



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:08 AM EDT

PDB ID : 4ANX / pdb_00004anx
Title : Complexes of PI3Kgamma with isoform selective inhibitors.
Authors : Foster, P.G.; Lougheed, J.C.
Deposited on : 2012-03-22
Resolution : 2.73 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

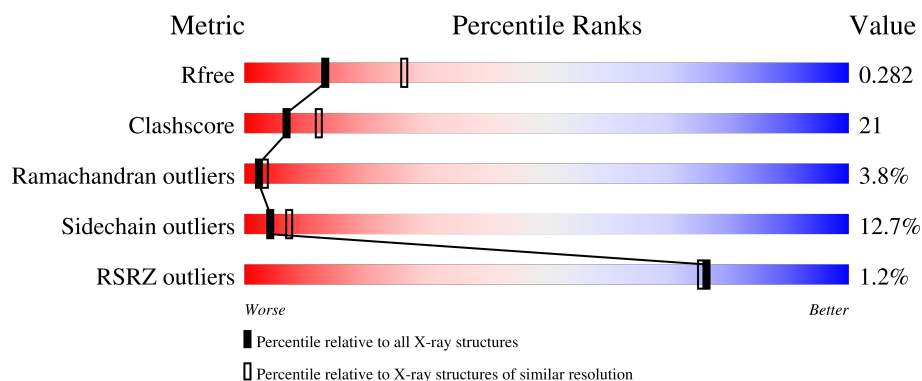
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6828 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.

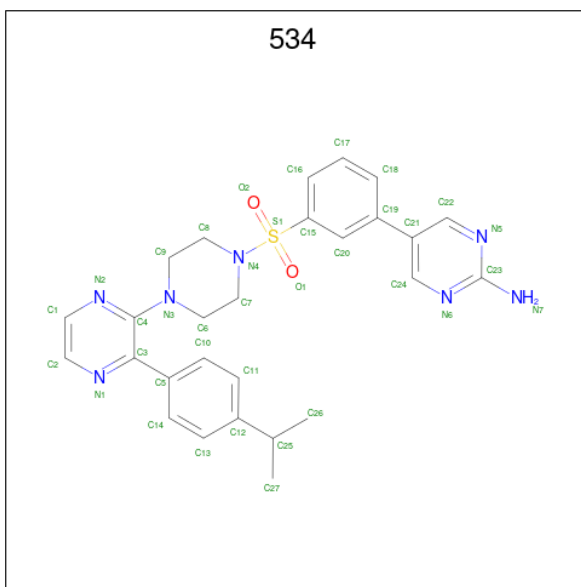
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

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 5-{3-[(4-{3-[4-(1-methylethyl)phenyl]pyrazin-2-yl}piperazin-1-yl)sulfonyl]phenyl}pyrimidin-2-amine (CCD ID: 534) (formula: C₂₇H₂₉N₇O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			37	27	7	2	1		

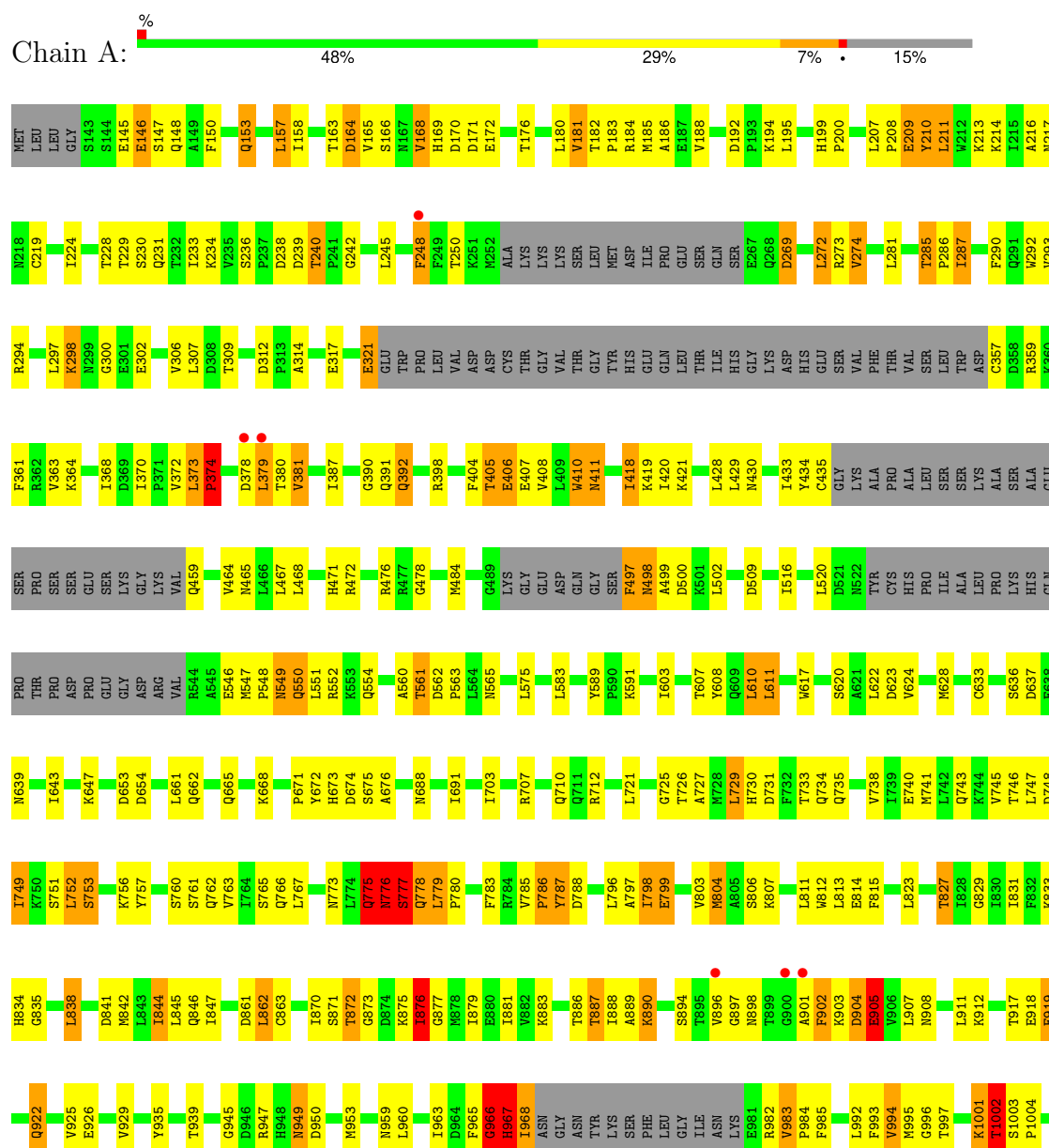
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		

