Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 01:00 pm BST

PDB ID	:	4ANV
Title	:	Complexes of PI3Kgamma with isoform selective inhibitors.
Authors	:	Foster, P.G.; Lougheed, J.C.
Deposited on	:	2012-03-22
Resolution	:	2.13 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

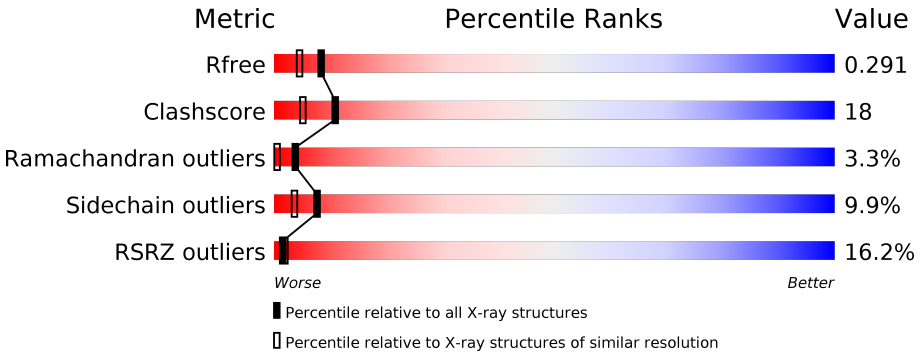
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.13 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	980	14% 56% 24% 6% • 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7111 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.

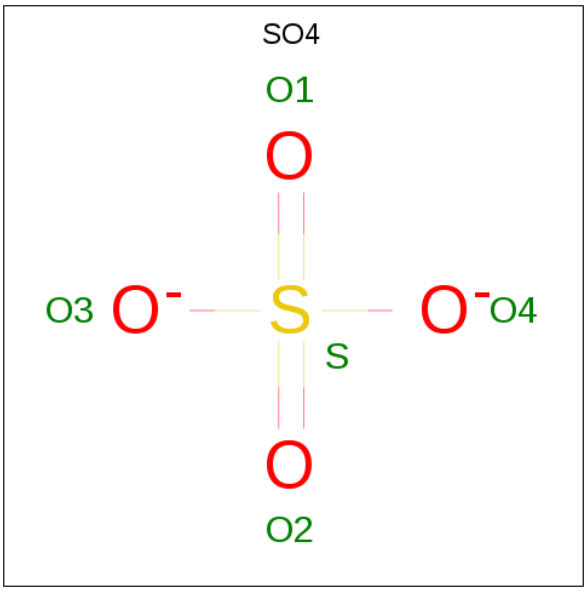
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	848	6893	4426	1179	1252	36	0	4	0

There are 21 discrepancies between the modelled and reference sequences:

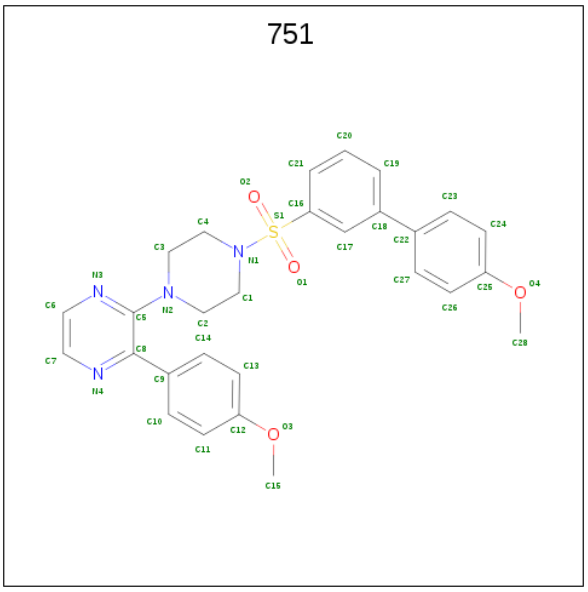
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	expression tag	UNP P48736
A	140	LEU	-	expression tag	UNP P48736
A	141	LEU	-	expression tag	UNP P48736
A	142	GLY	-	expression tag	UNP P48736
A	143	SER	-	expression tag	UNP P48736
A	1103	GLU	-	expression tag	UNP P48736
A	1104	PHE	-	expression 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 (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 2-{4-[(4'-METHOXYBIPHENYL-3-YL)SULFONYL]PIPERAZIN-1-YL}-3-(4-METHOXYPHENYL)PYRAZINE (three-letter code: 751) (formula: $C_{28}H_{28}N_4O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			37	28	4	4	1		

- Molecule 4 is water.

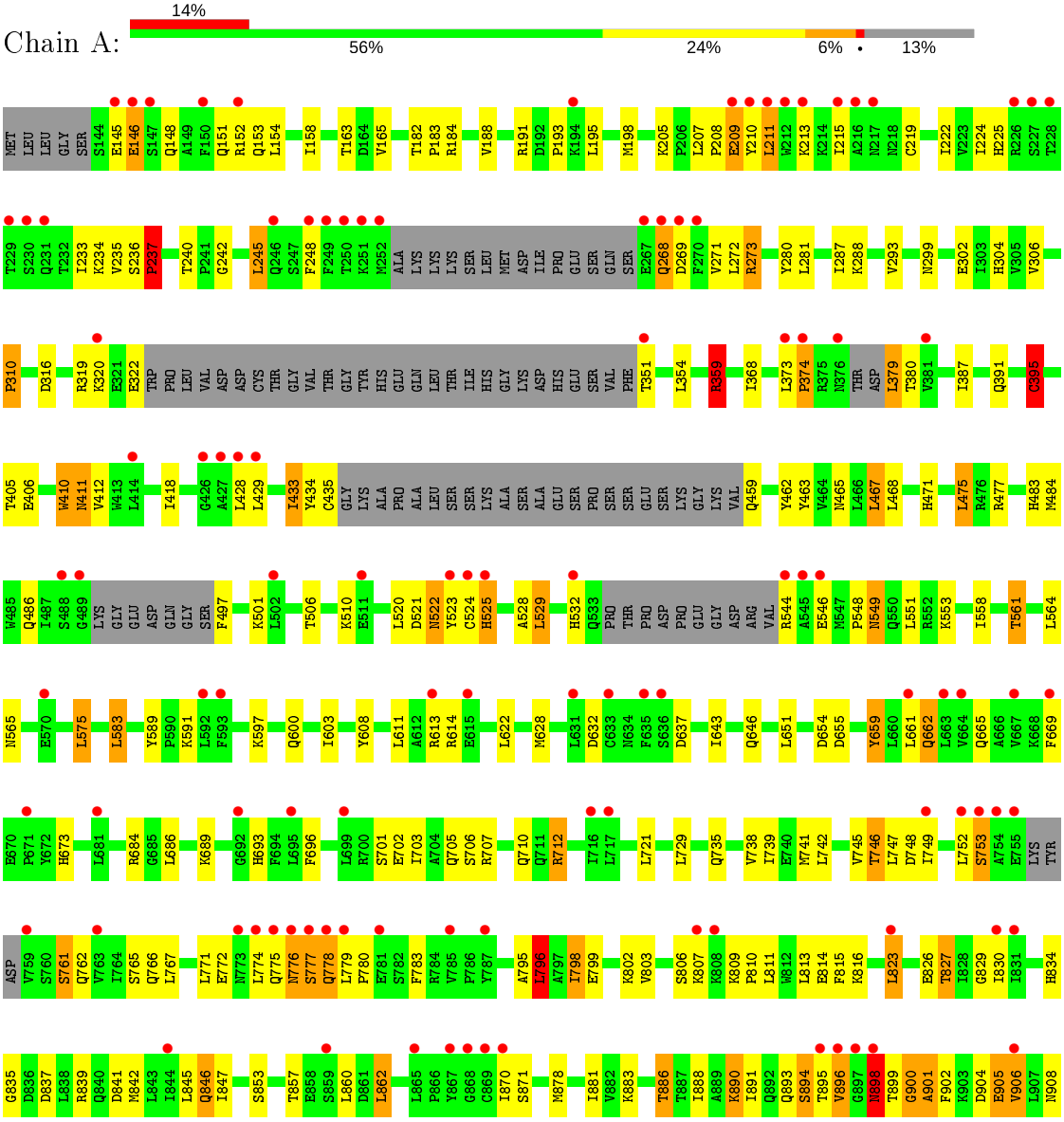
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	176	Total	O	0	0
			176	176		

