72	0.69
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.94	0.68
1:A:786:PRO:O	1:A:787:TYR:CG	2.46	0.68
1:A:165:VAL:HG12	1:A:165:VAL:O	1.94	0.68
1:A:602:GLU:O	1:A:605:ALA:HB3	1.92	0.67
1:A:653:ASP:O	1:A:656:VAL:N	2.27	0.67
1:A:775:GLN:HB3	1:A:776:ASN:HB2	1.76	0.67
1:A:1010:GLN:O	1:A:1014:VAL:HG23	1.93	0.67
1:A:1077:ASP:N	1:A:1078:LYS:HB2	2.09	0.67
1:A:738:VAL:HG12	1:A:742:LEU:CD1	2.24	0.67
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.24	0.67
1:A:561:THR:CG2	1:A:591:LYS:HE2	2.25	0.67
1:A:435:CYS:SG	1:A:461:LEU:HD12	2.35	0.67
1:A:724:CYS:SG	1:A:729:LEU:HD13	2.34	0.67
1:A:207:LEU:HD23	1:A:208:PRO:CD	2.24	0.66
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.76	0.66
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.78	0.66
1:A:271:VAL:HG12	1:A:282:VAL:HG12	1.76	0.66
1:A:966:GLY:CA	1:A:967:HIS:HB2	2.25	0.66
1:A:579:ARG:HD2	1:A:610:LEU:HD13	1.78	0.65
1:A:966:GLY:HA3	1:A:967:HIS:CB	2.26	0.65
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.37	0.65
1:A:746:THR:HG22	1:A:811:LEU:HD12	1.78	0.65
1:A:777:SER:HB3	1:A:778:GLN:HB2	1.79	0.64
1:A:560:ALA:HB3	4:A:2012:HOH:O	1.96	0.64
1:A:210:TYR:CD1	1:A:211:LEU:HD22	2.32	0.64
1:A:748:ASP:O	1:A:752:LEU:HD13	1.98	0.63
1:A:198:MET:HE3	1:A:282:VAL:HG11	1.79	0.63
1:A:831:ILE:HG22	1:A:831:ILE:O	1.99	0.63
1:A:767:LEU:HD11	1:A:771:LEU:HD11	1.79	0.62
1:A:844:ILE:CD1	1:A:1034:MET:SD	2.88	0.61
1:A:558:ILE:O	1:A:561:THR:HG22	2.00	0.61
1:A:198:MET:HE1	1:A:271:VAL:HG11	1.83	0.61
1:A:1052:ARG:HB2	1:A:1057:VAL:HG21	1.81	0.61
1:A:775:GLN:CB	1:A:776:ASN:HB2	2.29	0.61
1:A:775:GLN:OE1	1:A:795:ALA:HB1	2.00	0.61
1:A:198:MET:CE	1:A:282:VAL:HG11	2.31	0.61
1:A:944:ILE:HD12	1:A:965:PHE:HD2	1.65	0.61
1:A:212:TRP:CE3	1:A:215:ILE:HD12	2.36	0.60
1:A:216:ALA:HB3	1:A:219:CYS:HB3	1.83	0.60
1:A:1086:TRP:CE3	1:A:1087:PHE:HB2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:MET:O	1:A:805:ALA:C	2.44	0.60
1:A:1077:ASP:HB2	1:A:1078:LYS:HG2	1.84	0.60
1:A:860:LEU:HD22	1:A:862:LEU:HD21	1.82	0.59
1:A:151:GLN:HE21	1:A:163:THR:HG23	1.67	0.59
1:A:930:TYR:CD1	1:A:1012:ILE:HD13	2.37	0.59
1:A:777:SER:HB3	1:A:778:GLN:CB	2.33	0.59
1:A:558:ILE:HG21	1:A:575:LEU:HD21	1.85	0.58
1:A:786:PRO:O	1:A:787:TYR:CD2	2.57	0.58
1:A:158:ILE:HD11	1:A:718:GLU:HB2	1.86	0.57
1:A:170:ASP:OD1	1:A:170:ASP:C	2.47	0.57
1:A:571:ASP:O	1:A:575:LEU:HD23	2.05	0.57
1:A:661:LEU:O	1:A:665:GLN:HG2	2.04	0.57
1:A:653:ASP:O	1:A:654:ASP:C	2.47	0.57
1:A:550:GLN:HA	1:A:553:LYS:HG2	1.86	0.57
1:A:245:LEU:CD1	1:A:272:LEU:HD13	2.35	0.56
1:A:833:LYS:O	1:A:876:ILE:HD12	2.05	0.56
1:A:547:MET:HE2	1:A:552:ARG:N	2.20	0.56
1:A:222:ILE:HD12	1:A:235:VAL:HG21	1.88	0.56
1:A:379:LEU:HD13	1:A:380:THR:H	1.70	0.56
1:A:299:ASN:N	1:A:299:ASN:HD22	2.04	0.56
1:A:912:LYS:NZ	1:A:917:THR:O	2.39	0.56
1:A:775:GLN:CA	1:A:776:ASN:HB2	2.35	0.56
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.86	0.56
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.87	0.56
1:A:785:VAL:HG12	1:A:786:PRO:O	2.05	0.56
1:A:860:LEU:HD11	1:A:1015:LYS:HB3	1.88	0.56
1:A:150:PHE:CE2	1:A:154:LEU:HD21	2.42	0.55
1:A:745:VAL:O	1:A:749:ILE:HD13	2.06	0.55