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 GAMMA ISOFORM



Q1007	K1008	F1009	Q1010	V1014	Y1017	R1021	I1028	I1029	L1030	F1031	M1033	M1034	L1035	M1036	T1037	G1038	M1039	P1040	Q1041	L1042	T1043	S1044	K1045	E1046	D1047	I1048	E1049	D1053	G1058	K1059	D1063	K1066	Y1067	F1068	Q1071	I1072	R1076	D1077	K1078	G1079	Q1083	F1084	N1085	W1086	F1087	LEU	HIS									
LEU	VAL	LEU	GLY	ILE	LYS	GLN	GLY	GLU	LYS	HIS	SER	ALA	GLU	PHE	GLY	LEU	VAL	PRO	ARG	GLY	SER	GLY	HIS	HIS	HIS	HIS	HIS	HIS	LEU	VAL	GLY	ILE	LYS	GLN	GLY	GLU	LYS	HIS	SER	ALA	GLU	PHE	GLY	LEU	VAL	PRO	ARG	GLY	SER	GLY	HIS	HIS	HIS	HIS	LEU	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.42Å 68.53Å 106.26Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	32.60 – 2.73 32.60 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.5 (32.60-2.73) 99.4 (32.60-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.282 0.226 , 0.282	Depositor DCC
R_{free} test set	1375 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6828	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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:
534

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	0.85	1/6901 (0.0%)	1.05	27/9334 (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	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	HIS	C-N	-9.06	1.20	1.33

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	775	GLN	N-CA-C	11.90	123.99	111.14
1	A	210	TYR	N-CA-C	11.25	128.80	112.94
1	A	1077	ASP	N-CA-C	7.67	120.32	111.11
1	A	1077	ASP	CA-C-N	7.54	135.28	121.70
1	A	1077	ASP	C-N-CA	7.54	135.28	121.70
1	A	478	GLY	N-CA-C	6.49	118.69	110.38
1	A	410	TRP	N-CA-C	6.48	120.81	112.12
1	A	210	TYR	CA-C-N	6.28	133.01	121.70
1	A	210	TYR	C-N-CA	6.28	133.01	121.70
1	A	967	HIS	O-C-N	-6.27	112.97	123.00
1	A	777	SER	CA-C-N	6.17	133.32	121.54
1	A	777	SER	C-N-CA	6.17	133.32	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	983	VAL	N-CA-C	-6.07	104.22	109.19
1	A	381	VAL	N-CA-C	5.97	115.70	108.06
1	A	904	ASP	N-CA-C	5.72	118.00	111.02
1	A	181	VAL	CB-CA-C	-5.68	104.61	111.88
1	A	966	GLY	CA-C-N	5.45	131.51	121.70
1	A	966	GLY	C-N-CA	5.45	131.51	121.70
1	A	786	PRO	N-CA-C	-5.44	103.61	111.22
1	A	804	MET	N-CA-C	5.40	119.97	113.17
1	A	1077	ASP	CA-C-O	-5.30	115.23	120.90
1	A	163	THR	N-CA-C	-5.12	107.20	113.50
1	A	777	SER	CB-CA-C	5.10	120.58	110.42
1	A	775	GLN	CA-C-N	5.09	130.87	121.70
1	A	775	GLN	C-N-CA	5.09	130.87	121.70
1	A	844	ILE	CB-CA-C	-5.06	105.31	112.14
1	A	876	ILE	N-CA-C	5.04	115.91	108.45

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	209	GLU	Peptide
1	A	210	TYR	Peptide
1	A	777	SER	Peptide
1	A	965	PHE	Peptide

