



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:04 PM GMT

PDB ID : 4ANX  
Title : Complexes of PI3Kgamma with isoform selective inhibitors.  
Authors : Foster, P.G.; Loughheed, J.C.  
Deposited on : 2012-03-22  
Resolution : 2.73 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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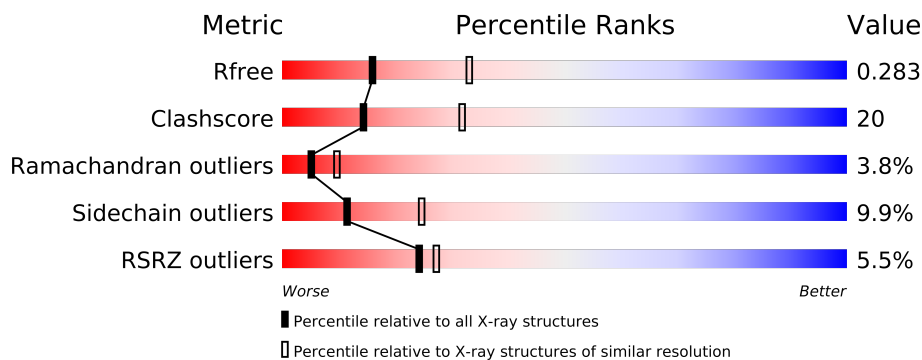
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2164 (2.78-2.70)
Clashscore	79885	2639 (2.78-2.70)
Ramachandran outliers	78287	2594 (2.78-2.70)
Sidechain outliers	78261	2595 (2.78-2.70)
RSRZ outliers	66119	2166 (2.78-2.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 hydrogen and 0 are deuterium.

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.

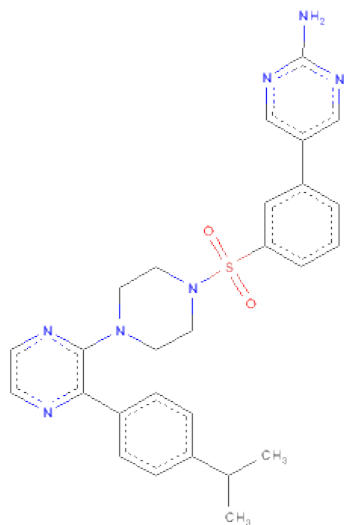
- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE3-KINASE CATALYTIC SUBUNIT GAMMA ISOFORM.

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 (three-letter code: 534) (formula: C<sub>27</sub>H<sub>29</sub>N<sub>7</sub>O<sub>2</sub>S).



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

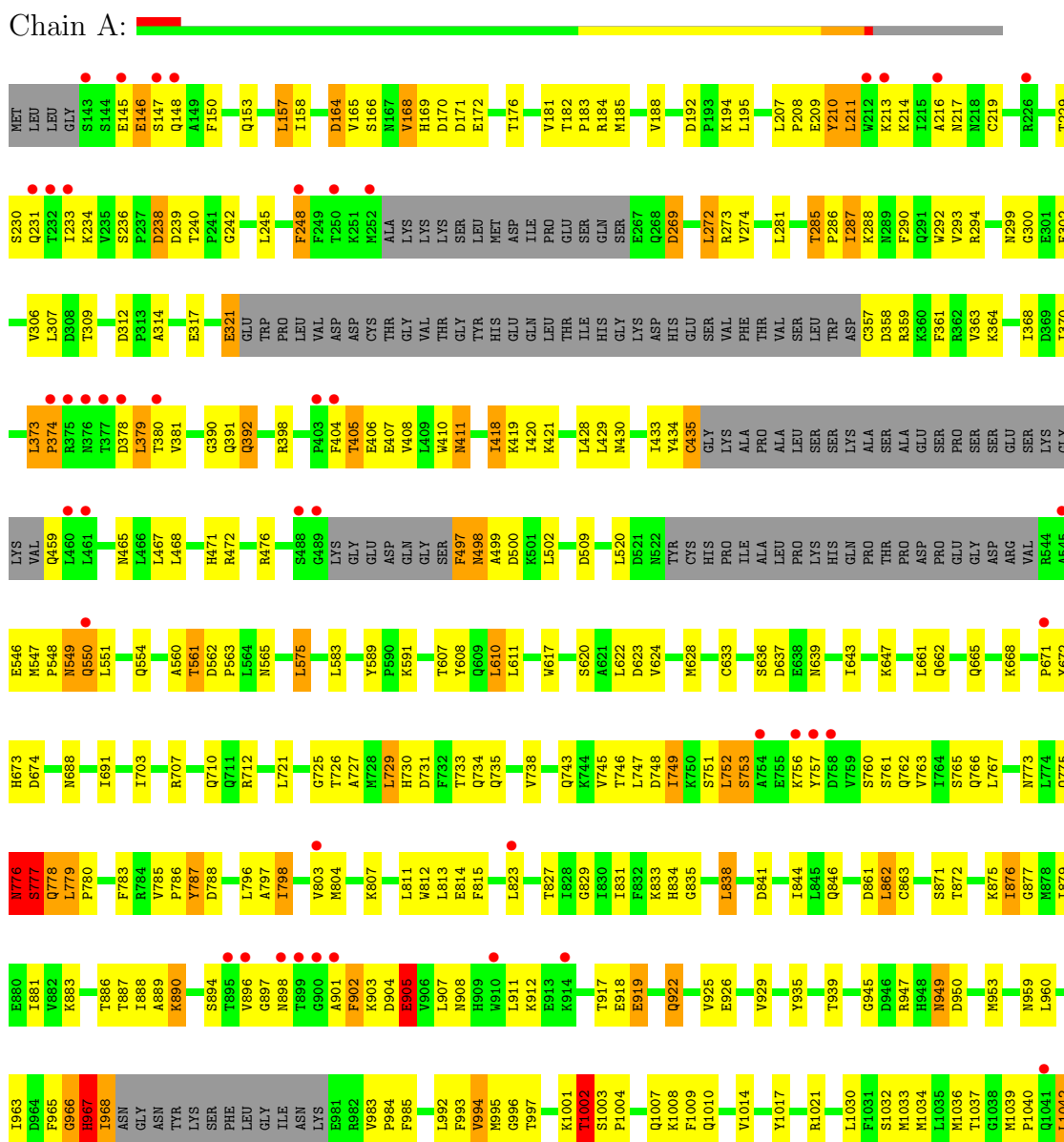
- Molecule 3 is water.