1:A:434:TYR:HA	1:A:459:GLN:O	2.07	0.55
1:A:829:GLY:C	1:A:881:ILE:HD12	2.31	0.55
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.87	0.55
1:A:157:LEU:HD11	1:A:733:THR:HA	1.88	0.55
1:A:210:TYR:HE1	1:A:211:LEU:HD22	1.64	0.55
1:A:512:ASN:N	1:A:512:ASN:HD22	2.05	0.55
1:A:198:MET:HE3	1:A:282:VAL:HG21	1.88	0.54
1:A:199:HIS:O	1:A:200:PRO:C	2.51	0.54
1:A:582:SER:CB	1:A:592:LEU:HD22	2.38	0.54
1:A:905:GLU:O	1:A:906:VAL:HG23	2.08	0.53
1:A:462:TYR:HA	1:A:485:TRP:O	2.08	0.53
1:A:212:TRP:CZ3	1:A:215:ILE:HD12	2.43	0.53
1:A:365:ILE:HD13	1:A:518:ILE:HG22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:ASP:O	1:A:845:LEU:HD22	2.08	0.53
1:A:498:ASN:OD1	1:A:498:ASN:C	2.51	0.53
1:A:873:GLY:C	1:A:876:ILE:HG22	2.33	0.53
1:A:181:VAL:HG22	1:A:184:ARG:NH2	2.23	0.53
1:A:611:LEU:O	1:A:614:ARG:HG3	2.08	0.53
1:A:741:MET:HE2	1:A:778:GLN:HG3	1.91	0.53
1:A:245:LEU:HD21	1:A:272:LEU:HD13	1.90	0.52
1:A:741:MET:SD	1:A:774:LEU:HD11	2.50	0.52
1:A:746:THR:HG21	1:A:832:PHE:HB3	1.92	0.52
1:A:544:ARG:O	1:A:545:ALA:HB3	2.10	0.52
1:A:583:LEU:HD22	1:A:589:TYR:OH	2.10	0.52
1:A:622:LEU:HD12	1:A:623:ASP:N	2.25	0.52
1:A:929:VAL:HG13	1:A:1009:PHE:HB2	1.92	0.51
1:A:1010:GLN:HE21	1:A:1069:LEU:HD22	1.75	0.51
1:A:157:LEU:O	1:A:700:ARG:NE	2.43	0.51
1:A:208:PRO:CG	1:A:211:LEU:HD23	2.39	0.51
1:A:390:GLY:C	1:A:392:GLN:H	2.18	0.51
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.41	0.51
1:A:628:MET:HE3	1:A:1030:LEU:HD22	1.86	0.51
1:A:689:LYS:O	1:A:690:ARG:C	2.54	0.51
1:A:845:LEU:O	1:A:846:GLN:C	2.54	0.51
1:A:476:ARG:HD2	1:A:480:TYR:OH	2.11	0.50
1:A:827:THR:CG2	1:A:883:LYS:NZ	2.74	0.50
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.12	0.50
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.77	0.50
1:A:360:LYS:HD3	1:A:416:PHE:O	2.10	0.50
1:A:435:CYS:SG	1:A:461:LEU:CD1	2.98	0.50
1:A:932:CYS:O	1:A:936:CYS:SG	2.56	0.50
1:A:948:HIS:ND1	1:A:950:ASP:OD1	2.44	0.50
1:A:593:PHE:CZ	1:A:611:LEU:HD21	2.45	0.50
1:A:775:GLN:O	1:A:779:LEU:HB3	2.12	0.50
1:A:240:THR:HG22	1:A:242:GLY:N	2.16	0.50
1:A:281:LEU:N	1:A:281:LEU:CD1	2.74	0.50
1:A:804:MET:O	1:A:806:SER:N	2.44	0.50
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.93	0.50
1:A:180:LEU:C	1:A:183:PRO:HD2	2.37	0.50
1:A:967:HIS:HB3	1:A:968:ILE:HG13	1.93	0.50
1:A:582:SER:HB2	1:A:592:LEU:HD22	1.94	0.50
1:A:888:ILE:HG21	4:A:2026:HOH:O	2.11	0.50
1:A:276:GLY:HA3	4:A:2003:HOH:O	2.12	0.49
1:A:583:LEU:HD22	1:A:589:TYR:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1040:PRO:O	1:A:1042:LEU:HD22	2.11	0.49
1:A:168:VAL:HG13	1:A:170:ASP:H	1.77	0.49
1:A:936:CYS:HB3	1:A:985:PHE:CD2	2.47	0.49
1:A:733:THR:HG22	1:A:737:GLN:NE2	2.26	0.49
1:A:834:HIS:HB2	1:A:876:ILE:HD13	1.95	0.49
1:A:896:VAL:O	1:A:896:VAL:CG1	2.61	0.49
1:A:212:TRP:C	1:A:214:LYS:H	2.20	0.49
1:A:666:ALA:HB3	1:A:677:LEU:HD21	1.94	0.49
1:A:759:VAL:HG12	1:A:764:ILE:HG12	1.94	0.49
1:A:834:HIS:HA	1:A:875:LYS:O	2.13	0.49
1:A:944:ILE:HB	1:A:968:ILE:HD13	1.95	0.49
1:A:165:VAL:O	1:A:165:VAL:CG1	2.61	0.49
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.48	0.49
1:A:481:VAL:HG22	1:A:517:SER:OG	2.13	0.49