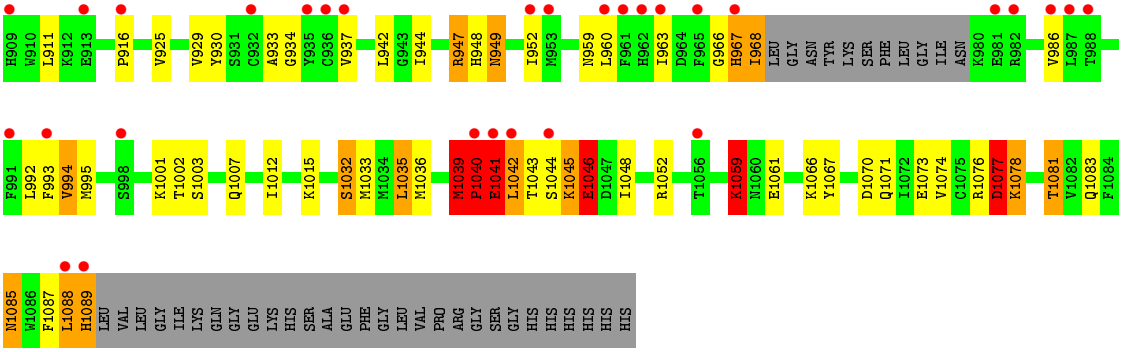
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

Chain A:




H909 W910 L911 K912 E913 P916 V925 V929 Y930 S931 C932 A933 G934 Y935 C936 V937 L942 G943 I944 R947 H948 N949 I952 M953 N959 L960 F961 H962 I963 D964 F965 G966 H967 I968 LEU GLY ASN TYR LYS SER PHE LEU GLY ILE ASN K980 E981 R982 V986 L987 T988
F991 L992 F993 V994 M995 S998 K1001 T1002 S1003 Q1007 I1012 K1015 S1032 M1033 M1034 L1035 M1036 M1039 P1040 E1041 L1042 T1043 S1044 K1045 E1046 D1047 I1048 R1052 T1056 K1059 N1060 E1061 K1066 Y1067 D1070 Q1071 I1072 E1073 V1074 C1075 R1076 D1077 K1078 T1081 V1082 Q1083 F1084
N1085 W1086 F1087 L1088 H1089 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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.34Å 68.73Å 106.77Å 90.00° 94.91° 90.00°	Depositor
Resolution (Å)	106.60 – 2.13 31.28 – 2.13	Depositor EDS
% Data completeness (in resolution range)	94.9 (106.60-2.13) 94.9 (31.28-2.13)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.297 0.236 , 0.291	Depositor DCC
R_{free} test set	2804 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7111	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 751, SO4

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	0.92	8/7045 (0.1%)	0.97	17/9529 (0.2%)

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	13

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	CYS	CB-SG	-11.77	1.62	1.82
1	A	1040	PRO	C-N	-7.39	1.17	1.34
1	A	659	TYR	CD1-CE1	-6.06	1.30	1.39
1	A	1046	GLU	C-N	-5.92	1.20	1.34
1	A	322	GLU	CB-CG	5.79	1.63	1.52
1	A	846	GLN	CD-NE2	5.71	1.47	1.32
1	A	900	GLY	C-N	-5.48	1.21	1.34
1	A	1089	HIS	C-O	5.10	1.33	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	237	PRO	O-C-N	-11.54	104.24	122.70
1	A	359	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	434	TYR	O-C-N	6.85	133.67	122.70
1	A	684	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	210	TYR	C-N-CA	6.46	137.84	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	TYR	N-CA-C	6.26	127.90	111.00
1	A	796	LEU	CA-CB-CG	6.13	129.40	115.30
1	A	467	LEU	CA-CB-CG	5.96	129.00	115.30
1	A	434	TYR	CA-C-N	-5.93	104.15	117.20
1	A	947	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	712	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	237	PRO	CA-C-N	5.59	129.51	117.20
1	A	947	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	1077	ASP	C-N-CA	5.41	135.22	121.70
1	A	210	TYR	CA-C-N	5.36	129.00	117.20
1	A	777	SER	C-N-CA	5.32	134.99	121.70
1	A	575	LEU	CA-CB-CG	5.09	127.00	115.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1039	MET	Peptide
1	A	1040	PRO	Mainchain,Peptide
1	A	1041	GLU	Peptide
1	A	1042	LEU	Peptide
1	A	1088	LEU	Peptide
1	A	209	GLU	Peptide
1	A	237	PRO	Mainchain
1	A	411	ASN	Peptide
1	A	528	ALA	Peptide
1	A	898	ASN	Peptide
1	A	901	ALA	Peptide
1	A	966	GLY	Peptide

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	6893	0	6903	249	0
2	A	5	0	0	1	0
3	A	37	0	28	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	176	0	0	25	0
All	All	7111	0	6931	253	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 18.