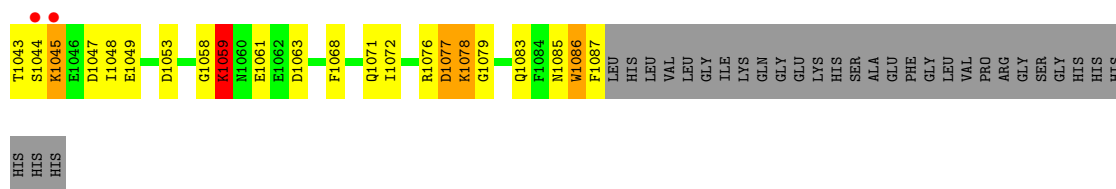
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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-BISPHOSPHATE3-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, $\alpha$ , $\beta$ , $\gamma$	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) 99.5 (32.60-2.73)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.51 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.225 , 0.282 0.226 , 0.283	Depositor DCC
$R_{free}$ test set	1375 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27394 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6828	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.67	2/6901 (0.0%)	0.79	5/9334 (0.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	967	HIS	C-N	-5.82	1.20	1.34
1	A	435	CYS	CB-SG	-5.02	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	LEU	CA-CB-CG	6.71	130.72	115.30
1	A	210	TYR	N-CA-C	6.59	128.80	111.00
1	A	967	HIS	O-C-N	-6.08	112.97	122.70
1	A	777	SER	CB-CA-C	5.51	120.58	110.10
1	A	1077	ASP	C-N-CA	5.43	135.28	121.70