1:A:1023:HIS:O	1:A:1024:THR:C	2.56	0.49
1:A:145:GLU:CA	1:A:146:GLU:O	2.60	0.49
1:A:168:VAL:HG13	1:A:169:HIS:N	2.28	0.49
1:A:219:CYS:SG	1:A:234:LYS:HB2	2.52	0.49
1:A:375:ARG:HG3	1:A:376:ASN:H	1.77	0.49
1:A:632:ASP:C	1:A:632:ASP:OD1	2.56	0.49
1:A:842:MET:HE3	1:A:870:ILE:HD13	1.95	0.49
1:A:1077:ASP:HB2	1:A:1078:LYS:HG3	1.92	0.49
1:A:993:PHE:O	1:A:994:VAL:HB	2.13	0.48
1:A:373:LEU:O	1:A:375:ARG:N	2.47	0.48
1:A:749:ILE:HD11	1:A:770:LYS:HD2	1.95	0.48
1:A:731:ASP:O	1:A:735:GLN:HG3	2.12	0.48
1:A:380:THR:O	1:A:435:CYS:HA	2.13	0.48
1:A:235:VAL:HG12	1:A:236:SER:N	2.29	0.48
1:A:850:ILE:HD13	1:A:1030:LEU:CD1	2.44	0.48
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.41	0.47
1:A:844:ILE:HD11	1:A:1034:MET:SD	2.54	0.47
1:A:509:ASP:C	1:A:509:ASP:OD1	2.57	0.47
1:A:735:GLN:O	1:A:739:ILE:HD13	2.14	0.47
1:A:423:LEU:HD13	1:A:468:LEU:HD13	1.96	0.47
1:A:887:THR:HG22	1:A:889:ALA:N	2.29	0.47
1:A:161:ASP:HB3	1:A:164:ASP:HB3	1.97	0.47
1:A:285:THR:HB	1:A:290:PHE:CE1	2.49	0.47
1:A:759:VAL:HG13	1:A:763:VAL:HG11	1.97	0.47
1:A:844:ILE:O	1:A:848:LEU:HG	2.15	0.47
1:A:588:ALA:O	1:A:589:TYR:C	2.57	0.47
1:A:905:GLU:O	1:A:906:VAL:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:ALA:HB1	1:A:902:PHE:CD2	2.50	0.46
1:A:1043:THR:O	1:A:1048:ILE:HD12	2.14	0.46
1:A:146:GLU:O	1:A:148:GLN:N	2.38	0.46
1:A:625:GLY:O	1:A:629:GLN:HG3	2.15	0.46
1:A:245:LEU:HD11	1:A:272:LEU:CD1	2.42	0.46
1:A:887:THR:HG23	1:A:950:ASP:HA	1.97	0.46
1:A:989:PRO:HG2	1:A:1080:TRP:CD1	2.51	0.46
1:A:280:TYR:HB3	1:A:282:VAL:HG13	1.98	0.46
1:A:361:PHE:HD1	1:A:416:PHE:CD1	2.34	0.46
1:A:370:ILE:HD12	1:A:371:PRO:HD2	1.97	0.46
1:A:483:HIS:CD2	1:A:510:LYS:HD2	2.51	0.46
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.21	0.46
1:A:468:LEU:O	1:A:476:ARG:HB2	2.15	0.46
1:A:997:THR:CG2	1:A:1001:LYS:H	2.29	0.46
1:A:163:THR:O	1:A:165:VAL:HG23	2.15	0.46
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.39	0.46
1:A:470:ASP:OD1	1:A:470:ASP:C	2.58	0.45
1:A:988:THR:O	1:A:991:PHE:N	2.47	0.45
1:A:544:ARG:O	1:A:545:ALA:CB	2.65	0.45
1:A:628:MET:CE	1:A:1030:LEU:CD2	2.65	0.45
1:A:212:TRP:O	1:A:214:LYS:N	2.49	0.45
1:A:952:ILE:HD11	1:A:986:VAL:HG21	1.98	0.45
1:A:1052:ARG:O	1:A:1057:VAL:HG23	2.17	0.45
1:A:182:THR:N	1:A:183:PRO:CD	2.80	0.45
1:A:460:LEU:HD12	1:A:461:LEU:H	1.82	0.45
1:A:214:LYS:O	1:A:214:LYS:HG2	2.16	0.45
1:A:373:LEU:HD21	1:A:406:GLU:HA	1.98	0.45
1:A:585:HIS:O	1:A:586:PRO:C	2.56	0.44
1:A:582:SER:HB3	1:A:592:LEU:HD22	1.99	0.44
1:A:738:VAL:CG1	1:A:742:LEU:CD1	2.95	0.44
1:A:236:SER:O	1:A:239:ASP:OD1	2.35	0.44
1:A:1082:VAL:HG12	1:A:1082:VAL:O	2.16	0.44
1:A:430:ASN:HD22	1:A:465:ASN:HD21	1.64	0.44
1:A:228:THR:O	1:A:228:THR:HG22	2.18	0.44
1:A:748:ASP:O	1:A:752:LEU:CD1	2.65	0.44
1:A:862:LEU:HD12	1:A:934:GLY:HA2	1.98	0.44
1:A:916:PRO:HG2	1:A:920:LYS:HZ1	1.83	0.44
1:A:878:MET:C	1:A:879:ILE:HD12	2.43	0.44
1:A:381:VAL:HG11	1:A:404:PHE:CD1	2.53	0.43
1:A:695:LEU:HD12	1:A:699:LEU:HG	2.00	0.43
1:A:390:GLY:C	1:A:392:GLN:N	2.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.99	0.43
1:A:876:ILE:O	1:A:876:ILE:HG23	2.18	0.43
1:A:1080:TRP:O	1:A:1081:THR:C	2.60	0.43