All (253) 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:814:GLU:OE1	1:A:827:THR:HG21	1.45	1.17
1:A:898:ASN:HB3	1:A:899:THR:HA	1.24	1.13
1:A:895:THR:HA	1:A:896:VAL:HB	1.23	1.12
1:A:693:HIS:O	4:A:2127:HOH:O	1.67	1.11
1:A:497:PHE:HB3	1:A:1043:THR:O	1.49	1.11
1:A:899:THR:N	1:A:900:GLY:HA3	1.63	1.09
1:A:1040:PRO:HA	1:A:1041:GLU:C	1.69	1.09
1:A:742:LEU:O	1:A:746:THR:HG23	1.55	1.07
1:A:1036:MET:HE1	4:A:2172:HOH:O	1.65	0.97
1:A:696:PHE:HB3	4:A:2127:HOH:O	1.69	0.92
1:A:947:ARG:NH2	1:A:963:ILE:O	2.04	0.91
1:A:967:HIS:C	1:A:968:ILE:N	2.24	0.91
1:A:673:HIS:HD2	1:A:712:ARG:HE	1.19	0.89
1:A:219:CYS:SG	1:A:234:LYS:HG3	2.12	0.89
1:A:895:THR:CA	1:A:896:VAL:HB	2.03	0.89
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.55	0.89
1:A:846:GLN:NE2	4:A:2113:HOH:O	1.87	0.86
1:A:899:THR:H	1:A:900:GLY:HA3	1.42	0.83
1:A:898:ASN:CB	1:A:899:THR:HA	2.08	0.83
1:A:777:SER:HB3	1:A:778:GLN:HB3	1.62	0.80
1:A:895:THR:HA	1:A:896:VAL:CB	2.10	0.79
1:A:613:ARG:NH1	4:A:2086:HOH:O	2.17	0.78
1:A:890:LYS:NZ	4:A:2151:HOH:O	2.05	0.78
1:A:240:THR:HG22	1:A:242:GLY:H	1.48	0.77
1:A:558:ILE:O	1:A:561:THR:HG22	1.85	0.76
1:A:428:LEU:HD22	1:A:465:ASN:HB3	1.65	0.75
1:A:746:THR:HG22	1:A:811:LEU:HD11	1.66	0.75
1:A:662:GLN:CG	4:A:2114:HOH:O	2.33	0.75
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.68	0.75
1:A:901:ALA:HB1	1:A:902:PHE:HD2	1.52	0.75
1:A:1040:PRO:HA	1:A:1041:GLU:O	1.87	0.75
1:A:240:THR:HG22	1:A:242:GLY:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:VAL:O	1:A:749:ILE:HD13	1.88	0.74
1:A:611:LEU:O	1:A:614:ARG:HG3	1.88	0.74
1:A:433:ILE:HD12	1:A:484:MET:CE	2.18	0.74
1:A:662:GLN:HG3	4:A:2114:HOH:O	1.86	0.74
1:A:433:ILE:HD12	1:A:484:MET:SD	2.28	0.73
1:A:901:ALA:HB1	1:A:902:PHE:CD2	2.24	0.73
1:A:233:ILE:HG22	1:A:235:VAL:HG23	1.69	0.73
1:A:316:ASP:O	4:A:2018:HOH:O	2.08	0.72
1:A:299:ASN:ND2	4:A:2038:HOH:O	2.22	0.71
1:A:435:CYS:HB3	1:A:459:GLN:HG3	1.72	0.71
1:A:148:GLN:O	1:A:152:ARG:HG3	1.91	0.71
1:A:775:GLN:HE22	1:A:798:ILE:HG13	1.56	0.71
1:A:777:SER:HB3	1:A:778:GLN:CB	2.21	0.70
1:A:435:CYS:HB3	1:A:459:GLN:CG	2.21	0.70
1:A:814:GLU:OE1	1:A:827:THR:CG2	2.32	0.70
1:A:748:ASP:O	1:A:752:LEU:HD13	1.93	0.69
1:A:860:LEU:HD21	1:A:1015:LYS:HD3	1.73	0.69
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.74	0.68
1:A:207:LEU:HD21	1:A:211:LEU:HB3	1.76	0.68
1:A:379:LEU:HD12	1:A:380:THR:H	1.59	0.67
1:A:1036:MET:CE	4:A:2172:HOH:O	2.30	0.67
1:A:215:ILE:HG23	1:A:219:CYS:O	1.95	0.67
1:A:742:LEU:O	1:A:746:THR:CG2	2.39	0.66
1:A:806:SER:O	1:A:809:LYS:HD3	1.97	0.64
1:A:1044:SER:O	1:A:1045:LYS:C	2.35	0.64
1:A:746:THR:HG22	1:A:811:LEU:CD1	2.27	0.63
3:A:1201:751:H31C	3:A:1201:751:C9	2.29	0.63
1:A:846:GLN:CD	4:A:2115:HOH:O	2.36	0.62
1:A:207:LEU:CD2	1:A:211:LEU:HB3	2.30	0.62
1:A:207:LEU:HD23	1:A:207:LEU:C	2.20	0.62
1:A:410:TRP:HB3	1:A:412:VAL:HG22	1.82	0.62
1:A:779:LEU:HD22	1:A:780:PRO:HD2	1.82	0.62
1:A:1045:LYS:O	1:A:1046:GLU:CB	2.47	0.62
1:A:316:ASP:OD1	1:A:689:LYS:NZ	2.26	0.61
1:A:208:PRO:HG2	1:A:211:LEU:HD22	1.80	0.61
1:A:387:ILE:HD12	1:A:468:LEU:HD11	1.82	0.61
1:A:775:GLN:HB3	1:A:776:ASN:HB2	1.83	0.61
1:A:1032:SER:O	1:A:1036:MET:HG3	1.99	0.61
1:A:827:THR:HG22	1:A:883:LYS:NZ	2.15	0.61
1:A:905:GLU:O	1:A:906:VAL:CB	2.47	0.61
1:A:949:ASN:HD22	1:A:949:ASN:C	2.04	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:CYS:SG	1:A:234:LYS:CG	2.88	0.60
1:A:1074:VAL:O	1:A:1078:LYS:HG3	2.01	0.60
1:A:184:ARG:O	1:A:188:VAL:HG23	2.02	0.59
1:A:891:ILE:HG22	1:A:906:VAL:HG12	1.84	0.59
1:A:901:ALA:CB	1:A:902:PHE:CD2	2.85	0.59
1:A:673:HIS:CD2	1:A:712:ARG:HE	2.10	0.59
1:A:561:THR:CG2	1:A:591:LYS:HE2	2.32	0.59
1:A:905:GLU:O	1:A:906:VAL:HB	2.02	0.59
1:A:905:GLU:O	1:A:906:VAL:HG23	2.03	0.59
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.31	0.59
1:A:701:SER:HB3	4:A:2129:HOH:O	2.02	0.58