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	6757	0	6789	287	0
2	A	37	0	29	4	0
3	A	34	0	0	4	0
All	All	6828	0	6818	287	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (287) 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:967:HIS:H	1:A:968:ILE:HA	1.07	1.11
1:A:775:GLN:HE22	1:A:798:ILE:HD11	1.21	1.02
1:A:827:THR:HG22	1:A:883:LYS:NZ	1.81	0.95
1:A:561:THR:HG22	1:A:591:LYS:NZ	1.81	0.95
1:A:967:HIS:N	1:A:968:ILE:HA	1.73	0.94
1:A:827:THR:HG22	1:A:883:LYS:HZ2	1.38	0.89
1:A:967:HIS:H	1:A:968:ILE:CA	1.86	0.89
1:A:925:VAL:O	1:A:929:VAL:HG23	1.73	0.88
1:A:966:GLY:HA3	1:A:967:HIS:HB2	1.54	0.87
1:A:430:ASN:HD22	1:A:465:ASN:HD21	1.23	0.86
1:A:145:GLU:HA	1:A:146:GLU:O	1.75	0.86
1:A:777:SER:HB3	1:A:778:GLN:CB	2.06	0.85
1:A:907:LEU:HD23	1:A:994:VAL:HG21	1.58	0.83
1:A:233:ILE:HG22	1:A:234:LYS:O	1.81	0.81
1:A:561:THR:HG22	1:A:591:LYS:HZ3	1.43	0.81
1:A:903:LYS:HG2	1:A:905:GLU:OE2	1.82	0.80
1:A:1077:ASP:N	1:A:1078:LYS:HB2	1.98	0.79
1:A:620:SER:O	1:A:647:LYS:NZ	2.17	0.78
1:A:814:GLU:OE1	1:A:827:THR:HG21	1.84	0.77
1:A:775:GLN:N	1:A:776:ASN:HB2	1.99	0.77
1:A:497:PHE:O	1:A:1042:LEU:HD11	1.83	0.77
1:A:777:SER:CB	1:A:778:GLN:HB2	2.15	0.77
1:A:430:ASN:HD22	1:A:465:ASN:ND2	1.82	0.77
1:A:926:GLU:OE2	1:A:1008:LYS:NZ	2.18	0.76
1:A:777:SER:HB3	1:A:778:GLN:HB3	1.67	0.76
1:A:811:LEU:HB3	1:A:813:LEU:HD21	1.68	0.75
1:A:168:VAL:HG13	1:A:170:ASP:H	1.52	0.75
1:A:165:VAL:HG12	1:A:165:VAL:O	1.87	0.75
1:A:907:LEU:O	1:A:911:LEU:HD23	1.87	0.75
1:A:146:GLU:O	1:A:148:GLN:N	2.20	0.74
1:A:245:LEU:HD21	1:A:272:LEU:HD22	1.70	0.74
1:A:775:GLN:CA	1:A:776:ASN:HB2	2.18	0.73
1:A:182:THR:HB	1:A:183:PRO:HD3	1.72	0.72
1:A:498:ASN:OD1	1:A:498:ASN:C	2.32	0.72
1:A:236:SER:OG	1:A:239:ASP:OD1	2.08	0.71
1:A:748:ASP:O	1:A:752:LEU:HD13	1.88	0.71
1:A:777:SER:HB3	1:A:778:GLN:HB2	1.70	0.71
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.73	0.70
1:A:966:GLY:CA	1:A:967:HIS:HB2	2.22	0.70
1:A:761:SER:O	1:A:765:SER:N	2.26	0.69
1:A:907:LEU:O	1:A:911:LEU:CD2	2.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:MET:O	1:A:960:LEU:HD12	1.93	0.69
1:A:673:HIS:HD2	1:A:712:ARG:HE	1.39	0.68
1:A:583:LEU:HD22	1:A:589:TYR:OH	1.92	0.68
1:A:624:VAL:HG12	1:A:628:MET:HE2	1.75	0.68
1:A:662:GLN:OE1	1:A:1030:LEU:HD22	1.93	0.68
1:A:741:MET:HE2	1:A:778:GLN:HG3	1.76	0.68
1:A:405:THR:HG23	1:A:408:VAL:HG22	1.76	0.68
1:A:561:THR:HG22	1:A:591:LYS:CE	2.23	0.68
1:A:947:ARG:NH2	1:A:963:ILE:O	2.26	0.68
1:A:731:ASP:O	1:A:735:GLN:HG3	1.95	0.67
1:A:997:THR:HG23	1:A:1002:THR:N	2.08	0.67
1:A:834:HIS:CA	1:A:876:ILE:HD12	2.24	0.67
1:A:240:THR:HG22	1:A:242:GLY:N	2.10	0.67
1:A:775:GLN:NE2	1:A:798:ILE:HD11	2.04	0.67
1:A:812:TRP:C	1:A:813:LEU:HD23	2.20	0.66
1:A:1077:ASP:HB2	1:A:1078:LYS:HG2	1.78	0.66
1:A:561:THR:HG23	1:A:565:ASN:HB3	1.78	0.65
1:A:181:VAL:HG13	1:A:185:MET:HE3	1.78	0.65
1:A:1048:ILE:HD12	1:A:1048:ILE:H	1.62	0.65
1:A:185:MET:CE	1:A:321:GLU:HG3	2.26	0.65
1:A:245:LEU:CD2	1:A:272:LEU:HD22	2.26	0.64
1:A:673:HIS:CD2	1:A:712:ARG:HE	2.15	0.64
1:A:379:LEU:HD13	1:A:380:THR:HG22	1.80	0.64
1:A:725:GLY:O	1:A:729:LEU:HD22	1.98	0.63
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.78	0.63
1:A:561:THR:CG2	1:A:565:ASN:HB3	2.28	0.63
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.80	0.63
1:A:775:GLN:H	1:A:776:ASN:HB2	1.64	0.63
1:A:1068:PHE:O	1:A:1071:GLN:HB2	1.99	0.62
1:A:844:ILE:HD13	1:A:1034:MET:SD	2.39	0.62
1:A:287:ILE:HG22	1:A:293:VAL:HG21	1.81	0.62
1:A:834:HIS:N	1:A:876:ILE:HD12	2.15	0.62
1:A:171:ASP:OD2	1:A:472:ARG:NH2	2.32	0.61
1:A:966:GLY:HA3	1:A:967:HIS:CB	2.26	0.61
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.47	0.61
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.36	0.61
1:A:476:ARG:O	1:A:520:LEU:HD23	2.02	0.60
1:A:827:THR:CG2	1:A:883:LYS:NZ	2.62	0.60
1:A:671:PRO:HD2	3:A:2024:HOH:O	2.00	0.60
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.84	0.60
1:A:207:LEU:C	1:A:207:LEU:HD23	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:ILE:HD12	1:A:287:ILE:H	1.67	0.60
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.84	0.59
1:A:950:ASP:HB2	2:A:2088:534:C2	2.32	0.59
1:A:862:LEU:CD2	1:A:862:LEU:N	2.65	0.59
1:A:887:THR:HG22	1:A:890:LYS:H	1.68	0.59
1:A:207:LEU:HD23	1:A:208:PRO:N	2.17	0.58
1:A:560:ALA:HB3	3:A:2013:HOH:O	2.03	0.58
1:A:1010:GLN:O	1:A:1014:VAL:HG23	2.04	0.58
1:A:312:ASP:OD2	1:A:314:ALA:HB3	2.03	0.58
1:A:804:MET:HE3	2:A:2088:534:H261	1.85	0.57