1:A:420:ILE:HD11	1:A:522:ASN:HD22	1.82	0.43
1:A:966:GLY:HA3	1:A:967:HIS:CG	2.52	0.43
1:A:379:LEU:CD1	1:A:380:THR:H	2.32	0.43
1:A:430:ASN:HD22	1:A:465:ASN:ND2	2.15	0.43
1:A:624:VAL:O	1:A:628:MET:HB2	2.18	0.43
1:A:625:GLY:O	1:A:629:GLN:CG	2.67	0.43
1:A:271:VAL:HG22	1:A:310:PRO:HD3	2.01	0.43
1:A:953:MET:HE1	3:A:2089:EM7:C12	2.49	0.43
1:A:172:GLU:HB2	1:A:471:HIS:CD2	2.54	0.43
1:A:241:PRO:O	1:A:245:LEU:HD23	2.19	0.43
1:A:564:LEU:HG	1:A:1028:ILE:HG21	1.99	0.43
1:A:607:THR:O	1:A:610:LEU:CD2	2.64	0.43
1:A:836:ASP:O	1:A:875:LYS:HA	2.18	0.43
1:A:245:LEU:CD2	1:A:272:LEU:HD13	2.48	0.43
1:A:183:PRO:O	1:A:184:ARG:C	2.62	0.43
1:A:168:VAL:CG1	1:A:169:HIS:N	2.81	0.42
1:A:482:LEU:HB2	1:A:516:ILE:HG23	2.01	0.42
1:A:939:THR:HB	1:A:945:GLY:HA2	2.01	0.42
1:A:806:SER:OG	1:A:807:LYS:N	2.51	0.42
1:A:175:PHE:HD2	1:A:471:HIS:HD1	1.66	0.42
1:A:734:GLN:O	1:A:735:GLN:C	2.62	0.42
1:A:777:SER:OG	1:A:778:GLN:HB2	2.19	0.42
1:A:787:TYR:CD1	1:A:787:TYR:C	2.97	0.42
1:A:1025:ASN:O	1:A:1029:ILE:HG22	2.20	0.42
1:A:180:LEU:O	1:A:183:PRO:HD2	2.20	0.42
1:A:498:ASN:OD1	1:A:499:ALA:N	2.53	0.42
1:A:146:GLU:CD	1:A:147:SER:H	2.28	0.42
1:A:569:ALA:O	1:A:570:GLU:C	2.62	0.42
1:A:756:LYS:HE3	1:A:756:LYS:HA	2.01	0.42
1:A:905:GLU:O	1:A:906:VAL:HB	2.20	0.42
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	2.01	0.42
1:A:1086:TRP:CG	1:A:1087:PHE:N	2.88	0.42
1:A:801:CYS:HA	1:A:812:TRP:O	2.20	0.42
1:A:1081:THR:O	1:A:1085:ASN:ND2	2.53	0.42
1:A:498:ASN:HB2	1:A:1042:LEU:HD11	2.02	0.41
1:A:1018:LEU:HD22	1:A:1061:GLU:HG3	2.02	0.41
1:A:922:GLN:HE21	1:A:922:GLN:CA	2.32	0.41
1:A:927:ARG:O	1:A:931:SER:OG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:N	1:A:409:LEU:HD12	2.34	0.41
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.20	0.41
1:A:1021:ARG:C	1:A:1023:HIS:H	2.28	0.41
1:A:272:LEU:HG	1:A:305:VAL:HG21	2.03	0.41
1:A:852:GLU:O	1:A:855:TRP:N	2.53	0.41
1:A:930:TYR:CE1	1:A:1012:ILE:HD11	2.55	0.41
1:A:232:THR:HG22	1:A:233:ILE:N	2.36	0.41
1:A:370:ILE:HG23	1:A:370:ILE:O	2.21	0.41
1:A:623:ASP:C	1:A:623:ASP:OD1	2.61	0.41
1:A:764:ILE:O	1:A:768:LYS:CG	2.69	0.41
1:A:1071:GLN:NE2	1:A:1071:GLN:HA	2.36	0.41
1:A:726:THR:HA	1:A:729:LEU:HD22	2.03	0.41
1:A:888:ILE:HD11	1:A:960:LEU:HD11	2.02	0.41
1:A:997:THR:HG22	1:A:997:THR:O	2.20	0.41
1:A:150:PHE:CD2	1:A:154:LEU:HD21	2.56	0.41
1:A:418:ILE:CD1	1:A:423:LEU:HD23	2.50	0.41
1:A:547:MET:HE2	1:A:552:ARG:CA	2.51	0.41
1:A:920:LYS:O	1:A:923:ALA:CB	2.65	0.41
1:A:650:SER:O	1:A:651:LEU:C	2.64	0.40
1:A:405:THR:CG2	1:A:408:VAL:HG22	2.45	0.40
1:A:827:THR:CG2	1:A:883:LYS:HZ1	2.34	0.40
1:A:1073:GLU:O	1:A:1074:VAL:C	2.64	0.40
1:A:1077:ASP:CA	1:A:1078:LYS:HB2	2.50	0.40
1:A:887:THR:HG21	1:A:889:ALA:HB3	2.04	0.40
1:A:211:LEU:HD12	1:A:211:LEU:HA	1.77	0.40
1:A:292:TRP:O	1:A:295:HIS:HB3	2.21	0.40
1:A:403:PRO:O	1:A:405:THR:HG22	2.22	0.40
1:A:465:ASN:HB2	1:A:503:THR:O	2.21	0.40
1:A:203:THR:HG21	1:A:291:GLN:HE21	1.86	0.40
1:A:824:SER:OG	1:A:825:ASN:N	2.54	0.40
1:A:996:GLY:O	1:A:997:THR:OG1	2.31	0.40
1:A:1077:ASP:HB2	1:A:1078:LYS:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	819/980 (84%)	688 (84%)	105 (13%)	26 (3%)	3 10