1:A:561:THR:HG22	1:A:591:LYS:HE2	1.84	0.58
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.51	0.57
1:A:925:VAL:O	1:A:929:VAL:HG23	2.04	0.57
1:A:741:MET:HB3	1:A:774:LEU:HD21	1.86	0.57
3:A:1201:751:H31C	3:A:1201:751:C14	2.35	0.57
1:A:898:ASN:HB3	1:A:899:THR:CA	2.16	0.57
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.35	0.57
1:A:1077:ASP:N	1:A:1078:LYS:HB2	2.20	0.56
1:A:145:GLU:HA	1:A:146:GLU:O	2.05	0.56
1:A:948:HIS:CD2	1:A:1083:GLN:NE2	2.72	0.56
1:A:411:ASN:O	1:A:411:ASN:CG	2.43	0.56
1:A:899:THR:N	1:A:900:GLY:CA	2.48	0.56
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.70	0.56
1:A:893:GLN:C	1:A:895:THR:H	2.09	0.56
1:A:207:LEU:HD23	1:A:208:PRO:N	2.21	0.55
1:A:837:ASP:OD1	1:A:839:ARG:HD3	2.06	0.55
1:A:240:THR:CG2	1:A:242:GLY:H	2.19	0.55
1:A:288:LYS:NZ	2:A:1200:SO4:O4	2.36	0.55
1:A:583:LEU:HD22	1:A:589:TYR:OH	2.07	0.55
1:A:893:GLN:C	1:A:895:THR:N	2.60	0.55
1:A:944:ILE:O	4:A:2159:HOH:O	2.18	0.54
1:A:435:CYS:HB3	1:A:459:GLN:HG2	1.90	0.54
1:A:354:LEU:HB2	1:A:529:LEU:H	1.72	0.54
1:A:1044:SER:O	1:A:1046:GLU:N	2.41	0.54
1:A:986:VAL:HA	4:A:2166:HOH:O	2.08	0.54
1:A:888:ILE:HD11	1:A:960:LEU:HD11	1.89	0.53
1:A:304:HIS:CD2	1:A:823:LEU:HD23	2.44	0.53
1:A:497:PHE:CB	1:A:1043:THR:O	2.41	0.53
1:A:739:ILE:HG13	1:A:878:MET:HE1	1.91	0.53
1:A:222:ILE:HD12	1:A:235:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:GLU:H	1:A:799:GLU:CD	2.12	0.53
1:A:993:PHE:O	1:A:994:VAL:HB	2.09	0.53
1:A:1059:LYS:H	1:A:1059:LYS:HD2	1.73	0.53
1:A:1087:PHE:O	1:A:1089:HIS:HA	2.09	0.53
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.90	0.53
1:A:1067:TYR:O	1:A:1070:ASP:HB2	2.09	0.52
1:A:506:THR:OG1	4:A:2006:HOH:O	2.19	0.52
1:A:673:HIS:HD2	1:A:712:ARG:NE	1.99	0.52
1:A:379:LEU:CD1	1:A:380:THR:H	2.21	0.52
1:A:735:GLN:O	1:A:739:ILE:HD13	2.10	0.52
1:A:898:ASN:C	1:A:900:GLY:HA3	2.26	0.52
1:A:193:PRO:HD2	4:A:2019:HOH:O	2.09	0.52
1:A:772:GLU:O	1:A:776:ASN:HB3	2.10	0.52
1:A:796:LEU:HD13	1:A:815:PHE:CE2	2.45	0.51
1:A:236:SER:OG	1:A:237:PRO:HD2	2.10	0.51
1:A:993:PHE:O	1:A:994:VAL:CB	2.59	0.51
1:A:564:LEU:HD12	1:A:1052:ARG:HD2	1.93	0.51
1:A:1087:PHE:O	1:A:1089:HIS:CA	2.59	0.51
1:A:777:SER:CB	1:A:778:GLN:CB	2.88	0.51
1:A:233:ILE:HD11	1:A:248:PHE:HA	1.93	0.51
1:A:523:TYR:O	1:A:525:HIS:N	2.44	0.51
1:A:1035:LEU:HA	1:A:1039:MET:HB2	1.93	0.50
1:A:433:ILE:HD12	1:A:484:MET:HE1	1.92	0.50
1:A:520:LEU:O	1:A:522:ASN:N	2.44	0.50
1:A:853:SER:O	1:A:857:THR:HG23	2.12	0.50
1:A:891:ILE:HG13	4:A:2149:HOH:O	2.11	0.50
1:A:899:THR:O	1:A:899:THR:OG1	2.28	0.50
3:A:1201:751:C9	3:A:1201:751:C3	2.89	0.50
1:A:1081:THR:O	1:A:1085:ASN:N	2.38	0.50
1:A:151:GLN:HA	1:A:154:LEU:HD12	1.94	0.49
1:A:905:GLU:O	1:A:906:VAL:CG2	2.60	0.49
1:A:952:ILE:HD11	1:A:986:VAL:HG21	1.94	0.49
1:A:802[B]:LYS:NZ	4:A:2138:HOH:O	2.21	0.49
1:A:614:ARG:HA	4:A:2088:HOH:O	2.12	0.49
1:A:795:ALA:HB3	1:A:816:LYS:HD2	1.94	0.49
1:A:749:ILE:O	1:A:753:SER:OG	2.30	0.49
1:A:597:LYS:HD3	1:A:600:GLN:NE2	2.28	0.49
1:A:862:LEU:HD12	1:A:934:GLY:HA2	1.95	0.48
1:A:373:LEU:N	1:A:374:PRO:HD2	2.28	0.48
1:A:198:MET:SD	1:A:271:VAL:HG11	2.53	0.48
1:A:233:ILE:CG2	1:A:234:LYS:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:LEU:HD22	1:A:589:TYR:CZ	2.49	0.48
1:A:893:GLN:HA	1:A:895:THR:HG23	1.95	0.48
1:A:862:LEU:HD12	1:A:934:GLY:CA	2.44	0.47
1:A:967:HIS:CA	1:A:968:ILE:N	2.76	0.47
1:A:1073:GLU:OE1	1:A:1076:ARG:HD3	2.14	0.47
1:A:1077:ASP:CA	1:A:1078:LYS:HB2	2.44	0.47
1:A:549:ASN:HD21	1:A:553:LYS:NZ	2.13	0.47
1:A:165:VAL:O	1:A:165:VAL:HG12	2.15	0.47
1:A:163:THR:O	1:A:165:VAL:HG23	2.15	0.47
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.44	0.47
1:A:847:ILE:HG21	1:A:942:LEU:HD21	1.97	0.47
1:A:706:SER:O	1:A:710:GLN:HB3	2.15	0.47
1:A:1071:GLN:HA	1:A:1071:GLN:NE2	2.30	0.47
1:A:775:GLN:HE22	1:A:798:ILE:CG1	2.23	0.47
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.97	0.47