1:A:1032:SER:O	1:A:1036:MET:HG3	2.04	0.57
1:A:963:ILE:HB	2:A:2088:534:C17	2.35	0.57
1:A:172:GLU:HG3	1:A:471:HIS:CD2	2.39	0.57
1:A:207:LEU:CD2	1:A:211:LEU:HB3	2.34	0.57
1:A:548:PRO:O	1:A:549:ASN:C	2.48	0.57
1:A:608:TYR:OH	1:A:637:ASP:OD1	2.23	0.57
1:A:827:THR:HG22	1:A:883:LYS:HZ1	1.66	0.57
1:A:949:ASN:HD22	1:A:949:ASN:C	2.12	0.57
1:A:181:VAL:CG1	1:A:185:MET:HE3	2.34	0.57
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.35	0.57
1:A:150:PHE:O	1:A:153:GLN:N	2.39	0.56
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.06	0.56
1:A:1003:SER:OG	1:A:1004:PRO:HD2	2.05	0.56
1:A:831:ILE:HB	1:A:879:ILE:HB	1.88	0.56
1:A:561:THR:HG22	1:A:591:LYS:HE2	1.88	0.55
1:A:668:LYS:O	3:A:2023:HOH:O	2.18	0.55
1:A:185:MET:HE2	1:A:321:GLU:HG3	1.89	0.55
1:A:547:MET:HE2	1:A:552:ARG:N	2.21	0.55
1:A:661:LEU:O	1:A:665:GLN:HG2	2.07	0.55
1:A:381:VAL:HG12	1:A:435:CYS:SG	2.47	0.55
1:A:1072:ILE:O	1:A:1076:ARG:HG3	2.07	0.55
1:A:707:ARG:HH11	1:A:710:GLN:HE22	1.55	0.55
1:A:726:THR:O	1:A:727:ALA:C	2.47	0.54
1:A:887:THR:CG2	1:A:889:ALA:HB3	2.37	0.54
1:A:1017:TYR:CE2	1:A:1021:ARG:HD2	2.42	0.54
1:A:583:LEU:CD2	1:A:589:TYR:OH	2.54	0.54
1:A:1033:MET:O	1:A:1037:THR:HG23	2.07	0.54
1:A:165:VAL:O	1:A:165:VAL:CG1	2.55	0.54
1:A:804:MET:CE	2:A:2088:534:H261	2.38	0.54
1:A:498:ASN:OD1	1:A:500:ASP:N	2.39	0.54
1:A:390:GLY:C	1:A:392:GLN:H	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG13	1:A:170:ASP:N	2.20	0.54
1:A:363:VAL:HG23	1:A:520:LEU:HD12	1.89	0.54
1:A:561:THR:CG2	1:A:591:LYS:HE2	2.37	0.53
1:A:617:TRP:CE2	1:A:643:ILE:HD12	2.44	0.53
1:A:357:CYS:SG	1:A:359:ARG:NE	2.82	0.53
1:A:181:VAL:O	1:A:185:MET:HG3	2.09	0.53
1:A:996:GLY:O	1:A:1003:SER:HB2	2.09	0.53
1:A:622:LEU:HD12	1:A:623:ASP:H	1.72	0.52
1:A:1048:ILE:HD12	1:A:1048:ILE:N	2.24	0.52
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.91	0.52
1:A:434:TYR:HA	1:A:459:GLN:O	2.10	0.52
1:A:992:LEU:O	1:A:995:MET:HB2	2.09	0.52
1:A:428:LEU:CD2	1:A:467:LEU:HD12	2.40	0.52
1:A:192:ASP:CG	1:A:195:LEU:HD23	2.34	0.51
1:A:688:ASN:HB3	1:A:691:ILE:HD12	1.93	0.51
1:A:861:ASP:C	1:A:862:LEU:HD22	2.36	0.51
1:A:361:PHE:HA	1:A:420:ILE:HD11	1.92	0.51
1:A:379:LEU:HD13	1:A:380:THR:H	1.75	0.51
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.91	0.51
1:A:1043:THR:O	1:A:1045:LYS:N	2.43	0.51
1:A:777:SER:OG	1:A:778:GLN:HB2	2.11	0.51
1:A:827:THR:CG2	1:A:883:LYS:HZ1	2.22	0.51
1:A:391:GLN:NE2	1:A:633:CYS:SG	2.84	0.51
1:A:285:THR:HB	1:A:290:PHE:CE1	2.46	0.51
1:A:775:GLN:CB	1:A:776:ASN:HB2	2.41	0.51
1:A:919:GLU:HA	1:A:922:GLN:HB2	1.93	0.50
1:A:302:GLU:HG3	3:A:2008:HOH:O	2.11	0.50
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.76	0.50
1:A:184:ARG:O	1:A:188:VAL:HG23	2.11	0.50
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.47	0.50
1:A:373:LEU:O	1:A:374:PRO:C	2.55	0.50
1:A:786:PRO:O	1:A:787:TYR:CG	2.65	0.50
1:A:901:ALA:HB1	1:A:902:PHE:HA	1.92	0.50
1:A:1049:GLU:O	1:A:1053:ASP:OD2	2.30	0.49
1:A:1058:GLY:O	1:A:1059:LYS:O	2.29	0.49
1:A:192:ASP:C	1:A:192:ASP:OD1	2.55	0.49
1:A:269:ASP:O	1:A:309:THR:HG22	2.11	0.49
1:A:887:THR:HG21	1:A:889:ALA:HB3	1.95	0.49
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.95	0.49
1:A:726:THR:HA	1:A:729:LEU:HD23	1.94	0.49
1:A:993:PHE:O	1:A:994:VAL:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:PHE:O	1:A:994:VAL:HG23	2.13	0.48
1:A:760:SER:OG	1:A:763:VAL:HG23	2.13	0.48
1:A:993:PHE:O	1:A:994:VAL:HB	2.13	0.48
1:A:245:LEU:HD11	1:A:272:LEU:HD13	1.94	0.48
1:A:317:GLU:O	1:A:726:THR:HG23	2.14	0.48
1:A:904:ASP:O	1:A:905:GLU:O	2.30	0.48
1:A:370:ILE:HG23	1:A:370:ILE:O	2.12	0.48
1:A:411:ASN:CG	1:A:411:ASN:O	2.57	0.48
1:A:1077:ASP:CA	1:A:1078:LYS:HB2	2.43	0.48
1:A:779:LEU:HD13	1:A:780:PRO:HD2	1.96	0.48
1:A:835:GLY:O	1:A:875:LYS:HD3	2.14	0.48
1:A:207:LEU:HD23	1:A:208:PRO:CD	2.44	0.48
1:A:373:LEU:HD22	1:A:404:PHE:CE2	2.49	0.48
1:A:887:THR:HG22	1:A:889:ALA:N	2.29	0.48
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.95	0.48
1:A:797:ALA:O	1:A:798:ILE:C	2.57	0.47
1:A:997:THR:HG23	1:A:1002:THR:H	1.78	0.47
1:A:164:ASP:OD1	1:A:166:SER:OG	2.27	0.47
1:A:639:ASN:O	1:A:643:ILE:HG23	2.13	0.47
1:A:743:GLN:O	1:A:746:THR:HG22	2.14	0.47
1:A:498:ASN:OD1	1:A:499:ALA:N	2.47	0.47
1:A:1085:ASN:C	1:A:1087:PHE:H	2.23	0.47
1:A:171:ASP:HB3	1:A:471:HIS:CE1	2.50	0.47
1:A:467:LEU:HD23	1:A:672:TYR:CE1	2.49	0.47
1:A:1059:LYS:HG3	1:A:1063:ASP:HB2	1.96	0.47
1:A:607:THR:O	1:A:610:LEU:HD23	2.14	0.47