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6757	0	6789	266	0
2	A	37	0	29	4	0
3	A	34	0	0	4	0
All	All	6828	0	6818	266	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (266) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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
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:662:GLN:OE1	1:A:1030:LEU:HD22	1.93	0.68
1:A:185:MET:HE1	1:A:321:GLU:HG3	1.75	0.68
1:A:561:THR:HG22	1:A:591:LYS:CE	2.23	0.68
1:A:405:THR:HG23	1:A:408:VAL:HG22	1.76	0.68
1:A:947:ARG:NH2	1:A:963:ILE:O	2.26	0.68
1:A:561:THR:HG22	1:A:591:LYS:HZ1	1.58	0.67
1:A:731:ASP:O	1:A:735:GLN:HG3	1.95	0.67
1:A:498:ASN:C	1:A:498:ASN:OD1	2.32	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:775:GLN:NE2	1:A:798:ILE:HD11	2.04	0.67
1:A:240:THR:HG22	1:A:242:GLY:N	2.10	0.67
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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:775:GLN:H	1:A:776:ASN:HB2	1.64	0.63
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.80	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:812:TRP:C	1:A:813:LEU:HD23	2.20	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:287:ILE:H	1:A:287:ILE:HD12	1.67	0.60
1:A:950:ASP:HB2	2:A:2088:534:C2	2.32	0.59
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.84	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: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:827:THR:HG22	1:A:883:LYS:HZ1	1.66	0.57
1:A:608:TYR:OH	1:A:637:ASP:OD1	2.23	0.57
1:A:829:GLY:CA	1:A:881:ILE:HD12	2.35	0.57
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.06	0.56
1:A:150:PHE:O	1:A:153:GLN:N	2.39	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:661:LEU:O	1:A:665:GLN:HG2	2.07	0.55
1:A:207:LEU:HD23	1:A:207:LEU:C	2.27	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: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: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:967:HIS:N	1:A:968:ILE:CA	2.55	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:N	1:A:1048:ILE:HD12	2.24	0.52
1:A:949:ASN:C	1:A:949:ASN:HD22	2.12	0.52
1:A:158:ILE:HG23	1:A:703:ILE:HD13	1.91	0.52
1:A:548:PRO:O	1:A:549:ASN:C	2.48	0.52
1:A:547:MET:HE2	1:A:551:LEU:HB3	1.92	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:688:ASN:HB3	1:A:691:ILE:HD12	1.93	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:726:THR:O	1:A:727:ALA:C	2.47	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:827:THR:CG2	1:A:883:LYS:HZ1	2.22	0.51
1:A:777:SER:OG	1:A:778:GLN:HB2	2.11	0.51
1:A:391:GLN:NE2	1:A:633:CYS:SG	2.84	0.51
1:A:775:GLN:CB	1:A:776:ASN:HB2	2.41	0.51
1:A:285:THR:HB	1:A:290:PHE:CE1	2.46	0.51
1:A:561:THR:HG22	1:A:591:LYS:HZ3	1.69	0.51
1:A:919:GLU:HA	1:A:922:GLN:HB2	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1009:PHE:HE2	1:A:1072:ILE:HD13	1.76	0.50
1:A:302:GLU:HG3	3:A:2008:HOH:O	2.11	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: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:887:THR:HG21	1:A:889:ALA:HB3	1.95	0.49
1:A:390:GLY:C	1:A:392:GLN:H	2.16	0.49
1:A:269:ASP:O	1:A:309:THR:HG22	2.11	0.49
1:A:829:GLY:HA3	1:A:881:ILE:HD12	1.95	0.49
1:A:993:PHE:O	1:A:994:VAL:CB	2.61	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:HG23	2.13	0.48
1:A:993:PHE:O	1:A:994:VAL:HB	2.13	0.48
1:A:760:SER:OG	1:A:763:VAL:HG23	2.13	0.48
1:A:245:LEU:HD11	1:A:272:LEU:HD13	1.94	0.48
1:A:904:ASP:O	1:A:905:GLU:O	2.30	0.48
1:A:317:GLU:O	1:A:726:THR:HG23	2.14	0.48
1:A:1077:ASP:CA	1:A:1078:LYS:HB2	2.43	0.48
1:A:370:ILE:O	1:A:370:ILE:HG23	2.12	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:498:ASN:OD1	1:A:499:ALA:N	2.47	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:373:LEU:HD22	1:A:404:PHE:CE2	2.49	0.48