1:A:893:GLN:HA	1:A:895:THR:CG2	2.45	0.47
1:A:632:ASP:HB3	1:A:1033:MET:HE2	1.97	0.46
1:A:182:THR:HB	1:A:183:PRO:CD	2.45	0.46
1:A:895:THR:HG21	1:A:898:ASN:ND2	2.31	0.46
1:A:933:ALA:O	1:A:937:VAL:HG23	2.15	0.46
1:A:359:ARG:HH11	1:A:359:ARG:HG3	1.80	0.46
1:A:608:TYR:OH	1:A:637:ASP:OD1	2.29	0.46
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.96	0.46
1:A:483:HIS:CD2	1:A:510:LYS:HD3	2.51	0.46
1:A:930:TYR:CE1	1:A:1012:ILE:HD13	2.50	0.46
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.50	0.46
1:A:433:ILE:CD1	1:A:484:MET:SD	3.00	0.46
1:A:886:THR:CB	4:A:2149:HOH:O	2.64	0.45
1:A:287:ILE:HG13	1:A:293:VAL:HG21	1.96	0.45
1:A:827:THR:HG22	1:A:883:LYS:HZ3	1.81	0.45
1:A:622:LEU:HD21	1:A:651:LEU:HG	1.98	0.45
1:A:591:LYS:NZ	4:A:2089:HOH:O	2.46	0.45
1:A:662:GLN:HB3	1:A:662:GLN:HE21	1.56	0.45
1:A:405:THR:HG22	1:A:406:GLU:H	1.81	0.45
1:A:738:VAL:HG21	1:A:783:PHE:CD1	2.51	0.45
1:A:661:LEU:O	1:A:665:GLN:HG2	2.16	0.45
1:A:745:VAL:HG12	1:A:745:VAL:O	2.16	0.45
1:A:771:LEU:HB2	1:A:798:ILE:HD13	1.99	0.45
1:A:497:PHE:N	1:A:501[A]:LYS:HZ3	2.15	0.44
1:A:881:ILE:HG23	3:A:1201:751:H282	2.00	0.44
1:A:735:GLN:O	1:A:739:ILE:CD1	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:THR:CG2	1:A:565:ASN:HD22	2.30	0.44
1:A:862:LEU:CD2	1:A:862:LEU:N	2.81	0.44
1:A:207:LEU:C	1:A:207:LEU:CD2	2.85	0.44
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.14	0.44
1:A:463:TYR:CE2	1:A:501[B]:LYS:HA	2.53	0.43
1:A:236:SER:OG	1:A:237:PRO:CD	2.66	0.43
1:A:1044:SER:O	1:A:1046:GLU:CB	2.66	0.43
1:A:158:ILE:HG23	1:A:703:ILE:HD13	2.00	0.43
1:A:1036:MET:HE2	1:A:1036:MET:HB2	1.76	0.43
1:A:523:TYR:C	1:A:525:HIS:H	2.22	0.43
1:A:701:SER:CB	4:A:2129:HOH:O	2.64	0.43
1:A:827:THR:HG22	1:A:883:LYS:HZ1	1.82	0.43
1:A:608:TYR:N	1:A:608:TYR:CD1	2.86	0.43
1:A:702:GLU:O	1:A:706:SER:HB3	2.19	0.43
1:A:830:ILE:CG2	1:A:878:MET:HB2	2.49	0.43
1:A:701:SER:OG	1:A:871:SER:HB3	2.18	0.43
1:A:898:ASN:CB	1:A:899:THR:CA	2.88	0.43
1:A:829:GLY:HA3	1:A:881:ILE:HD12	2.02	0.42
1:A:949:ASN:ND2	1:A:949:ASN:C	2.72	0.42
1:A:302:GLU:HB2	1:A:304:HIS:HE1	1.84	0.42
1:A:669:PHE:CE1	1:A:1036:MET:HE3	2.54	0.42
1:A:901:ALA:HA	1:A:902:PHE:CD2	2.54	0.42
1:A:205:LYS:NZ	1:A:654:ASP:OD2	2.40	0.42
1:A:834:HIS:CG	1:A:835:GLY:N	2.88	0.42
1:A:904:ASP:OD1	1:A:904:ASP:N	2.53	0.42
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.49	0.42
1:A:891:ILE:HD11	4:A:2149:HOH:O	2.20	0.42
1:A:354:LEU:HD11	1:A:475:LEU:HD23	2.02	0.41
1:A:435:CYS:N	1:A:459:GLN:O	2.52	0.41
1:A:191:ARG:HD2	1:A:686:LEU:O	2.20	0.41
1:A:908:ASN:HD22	1:A:994:VAL:HG22	1.85	0.41
1:A:1071:GLN:HA	1:A:1071:GLN:HE21	1.84	0.41
1:A:739:ILE:HG13	1:A:878:MET:CE	2.49	0.41
1:A:810:PRO:HG2	3:A:1201:751:H42C	2.02	0.41
1:A:762:GLN:HA	1:A:765:SER:HB3	2.03	0.41
1:A:881:ILE:HG23	3:A:1201:751:C28	2.49	0.41
1:A:225:HIS:CE1	1:A:304:HIS:HD2	2.38	0.41
1:A:395:CYS:SG	1:A:418:ILE:HG22	2.60	0.41
1:A:462:TYR:CE2	1:A:486:GLN:HG3	2.56	0.41
1:A:471:HIS:H	1:A:471:HIS:CD2	2.39	0.41
1:A:1003:SER:O	1:A:1007:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:PHE:O	1:A:1089:HIS:N	2.53	0.41
1:A:992:LEU:O	1:A:995:MET:HB2	2.20	0.41
1:A:930:TYR:CD1	1:A:1012:ILE:HD13	2.56	0.41
1:A:224:ILE:HD12	1:A:248:PHE:CD1	2.55	0.41
1:A:273:ARG:HG3	1:A:280:TYR:CE1	2.55	0.41
1:A:405:THR:HG22	1:A:406:GLU:N	2.36	0.41
1:A:968:ILE:C	1:A:968:ILE:CD1	2.90	0.41
1:A:245:LEU:HA	1:A:245:LEU:HD13	1.94	0.40
1:A:1087:PHE:O	1:A:1088:LEU:C	2.59	0.40
1:A:1032:SER:HB2	1:A:1048:ILE:HG23	2.02	0.40
3:A:1201:751:H283	3:A:1201:751:H24	1.82	0.40
1:A:655:ASP:O	1:A:659:TYR:HD2	2.05	0.40
1:A:862:LEU:HD12	1:A:934:GLY:N	2.37	0.40
1:A:883:LYS:HD3	4:A:2142:HOH:O	2.21	0.40
1:A:661:LEU:HD21	1:A:842:MET:HB3	2.03	0.40
1:A:145:GLU:CA	1:A:146:GLU:O	2.69	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	833/980 (85%)	751 (90%)	55 (7%)	27 (3%)	4 0