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.45	0.47
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.79	0.46
1:A:405:THR:HG23	1:A:407:GLU:O	2.15	0.46
1:A:464:VAL:HG12	1:A:484:MET:HE2	1.96	0.46
1:A:497:PHE:HB2	1:A:1042:LEU:HD21	1.96	0.46
1:A:813:LEU:HD23	1:A:813:LEU:N	2.30	0.46
1:A:168:VAL:HG13	1:A:169:HIS:N	2.30	0.46
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.98	0.46
1:A:745:VAL:O	1:A:749:ILE:HD13	2.16	0.46
1:A:786:PRO:C	1:A:788:ASP:H	2.24	0.46
1:A:361:PHE:HB2	1:A:420:ILE:HD12	1.98	0.45
1:A:787:TYR:CD1	1:A:787:TYR:C	2.95	0.45
1:A:796:LEU:HD13	1:A:815:PHE:CE2	2.50	0.45
1:A:623:ASP:OD1	1:A:623:ASP:C	2.58	0.45
1:A:509:ASP:C	1:A:509:ASP:OD1	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:SER:C	1:A:753:SER:H	2.24	0.45
1:A:738:VAL:HG21	1:A:783:PHE:CG	2.50	0.45
1:A:418:ILE:HG13	1:A:419:LYS:N	2.32	0.45
1:A:207:LEU:C	1:A:207:LEU:CD2	2.90	0.44
1:A:738:VAL:HG21	1:A:783:PHE:CB	2.47	0.44
1:A:239:ASP:HB2	1:A:287:ILE:HD11	2.00	0.44
1:A:380:THR:C	1:A:381:VAL:HG13	2.42	0.44
1:A:624:VAL:CG1	1:A:628:MET:HE2	2.46	0.44
1:A:145:GLU:CA	1:A:146:GLU:O	2.58	0.44
1:A:653:ASP:O	1:A:654:ASP:C	2.61	0.43
1:A:738:VAL:HG21	1:A:783:PHE:HB3	2.00	0.43
1:A:214:LYS:HE3	1:A:300:GLY:HA2	2.00	0.43
1:A:471:HIS:CD2	1:A:471:HIS:H	2.35	0.43
1:A:740:GLU:O	1:A:741:MET:C	2.61	0.43
1:A:779:LEU:HD13	1:A:780:PRO:N	2.33	0.43
1:A:192:ASP:OD2	1:A:195:LEU:HD23	2.18	0.43
1:A:207:LEU:CD2	1:A:208:PRO:O	2.66	0.43
1:A:561:THR:HG23	1:A:562:ASP:O	2.18	0.43
1:A:799:GLU:CD	1:A:799:GLU:H	2.26	0.43
1:A:834:HIS:HA	1:A:876:ILE:HD12	1.98	0.43
1:A:617:TRP:O	1:A:620:SER:OG	2.26	0.43
1:A:550:GLN:O	1:A:554:GLN:HG3	2.18	0.43
1:A:823:LEU:O	1:A:823:LEU:HG	2.18	0.43
1:A:551:LEU:O	1:A:552:ARG:C	2.61	0.43
1:A:842:MET:HE3	1:A:870:ILE:HA	2.00	0.43
1:A:1001:LYS:C	1:A:1002:THR:HG22	2.43	0.43
1:A:207:LEU:HD23	1:A:208:PRO:O	2.19	0.43
1:A:547:MET:HE2	1:A:551:LEU:C	2.44	0.43
1:A:297:LEU:O	1:A:298:LYS:C	2.60	0.42
1:A:357:CYS:SG	1:A:359:ARG:HG2	2.60	0.42
1:A:779:LEU:HD13	1:A:779:LEU:C	2.44	0.42
1:A:611:LEU:HD22	1:A:643:ILE:HG21	2.01	0.42
1:A:199:HIS:O	1:A:200:PRO:C	2.60	0.42
1:A:497:PHE:CD1	1:A:497:PHE:N	2.87	0.42
1:A:207:LEU:HD23	1:A:208:PRO:HD2	2.02	0.42
1:A:380:THR:O	1:A:381:VAL:HG13	2.20	0.42
1:A:862:LEU:N	1:A:862:LEU:HD22	2.34	0.42
1:A:779:LEU:HD13	1:A:780:PRO:CD	2.50	0.42
1:A:935:TYR:O	1:A:939:THR:HG23	2.19	0.42
1:A:785:VAL:HG12	1:A:786:PRO:O	2.19	0.42
1:A:1043:THR:OG1	1:A:1047:ASP:N	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:777:SER:CB	1:A:778:GLN:CB	2.78	0.42
1:A:896:VAL:HG12	1:A:896:VAL:O	2.20	0.42
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.42
1:A:238:ASP:HA	1:A:286:PRO:HB3	2.02	0.42
1:A:468:LEU:HD23	1:A:468:LEU:HA	1.90	0.42
1:A:829:GLY:C	1:A:881:ILE:HD12	2.45	0.42
1:A:1071:GLN:NE2	1:A:1071:GLN:HA	2.35	0.42
1:A:185:MET:O	1:A:186:ALA:C	2.63	0.41
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.85	0.41
1:A:273:ARG:HB3	1:A:306:VAL:HG13	2.03	0.41
1:A:611:LEU:CD2	1:A:643:ILE:HG21	2.50	0.41
1:A:373:LEU:HD22	1:A:404:PHE:CZ	2.55	0.41
1:A:373:LEU:HD11	1:A:406:GLU:N	2.36	0.41
1:A:806:SER:O	1:A:807:LYS:C	2.64	0.41
1:A:904:ASP:C	1:A:905:GLU:O	2.63	0.41
1:A:180:LEU:C	1:A:183:PRO:HD2	2.46	0.41
1:A:939:THR:HB	1:A:945:GLY:HA2	2.01	0.41
1:A:306:VAL:HG22	1:A:307:LEU:N	2.35	0.41
1:A:743:GLN:HA	1:A:746:THR:HG22	2.01	0.41
1:A:757:TYR:HE1	1:A:807:LYS:HA	1.86	0.41
1:A:216:ALA:HB3	1:A:219:CYS:HB3	2.03	0.41
1:A:245:LEU:O	1:A:248:PHE:HB3	2.21	0.41
1:A:364:LYS:HD3	1:A:411:ASN:HD21	1.86	0.41
1:A:834:HIS:HB2	1:A:876:ILE:CD1	2.50	0.41
1:A:844:ILE:CD1	1:A:1034:MET:SD	3.08	0.41
1:A:861:ASP:C	1:A:861:ASP:OD1	2.63	0.41
1:A:1078:LYS:O	1:A:1079:GLY:C	2.63	0.41
1:A:561:THR:CG2	1:A:591:LYS:CE	2.94	0.41
1:A:551:LEU:HD23	1:A:551:LEU:HA	1.83	0.40
1:A:873:GLY:C	1:A:876:ILE:HG22	2.45	0.40
1:A:157:LEU:HD11	1:A:733:THR:HA	2.02	0.40
1:A:182:THR:HB	1:A:183:PRO:CD	2.48	0.40
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.87	0.40
1:A:379:LEU:CD1	1:A:380:THR:H	2.34	0.40
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.51	0.40
1:A:833:LYS:O	1:A:876:ILE:HA	2.20	0.40
1:A:583:LEU:CD2	1:A:589:TYR:CZ	3.04	0.40
1:A:164:ASP:OD1	1:A:164:ASP:C	2.65	0.40
1:A:290:PHE:O	1:A:294:ARG:HG3	2.21	0.40
1:A:675:SER:O	1:A:676:ALA:C	2.65	0.40
1:A:1078:LYS:HD3	1:A:1078:LYS:HA	1.98	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%)	703 (86%)	85 (10%)	31 (4%)	2 3