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	211	LEU
1	A	216	ALA
1	A	374	PRO
1	A	778	GLN
1	A	894	SER
1	A	906	VAL
1	A	967	HIS
1	A	1040	PRO
1	A	1078	LYS
1	A	545	ALA
1	A	654	ASP
1	A	754	ALA
1	A	776	ASN
1	A	805	ALA
1	A	966	GLY
1	A	1079	GLY
1	A	213	LYS
1	A	227	SER
1	A	230	SER
1	A	855	TRP
1	A	300	GLY
1	A	997	THR
1	A	1077	ASP
1	A	916	PRO
1	A	989	PRO

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	749/874 (86%)	663 (88%)	86 (12%)	5 17

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	146	GLU
1	A	157	LEU
1	A	164	ASP
1	A	168	VAL
1	A	191	ARG
1	A	194	LYS
1	A	195	LEU
1	A	203	THR
1	A	207	LEU
1	A	211	LEU
1	A	217	ASN
1	A	244	ILE
1	A	269	ASP
1	A	271	VAL
1	A	272	LEU
1	A	273	ARG
1	A	281	LEU
1	A	299	ASN
1	A	307	LEU
1	A	359	ARG
1	A	377	THR
1	A	379	LEU
1	A	389	HIS
1	A	405	THR
1	A	410	TRP
1	A	420	ILE
1	A	421	LYS
1	A	435	CYS
1	A	459	GLN
1	A	467	LEU
1	A	475	LEU
1	A	497	PHE
1	A	502	LEU
1	A	512	ASN
1	A	544	ARG