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	374	PRO
1	A	521	ASP
1	A	761	SER
1	A	776	ASN
1	A	778	GLN

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	898	ASN
1	A	906	VAL
1	A	994	VAL
1	A	1042	LEU
1	A	1059	LYS
1	A	1078	LYS
1	A	146	GLU
1	A	213	LYS
1	A	268	GLN
1	A	1045	LYS
1	A	1046	GLU
1	A	1040	PRO
1	A	209	GLU
1	A	532	HIS
1	A	916	PRO
1	A	211	LEU
1	A	894	SER
1	A	1077	ASP
1	A	524	CYS
1	A	310	PRO
1	A	529	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	761/874 (87%)	686 (90%)	75 (10%)	8 3

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	195	LEU
1	A	245	LEU
1	A	268	GLN

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Mol	Chain	Res	Type
1	A	269	ASP
1	A	272	LEU
1	A	273	ARG
1	A	281	LEU
1	A	306	VAL
1	A	310	PRO
1	A	319	ARG
1	A	320	LYS
1	A	351	THR
1	A	359	ARG
1	A	379	LEU
1	A	391	GLN
1	A	395	CYS
1	A	410	TRP
1	A	433	ILE
1	A	467	LEU
1	A	475	LEU
1	A	477	ARG
1	A	522	ASN
1	A	525	HIS
1	A	544	ARG
1	A	546	GLU
1	A	549	ASN
1	A	561	THR
1	A	575	LEU
1	A	583	LEU
1	A	603	ILE
1	A	628	MET
1	A	643	ILE
1	A	646	GLN
1	A	662	GLN
1	A	705	GLN
1	A	707	ARG
1	A	721	LEU
1	A	729	LEU
1	A	746	THR
1	A	747	LEU
1	A	753	SER
1	A	761	SER
1	A	766	GLN
1	A	796	LEU
1	A	798	ILE

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Mol	Chain	Res	Type
1	A	807	LYS
1	A	823	LEU
1	A	826	GLU
1	A	827	THR
1	A	841	ASP
1	A	845	LEU
1	A	862	LEU
1	A	870	ILE
1	A	886	THR
1	A	890	LYS
1	A	894	SER
1	A	905	GLU
1	A	911	LEU
1	A	949	ASN
1	A	959	ASN
1	A	967	HIS
1	A	968	ILE
1	A	1001	LYS
1	A	1002	THR
1	A	1032	SER
1	A	1035	LEU
1	A	1039	MET
1	A	1040	PRO
1	A	1041	GLU
1	A	1059	LYS
1	A	1061	GLU
1	A	1066	LYS
1	A	1081	THR
1	A	1085	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	218	ASN
1	A	299	ASN
1	A	304	HIS
1	A	388	GLN
1	A	389	HIS
1	A	532	HIS
1	A	549	ASN
1	A	565	ASN

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Mol	Chain	Res	Type
1	A	600	GLN
1	A	619	GLN
1	A	646	GLN
1	A	662	GLN
1	A	673	HIS
1	A	705	GLN
1	A	766	GLN
1	A	775	GLN
1	A	776	ASN
1	A	840	GLN
1	A	893	GLN
1	A	898	ASN
1	A	908	ASN
1	A	922	GLN
1	A	949	ASN
1	A	951	ASN
1	A	1071	GLN
1	A	1083	GLN
1	A	1085	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	751	A	1201	-	41,41,41	2.27	7 (17%)	55,58,58	2.31	15 (27%)
2	SO4	A	1200	-	4,4,4	0.18	0	6,6,6	0.96	0

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	751	A	1201	-	-	14/28/38/38	0/5/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	751	C16-S1	9.15	1.89	1.76
3	A	1201	751	C9-C8	-6.15	1.42	1.49
3	A	1201	751	O2-S1	5.74	1.49	1.43
3	A	1201	751	C18-C22	-3.31	1.40	1.49
3	A	1201	751	S1-N1	2.96	1.67	1.63
3	A	1201	751	O1-S1	2.53	1.46	1.43
3	A	1201	751	C4-N1	-2.22	1.45	1.47

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1201	751	C16-S1-N1	-7.31	98.59	107.30
3	A	1201	751	O1-S1-N1	6.66	112.76	106.69
3	A	1201	751	C2-N2-C3	6.30	125.43	111.52
3	A	1201	751	C1-N1-S1	-4.80	108.33	117.05
3	A	1201	751	C21-C16-S1	4.27	124.25	119.76
3	A	1201	751	C1-N1-C4	3.92	116.50	112.17
3	A	1201	751	C21-C16-C17	-3.09	116.83	120.62
3	A	1201	751	C20-C21-C16	2.99	122.05	118.95
3	A	1201	751	O2-S1-C16	2.94	111.76	108.05
3	A	1201	751	C28-O4-C25	-2.89	111.23	117.51
3	A	1201	751	C6-N3-C5	2.82	121.67	115.14
3	A	1201	751	C7-N4-C8	2.80	122.30	116.81
3	A	1201	751	C15-O3-C12	2.54	123.02	117.51
3	A	1201	751	C4-C3-N2	2.54	115.62	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1201	751	C18-C17-C16	2.50	121.93	119.96

There are no chirality outliers.