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	SER
1	A	211	LEU
1	A	217	ASN
1	A	778	GLN
1	A	905	GLU
1	A	966	GLY
1	A	967	HIS
1	A	994	VAL
1	A	1045	LYS
1	A	1059	LYS
1	A	1078	LYS
1	A	248	PHE
1	A	374	PRO
1	A	378	ASP
1	A	549	ASN
1	A	752	LEU
1	A	776	ASN
1	A	898	ASN
1	A	1040	PRO
1	A	1079	GLY
1	A	231	GLN
1	A	894	SER
1	A	1002	THR
1	A	1044	SER
1	A	146	GLU

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Mol	Chain	Res	Type
1	A	897	GLY
1	A	1086	TRP
1	A	798	ILE
1	A	918	GLU
1	A	213	LYS
1	A	373	LEU

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%)	654 (87%)	95 (13%)	4 7

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	157	LEU
1	A	164	ASP
1	A	168	VAL
1	A	194	LYS
1	A	209	GLU
1	A	224	ILE
1	A	228	THR
1	A	229	THR
1	A	230	SER
1	A	240	THR
1	A	250	THR
1	A	269	ASP
1	A	272	LEU
1	A	274	VAL
1	A	281	LEU
1	A	285	THR
1	A	287	ILE
1	A	298	LYS
1	A	321	GLU

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Mol	Chain	Res	Type
1	A	372	VAL
1	A	374	PRO
1	A	379	LEU
1	A	387	ILE
1	A	392	GLN
1	A	398	ARG
1	A	405	THR
1	A	406	GLU
1	A	410	TRP
1	A	411	ASN
1	A	418	ILE
1	A	421	LYS
1	A	497	PHE
1	A	498	ASN
1	A	502	LEU
1	A	516	ILE
1	A	546	GLU
1	A	550	GLN
1	A	561	THR
1	A	575	LEU
1	A	603	ILE
1	A	610	LEU
1	A	611	LEU
1	A	636	SER
1	A	721	LEU
1	A	729	LEU
1	A	747	LEU
1	A	749	ILE
1	A	753	SER
1	A	756	LYS
1	A	762	GLN
1	A	766	GLN
1	A	773	ASN
1	A	775	GLN
1	A	776	ASN
1	A	779	LEU
1	A	787	TYR
1	A	799	GLU
1	A	827	THR
1	A	838	LEU
1	A	841	ASP
1	A	845	LEU

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Mol	Chain	Res	Type
1	A	846	GLN
1	A	847	ILE
1	A	862	LEU
1	A	863	CYS
1	A	871	SER
1	A	872	THR
1	A	876	ILE
1	A	886	THR
1	A	887	THR
1	A	888	ILE
1	A	890	LYS
1	A	902	PHE
1	A	905	GLU
1	A	908	ASN
1	A	912	LYS
1	A	917	THR
1	A	919	GLU
1	A	922	GLN
1	A	949	ASN
1	A	959	ASN
1	A	968	ILE
1	A	982	ARG
1	A	985	PHE
1	A	1001	LYS
1	A	1002	THR
1	A	1007	GLN
1	A	1028	ILE
1	A	1039	MET
1	A	1045	LYS
1	A	1059	LYS
1	A	1066	LYS
1	A	1071	GLN
1	A	1086	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	225	HIS
1	A	299	ASN
1	A	304	HIS
1	A	376	ASN