1:A:997:THR:HG23	1:A:1002:THR:H	1.78	0.47
1:A:192:ASP:CG	1:A:195:LEU:HD23	2.34	0.47
1:A:639:ASN:O	1:A:643:ILE:HG23	2.13	0.47
1:A:164:ASP:OD1	1:A:166:SER:OG	2.27	0.47
1:A:743:GLN:O	1:A:746:THR:HG22	2.14	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:861:ASP:C	1:A:862:LEU:HD22	2.36	0.47
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.45	0.47
1:A:607:THR:O	1:A:610:LEU:HD23	2.14	0.47
1:A:734:GLN:HE21	1:A:780:PRO:HB2	1.79	0.46
1:A:497:PHE:HB2	1:A:1042:LEU:HD21	1.96	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:813:LEU:HD23	1:A:813:LEU:N	2.30	0.46
1:A:405:THR:HG23	1:A:407:GLU:O	2.15	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:361:PHE:HB2	1:A:420:ILE:HD12	1.98	0.45
1:A:796:LEU:HD13	1:A:815:PHE:CE2	2.50	0.45
1:A:373:LEU:O	1:A:374:PRO:C	2.55	0.45
1:A:192:ASP:OD1	1:A:192:ASP:C	2.55	0.45
1:A:738:VAL:HG21	1:A:783:PHE:CG	2.50	0.45
1:A:703:ILE:HG22	1:A:703:ILE:O	2.17	0.45
1:A:418:ILE:HG13	1:A:419:LYS:N	2.32	0.45
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:804:MET:HE3	2:A:2088:534:H261	1.99	0.44
1:A:145:GLU:CA	1:A:146:GLU:O	2.58	0.44
1:A:738:VAL:HG21	1:A:783:PHE:HB3	2.00	0.43
1:A:471:HIS:H	1:A:471:HIS:CD2	2.35	0.43
1:A:779:LEU:HD13	1:A:780:PRO:N	2.33	0.43
1:A:214:LYS:HE3	1:A:300:GLY:HA2	2.00	0.43
1:A:561:THR:HG23	1:A:562:ASP:O	2.18	0.43
1:A:207:LEU:CD2	1:A:208:PRO:O	2.66	0.43
1:A:192:ASP:OD2	1:A:195:LEU:HD23	2.18	0.43
1:A:411:ASN:O	1:A:411:ASN:CG	2.57	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:823:LEU:O	1:A:823:LEU:HG	2.18	0.43
1:A:550:GLN:O	1:A:554:GLN:HG3	2.18	0.43
1:A:207:LEU:HD23	1:A:208:PRO:O	2.19	0.43
1:A:797:ALA:O	1:A:798:ILE:C	2.57	0.43
1:A:357:CYS:SG	1:A:359:ARG:HG2	2.60	0.42
1:A:611:LEU:HD22	1:A:643:ILE:HG21	2.01	0.42
1:A:1085:ASN:C	1:A:1087:PHE:H	2.23	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:HD22	1:A:862:LEU:N	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:1043:THR:OG1	1:A:1047:ASP:N	2.40	0.42
1:A:785:VAL:HG12	1:A:786:PRO:O	2.19	0.42
1:A:624:VAL:CG1	1:A:628:MET:HE1	2.49	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:777:SER:CB	1:A:778:GLN:CB	2.78	0.42
1:A:896:VAL:O	1:A:896:VAL:HG12	2.20	0.42
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.42
1:A:1071:GLN:HA	1:A:1071:GLN:NE2	2.35	0.42
1:A:468:LEU:HA	1:A:468:LEU:HD23	1.90	0.42
1:A:238:ASP:HA	1:A:286:PRO:HB3	2.02	0.42
1:A:1002:THR:OG1	1:A:1003:SER:N	2.53	0.41
1:A:561:THR:HG21	1:A:565:ASN:HD22	1.85	0.41
1:A:561:THR:CG2	1:A:591:LYS:HZ1	2.30	0.41
1:A:611:LEU:CD2	1:A:643:ILE:HG21	2.50	0.41
1:A:273:ARG:HB3	1:A:306:VAL:HG13	2.03	0.41
1:A:373:LEU:HD11	1:A:406:GLU:N	2.36	0.41
1:A:373:LEU:HD22	1:A:404:PHE:CZ	2.55	0.41
1:A:939:THR:HB	1:A:945:GLY:HA2	2.01	0.41
1:A:786:PRO:C	1:A:788:ASP:H	2.24	0.41
1:A:743:GLN:HA	1:A:746:THR:HG22	2.01	0.41
1:A:306:VAL:HG22	1:A:307:LEU:N	2.35	0.41
1:A:757:TYR:HE1	1:A:807:LYS:HA	1.86	0.41
1:A:168:VAL:CG1	1:A:169:HIS:N	2.84	0.41
1:A:245:LEU:O	1:A:248:PHE:HB3	2.21	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:787:TYR:C	1:A:787:TYR:CD1	2.95	0.41
1:A:364:LYS:HD3	1:A:411:ASN:HD21	1.86	0.41
1:A:216:ALA:HB3	1:A:219:CYS:HB3	2.03	0.41
1:A:561:THR:CG2	1:A:591:LYS:CE	2.94	0.41
1:A:551:LEU:HA	1:A:551:LEU:HD23	1.83	0.40
1:A:509:ASP:C	1:A:509:ASP:OD1	2.59	0.40
1:A:751:SER:C	1:A:753:SER:H	2.24	0.40
1:A:562:ASP:HB2	1:A:563:PRO:CD	2.51	0.40
1:A:623:ASP:OD1	1:A:623:ASP:C	2.58	0.40
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.87	0.40
1:A:182:THR:HB	1:A:183:PRO:CD	2.48	0.40
1:A:379:LEU:CD1	1:A:380:THR:H	2.34	0.40
1:A:157:LEU:HD11	1:A:733:THR:HA	2.02	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:1078:LYS:HA	1:A:1078:LYS:HD3	1.98	0.40
1:A:290:PHE:O	1:A:294:ARG:HG3	2.21	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%)	5 10