All (14) torsion outliers are listed below:

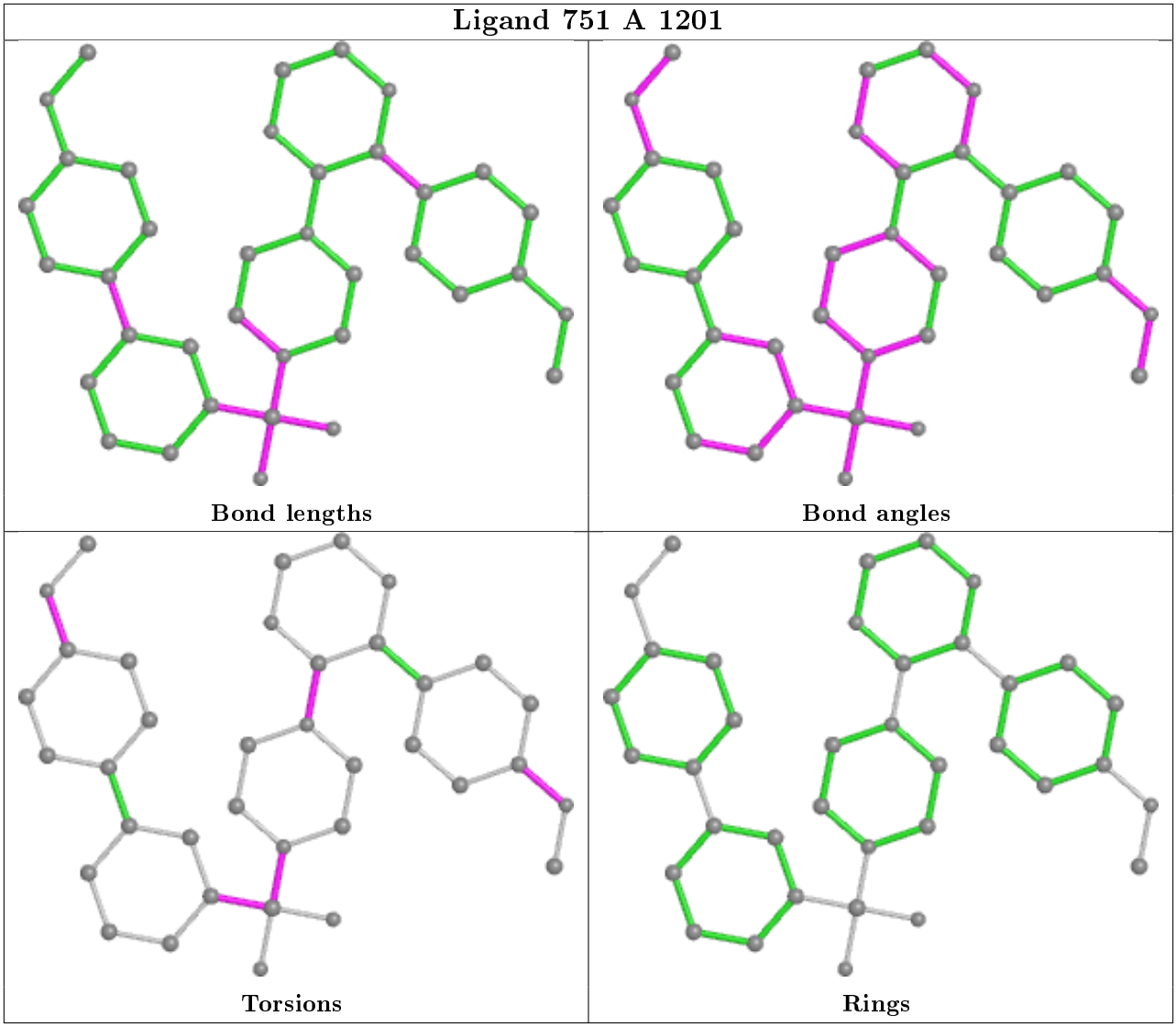
Mol	Chain	Res	Type	Atoms
3	A	1201	751	C8-C5-N2-C2
3	A	1201	751	C4-N1-S1-O2
3	A	1201	751	C4-N1-S1-C16
3	A	1201	751	N3-C5-N2-C2
3	A	1201	751	C4-N1-S1-O1
3	A	1201	751	C1-N1-S1-O2
3	A	1201	751	C26-C25-O4-C28
3	A	1201	751	C1-N1-S1-O1
3	A	1201	751	C24-C25-O4-C28
3	A	1201	751	C1-N1-S1-C16
3	A	1201	751	C11-C12-O3-C15
3	A	1201	751	C13-C12-O3-C15
3	A	1201	751	C17-C16-S1-O1
3	A	1201	751	C21-C16-S1-O1

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	751	7	0
2	A	1200	SO4	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

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	2.24
1	A	1046:GLU	C	1047:ASP	N	1.20
1	A	1040:PRO	C	1041:GLU	N	1.17

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	848/980 (86%)	0.93	137 (16%) 1 2	27, 50, 80, 91	0