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Mol	Chain	Res	Type
1	A	546	GLU
1	A	550	GLN
1	A	570	GLU
1	A	583	LEU
1	A	595	SER
1	A	603	ILE
1	A	616	VAL
1	A	629	GLN
1	A	638	GLU
1	A	650	SER
1	A	701	SER
1	A	721	LEU
1	A	728	MET
1	A	729	LEU
1	A	730	HIS
1	A	746	THR
1	A	747	LEU
1	A	753	SER
1	A	756	LYS
1	A	764	ILE
1	A	767	LEU
1	A	778	GLN
1	A	787	TYR
1	A	799	GLU
1	A	807	LYS
1	A	809	LYS
1	A	823	LEU
1	A	827	THR
1	A	845	LEU
1	A	847	ILE
1	A	862	LEU
1	A	887	THR
1	A	911	LEU
1	A	912	LYS
1	A	919	GLU
1	A	922	GLN
1	A	931	SER
1	A	949	ASN
1	A	959	ASN
1	A	968	ILE
1	A	1001	LYS
1	A	1002	THR

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Mol	Chain	Res	Type
1	A	1037	THR
1	A	1042	LEU
1	A	1051	ILE
1	A	1061	GLU
1	A	1066	LYS
1	A	1071	GLN
1	A	1072	ILE
1	A	1087	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	218	ASN
1	A	291	GLN
1	A	299	ASN
1	A	304	HIS
1	A	386	ASN
1	A	396	GLN
1	A	465	ASN
1	A	512	ASN
1	A	522	ASN
1	A	549	ASN
1	A	565	ASN
1	A	577	HIS
1	A	629	GLN
1	A	711	GLN
1	A	730	HIS
1	A	737	GLN
1	A	743	GLN
1	A	776	ASN
1	A	893	GLN
1	A	898	ASN
1	A	908	ASN
1	A	922	GLN
1	A	951	ASN
1	A	1010	GLN
1	A	1022	HIS

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 oligosaccharides 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	$\# Z > 2$
2	SO4	A	2088	-	4,4,4	0.25	0	6,6,6	0.24	0
3	EM7	A	2089	-	24,24,24	3.08	6 (25%)	31,33,33	1.32	4 (12%)

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	EM7	A	2089	-	-	4/14/14/14	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2089	EM7	N1-N4	-9.43	1.23	1.35
3	A	2089	EM7	N2-N3	-7.43	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2089	EM7	C7-C2	-5.91	1.39	1.49
3	A	2089	EM7	C9-C1	-4.17	1.39	1.47
3	A	2089	EM7	C5-C12	3.71	1.56	1.50
3	A	2089	EM7	N4-N3	-2.80	1.24	1.30

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2089	EM7	N1-C1-N2	-3.18	104.43	108.26
3	A	2089	EM7	C11-C10-C9	-2.35	118.06	120.36
3	A	2089	EM7	C5-N6-C2	2.17	122.00	118.45
3	A	2089	EM7	C5-C4-N5	2.10	120.91	119.78

There are no chirality outliers.

All (4) torsion outliers are listed below:

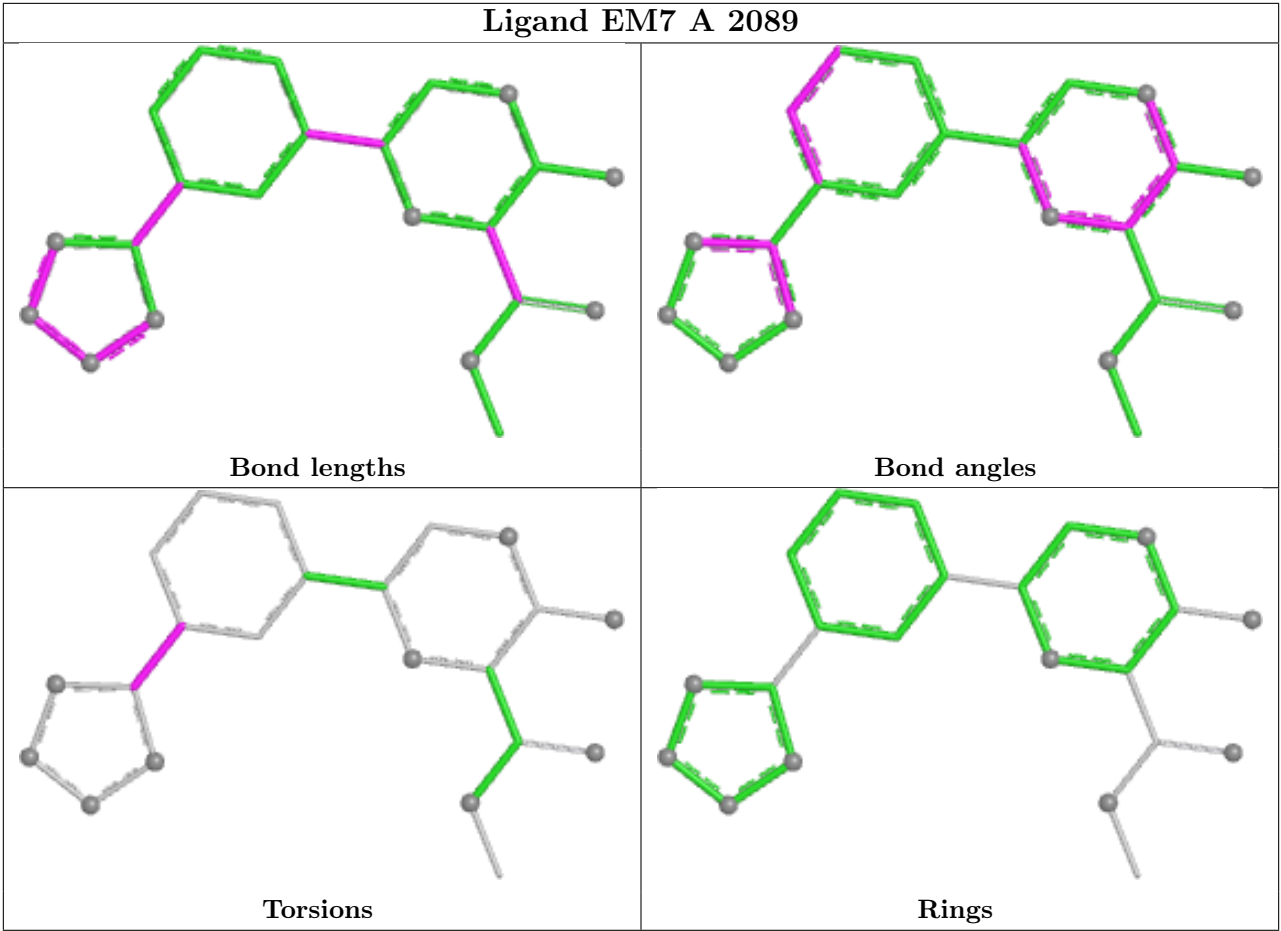
Mol	Chain	Res	Type	Atoms
3	A	2089	EM7	N2-C1-C9-C8
3	A	2089	EM7	N1-C1-C9-C8
3	A	2089	EM7	N2-C1-C9-C10
3	A	2089	EM7	N1-C1-C9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2089	EM7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	967:HIS	C	968:ILE	N	0.23

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	833/980 (85%)	0.69	47 (5%) 30 23	45, 73, 99, 110	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	859	SER	5.8
1	A	1044	SER	4.8
1	A	967	HIS	3.7
1	A	757	TYR	3.6
1	A	968	ILE	3.5
1	A	245	LEU	3.5
1	A	1079	GLY	3.4
1	A	987	LEU	3.3
1	A	1042	LEU	3.2
1	A	377	THR	3.2
1	A	966	GLY	3.1
1	A	1086	TRP	3.0
1	A	896	VAL	3.0
1	A	212	TRP	2.9
1	A	379	LEU	2.9
1	A	1046	GLU	2.8
1	A	1087	PHE	2.8
1	A	860	LEU	2.7
1	A	754	ALA	2.6
1	A	926	GLU	2.6
1	A	404	PHE	2.6
1	A	223	VAL	2.5
1	A	758	ASP	2.5
1	A	894	SER	2.5
1	A	895	THR	2.4
1	A	307	LEU	2.4
1	A	1043	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	646	GLN	2.3
1	A	761	SER	2.3
1	A	550	GLN	2.2
1	A	374	PRO	2.2
1	A	489	GLY	2.2
1	A	994	VAL	2.2
1	A	899	THR	2.2
1	A	931	SER	2.2
1	A	219	CYS	2.1
1	A	414	LEU	2.1
1	A	385	ALA	2.1
1	A	1057	VAL	2.1
1	A	316	ASP	2.1
1	A	897	GLY	2.1
1	A	898	ASN	2.1
1	A	1056	THR	2.1
1	A	393	VAL	2.0
1	A	315	LEU	2.0
1	A	900	GLY	2.0
1	A	1085	ASN	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](#)