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Mol	Chain	Res	Type
1	A	386	ASN
1	A	391	GLN
1	A	396	GLN
1	A	411	ASN
1	A	465	ASN
1	A	471	HIS
1	A	512	ASN
1	A	565	ASN
1	A	609	GLN
1	A	634	ASN
1	A	658	HIS
1	A	673	HIS
1	A	710	GLN
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	775	GLN
1	A	776	ASN
1	A	840	GLN
1	A	893	GLN
1	A	908	ASN
1	A	909	HIS
1	A	949	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1071	GLN
1	A	1083	GLN

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

1 ligand is 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	534	A	2088	-	41,41,41	2.43	7 (17%)	56,59,59	2.20	18 (32%)

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
2	534	A	2088	-	-	16/28/38/38	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2088	534	C5-C3	-9.81	1.38	1.49
2	A	2088	534	O2-S1	7.32	1.51	1.43
2	A	2088	534	O1-S1	6.53	1.50	1.43
2	A	2088	534	C21-C19	-3.76	1.40	1.49
2	A	2088	534	S1-N4	2.24	1.66	1.63
2	A	2088	534	C4-N3	2.16	1.43	1.37
2	A	2088	534	C6-N3	2.14	1.50	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2088	534	C15-S1-N4	-6.15	99.86	107.28
2	A	2088	534	O1-S1-N4	5.68	112.04	106.69
2	A	2088	534	O2-S1-O1	-5.65	110.77	119.59
2	A	2088	534	C6-N3-C9	4.70	122.13	111.57
2	A	2088	534	O2-S1-N4	4.42	110.85	106.69
2	A	2088	534	N6-C23-N5	-3.95	120.50	124.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2088	534	O2-S1-C15	3.60	112.58	108.10
2	A	2088	534	C1-N2-C4	3.49	122.96	115.05
2	A	2088	534	C2-N1-C3	2.79	122.30	116.84
2	A	2088	534	C2-C1-N2	-2.75	118.32	122.19
2	A	2088	534	C7-N4-S1	-2.67	112.10	117.06
2	A	2088	534	C24-N6-C23	2.65	120.96	116.29
2	A	2088	534	C21-C24-N6	-2.57	120.19	124.28
2	A	2088	534	N7-C23-N5	2.40	119.88	117.40
2	A	2088	534	C22-N5-C23	2.21	120.17	116.29
2	A	2088	534	C21-C22-N5	-2.18	120.82	124.28
2	A	2088	534	C6-C7-N4	-2.14	106.69	108.97
2	A	2088	534	N7-C23-N6	2.13	119.61	117.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2088	534	C3-C4-N3-C6
2	A	2088	534	C8-N4-S1-O2
2	A	2088	534	C7-N4-S1-O1
2	A	2088	534	C8-N4-S1-C15
2	A	2088	534	C8-N4-S1-O1
2	A	2088	534	N2-C4-N3-C6
2	A	2088	534	C7-N4-S1-O2
2	A	2088	534	C7-N4-S1-C15
2	A	2088	534	N1-C3-C5-C14
2	A	2088	534	N1-C3-C5-C10
2	A	2088	534	C4-C3-C5-C14
2	A	2088	534	C4-C3-C5-C10
2	A	2088	534	C20-C19-C21-C24
2	A	2088	534	C18-C19-C21-C22
2	A	2088	534	C20-C19-C21-C22
2	A	2088	534	C18-C19-C21-C24

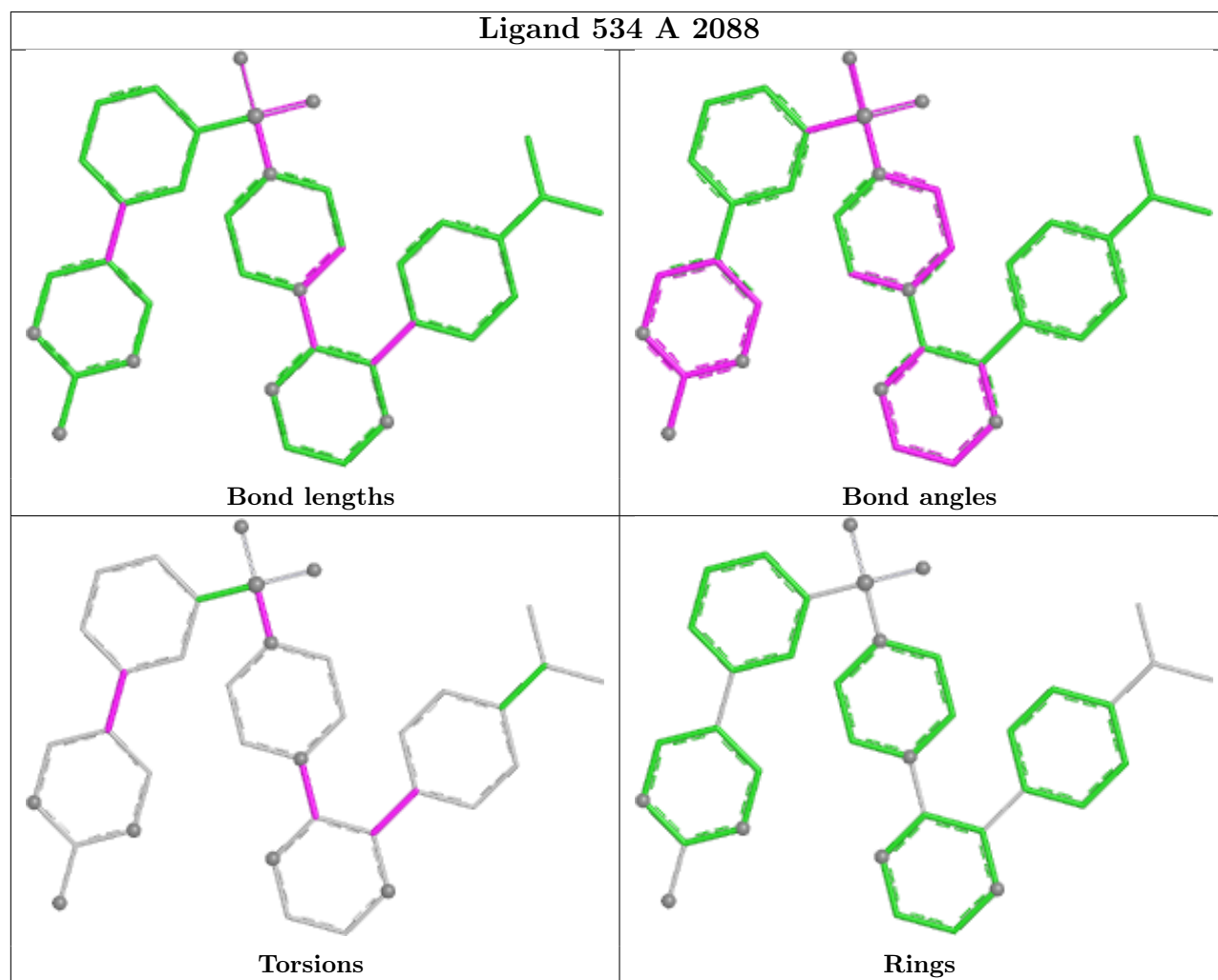
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2088	534	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 ⓘ