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	376	ASN	7.2
1	A	896	VAL	7.0
1	A	489	GLY	6.8
1	A	147	SER	6.1
1	A	228	THR	6.0
1	A	268	GLN	5.5
1	A	763	VAL	5.1
1	A	544	ARG	5.0
1	A	215	ILE	4.9
1	A	229	THR	4.8
1	A	859	SER	4.7
1	A	753	SER	4.7
1	A	779	LEU	4.6
1	A	1044	SER	4.5
1	A	952	ILE	4.4
1	A	488	SER	4.3
1	A	776	ASN	4.3
1	A	823	LEU	4.2
1	A	249	PHE	4.1
1	A	754	ALA	4.1
1	A	774	LEU	4.1
1	A	216	ALA	4.0
1	A	227	SER	4.0
1	A	250	THR	3.9
1	A	1088	LEU	3.9
1	A	991	PHE	3.8
1	A	960	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	374	PRO	3.7
1	A	759	VAL	3.7
1	A	636	SER	3.7
1	A	986	VAL	3.7
1	A	270	PHE	3.6
1	A	870	ILE	3.6
1	A	213	LYS	3.6
1	A	524	CYS	3.5
1	A	897	GLY	3.5
1	A	226	ARG	3.5
1	A	998	SER	3.5
1	A	993	PHE	3.4
1	A	775	GLN	3.4
1	A	1041	GLU	3.4
1	A	211	LEU	3.4
1	A	869	CYS	3.3
1	A	936	CYS	3.3
1	A	755	GLU	3.3
1	A	1042	LEU	3.2
1	A	778	GLN	3.2
1	A	570	GLU	3.2
1	A	150	PHE	3.1
1	A	252	MET	3.1
1	A	664	VAL	3.1
1	A	427	ALA	3.0
1	A	895	THR	3.0
1	A	830	ILE	3.0
1	A	777	SER	3.0
1	A	511	GLU	3.0
1	A	898	ASN	3.0
1	A	987	LEU	3.0
1	A	867	TYR	3.0
1	A	961	PHE	2.9
1	A	807	LYS	2.9
1	A	525	HIS	2.9
1	A	967	HIS	2.9
1	A	935	TYR	2.9
1	A	251	LYS	2.9
1	A	146	GLU	2.9
1	A	592	LEU	2.9
1	A	932	CYS	2.9
1	A	145	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	613	ARG	2.8
1	A	865	LEU	2.8
1	A	546	GLU	2.8
1	A	981	GLU	2.8
1	A	667	VAL	2.8
1	A	248	PHE	2.8
1	A	267	GLU	2.8
1	A	532	HIS	2.8
1	A	962[A]	HIS	2.8
1	A	152	ARG	2.8
1	A	749	ILE	2.7
1	A	210	TYR	2.7
1	A	963	ILE	2.7
1	A	1089	HIS	2.7
1	A	695	LEU	2.7
1	A	523	TYR	2.7
1	A	1056	THR	2.6
1	A	320	LYS	2.6
1	A	906	VAL	2.6
1	A	787	TYR	2.6
1	A	671	PRO	2.6
1	A	717	LEU	2.6
1	A	428	LEU	2.5
1	A	429	LEU	2.5
1	A	868	GLY	2.5
1	A	982	ARG	2.5
1	A	217	ASN	2.5
1	A	831	ILE	2.5
1	A	545	ALA	2.5
1	A	752	LEU	2.5
1	A	633	CYS	2.5
1	A	231	GLN	2.4
1	A	212	TRP	2.4
1	A	230	SER	2.4
1	A	808	LYS	2.4
1	A	953	MET	2.4
1	A	502	LEU	2.4
1	A	965	PHE	2.3
1	A	615	GLU	2.3
1	A	909	HIS	2.3
1	A	1040	PRO	2.3
1	A	351	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	692	GLY	2.2
1	A	373	LEU	2.2
1	A	699	LEU	2.2
1	A	781	GLU	2.2
1	A	414	LEU	2.2
1	A	631	LEU	2.2
1	A	661	LEU	2.2
1	A	913	GLU	2.2
1	A	844	ILE	2.2
1	A	593	PHE	2.2
1	A	716	ILE	2.2
1	A	246	GLN	2.2
1	A	635	PHE	2.2
1	A	663	LEU	2.1
1	A	937	VAL	2.1
1	A	426	GLY	2.1
1	A	916	PRO	2.1
1	A	681	LEU	2.1
1	A	785	VAL	2.1
1	A	194	LYS	2.1
1	A	209	GLU	2.1
1	A	773	ASN	2.1
1	A	381	VAL	2.1
1	A	988	THR	2.1
1	A	669	PHE	2.0
1	A	269	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

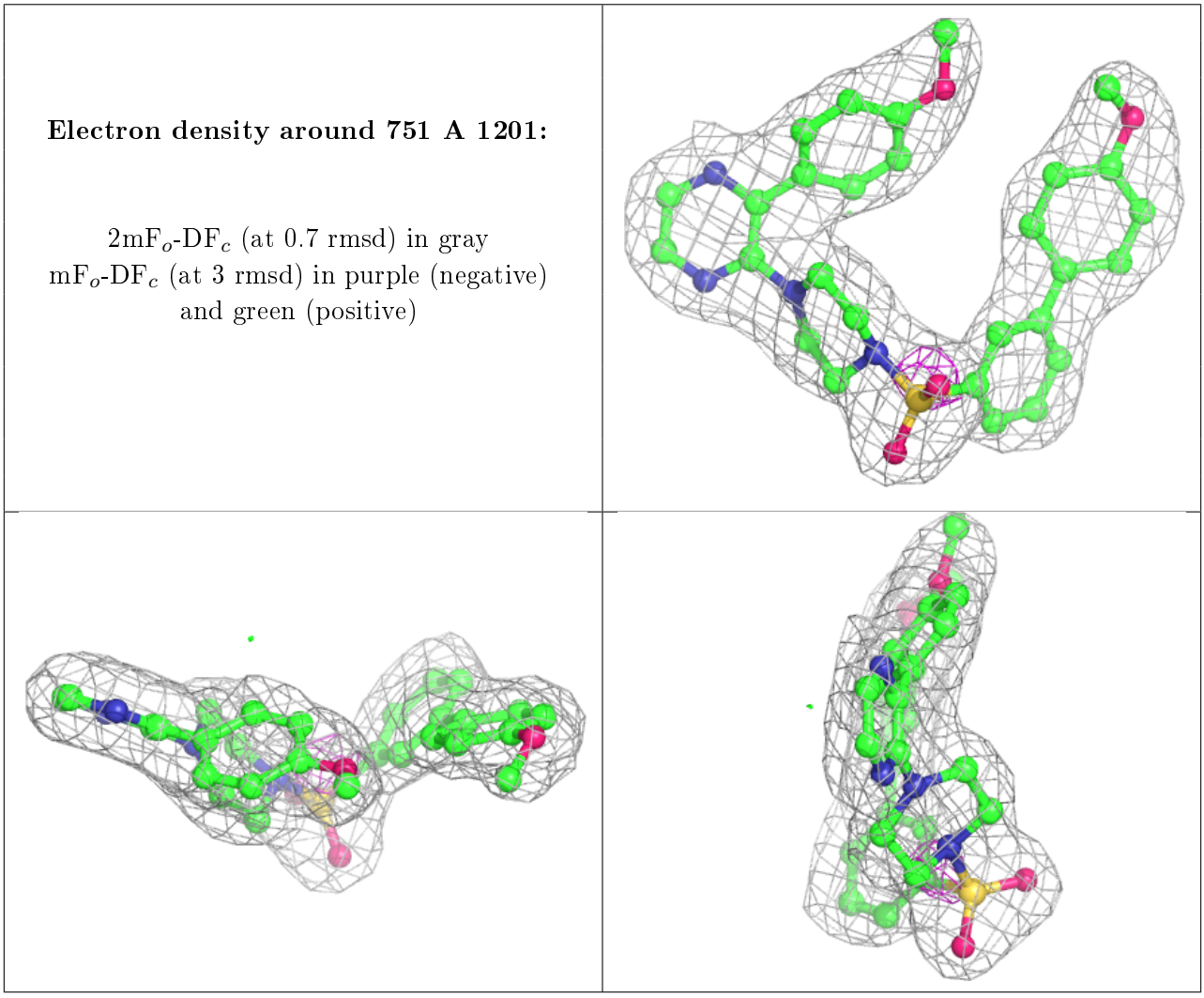
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	751	A	1201	37/37	0.96	0.11	35,42,47,48	0
2	SO4	A	1200	5/5	0.98	0.07	56,56,57,60	0

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

Electron density around 751 A 1201:

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



6.5 Other polymers

There are no such residues in this entry.