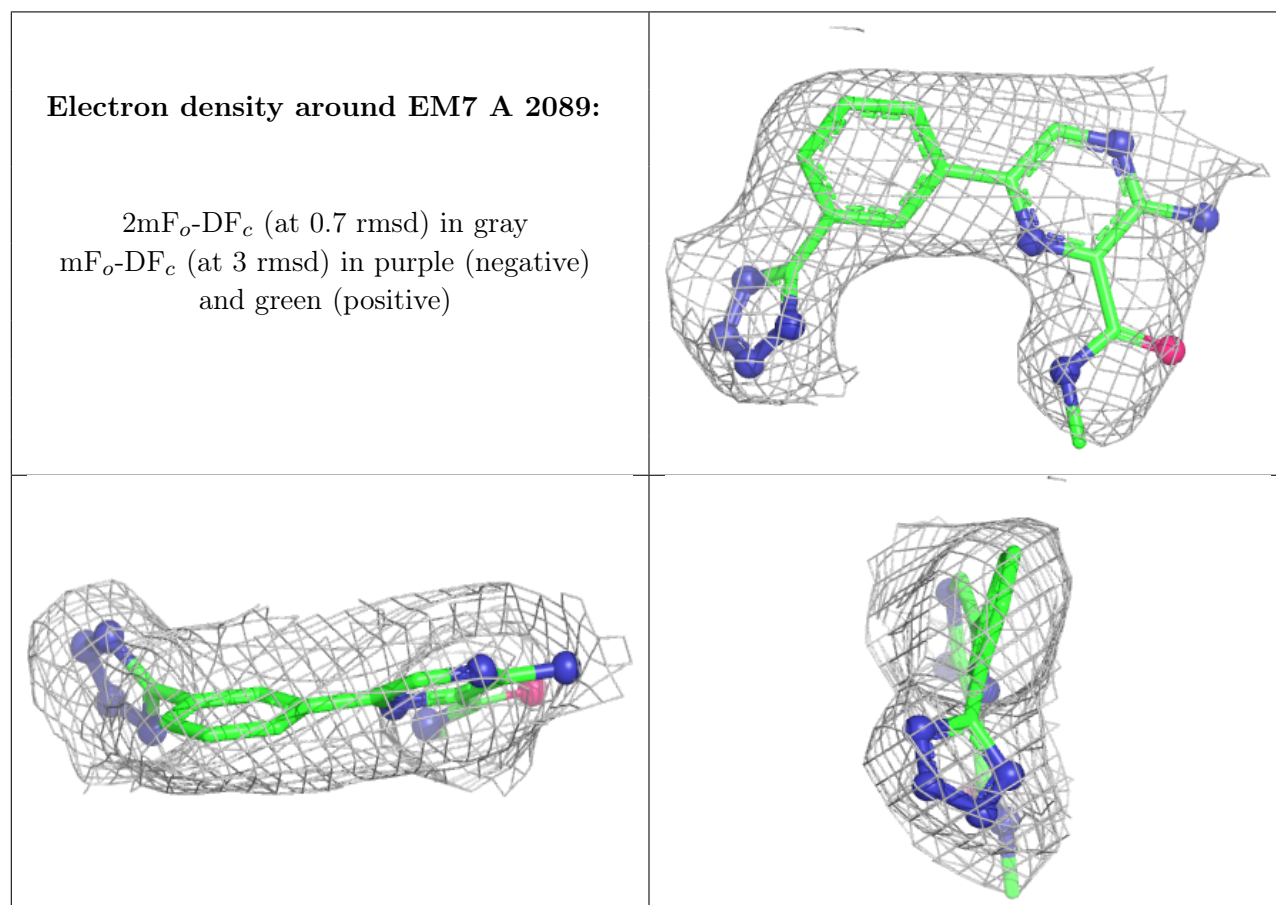
There are no oligosaccharides in this entry.

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
2	SO4	A	2088	5/5	0.83	0.12	97,98,98,99	0
3	EM7	A	2089	22/22	0.87	0.10	70,72,79,80	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 ⓘ

There are no such residues in this entry.