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	833/980 (85%)	0.05	10 (1%) 76 75	39, 70, 106, 120	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1044	SER	4.8
1	A	1042	LEU	3.6
1	A	901	ALA	3.4
1	A	900	GLY	3.2
1	A	1087	PHE	2.8
1	A	379	LEU	2.8
1	A	1086	TRP	2.7
1	A	378	ASP	2.7
1	A	896	VAL	2.5
1	A	248	PHE	2.5

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](#)

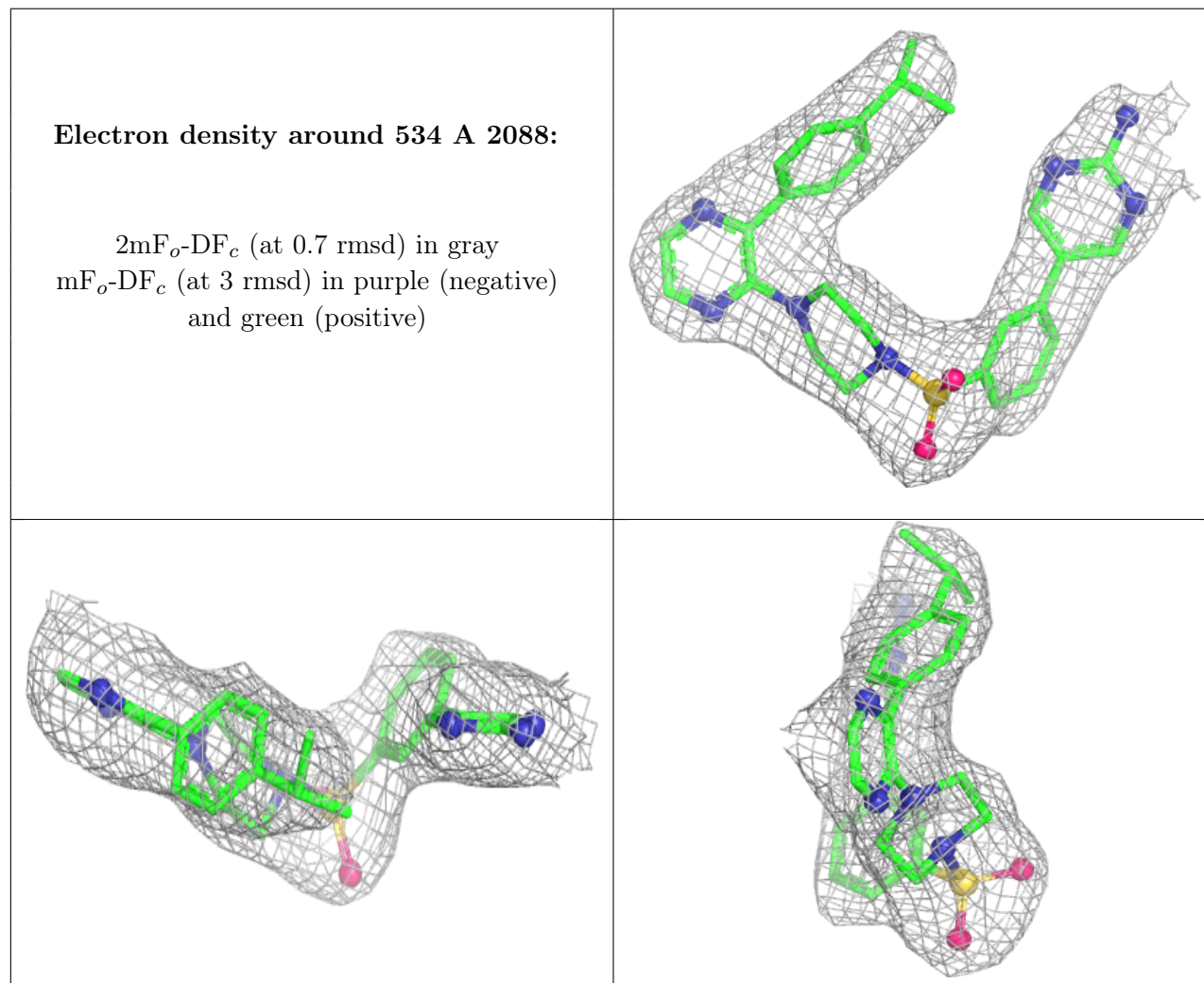
There are no oligosaccharides in this entry.

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	534	A	2088	37/37	0.96	0.08	61,66,70,71	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.