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
1	A	897	GLY
1	A	1086	TRP
1	A	798	ILE
1	A	918	GLU

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Mol	Chain	Res	Type
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%)	675 (90%)	74 (10%)	11	25

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	LEU
1	A	164	ASP
1	A	168	VAL
1	A	194	LYS
1	A	229	THR
1	A	230	SER
1	A	238	ASP
1	A	269	ASP
1	A	272	LEU
1	A	281	LEU
1	A	285	THR
1	A	287	ILE
1	A	288	LYS
1	A	299	ASN
1	A	321	GLU
1	A	358	ASP
1	A	379	LEU
1	A	392	GLN
1	A	398	ARG
1	A	405	THR
1	A	410	TRP
1	A	411	ASN
1	A	418	ILE
1	A	421	LYS
1	A	497	PHE
1	A	498	ASN

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Mol	Chain	Res	Type
1	A	502	LEU
1	A	546	GLU
1	A	550	GLN
1	A	561	THR
1	A	575	LEU
1	A	610	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	776	ASN
1	A	779	LEU
1	A	787	TYR
1	A	838	LEU
1	A	841	ASP
1	A	846	GLN
1	A	862	LEU
1	A	863	CYS
1	A	871	SER
1	A	876	ILE
1	A	886	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	985	PHE
1	A	1001	LYS
1	A	1002	THR

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Mol	Chain	Res	Type
1	A	1007	GLN
1	A	1039	MET
1	A	1042	LEU
1	A	1059	LYS
1	A	1061	GLU
1	A	1086	TRP

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

Mol	Chain	Res	Type
1	A	299	ASN
1	A	304	HIS
1	A	391	GLN
1	A	411	ASN
1	A	465	ASN
1	A	471	HIS
1	A	512	ASN
1	A	565	ASN
1	A	634	ASN
1	A	646	GLN
1	A	658	HIS
1	A	673	HIS
1	A	710	GLN
1	A	734	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	949	ASN
1	A	951	ASN
1	A	1071	GLN
1	A	1083	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	2.23	8 (19%)	59,59,59	2.26	19 (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	-	-	0/28/38/38	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2088	534	C5-C3	-9.56	1.38	1.48
2	A	2088	534	O2-S1	6.09	1.51	1.43
2	A	2088	534	O1-S1	5.42	1.50	1.43
2	A	2088	534	C21-C19	-3.21	1.40	1.49
2	A	2088	534	C4-N3	2.69	1.43	1.36
2	A	2088	534	C6-N3	2.43	1.50	1.46
2	A	2088	534	C9-N3	2.09	1.49	1.46
2	A	2088	534	S1-N4	2.03	1.66	1.63

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2088	534	C15-S1-N4	-5.85	99.86	107.29
2	A	2088	534	O1-S1-N4	5.22	112.04	106.71
2	A	2088	534	C6-N3-C9	5.09	122.13	111.67
2	A	2088	534	O2-S1-O1	-4.82	110.77	119.38
2	A	2088	534	N6-C23-N5	-4.06	120.50	124.57
2	A	2088	534	O2-S1-N4	4.06	110.85	106.71
2	A	2088	534	C24-N6-C23	4.02	120.96	115.90
2	A	2088	534	C3-C4-N2	-3.97	117.42	122.51
2	A	2088	534	O2-S1-C15	3.50	112.58	107.94
2	A	2088	534	C1-N2-C4	3.40	122.96	115.44
2	A	2088	534	C22-N5-C23	3.40	120.17	115.90
2	A	2088	534	C2-C1-N2	-3.03	118.32	122.28
2	A	2088	534	C6-C7-N4	-2.94	106.69	109.02
2	A	2088	534	C2-N1-C3	2.91	122.30	116.58
2	A	2088	534	N7-C23-N5	2.73	119.88	117.42
2	A	2088	534	C7-N4-S1	-2.70	112.10	117.00
2	A	2088	534	C21-C24-N6	-2.46	120.19	124.33
2	A	2088	534	N7-C23-N6	2.42	119.61	117.42
2	A	2088	534	C21-C22-N5	-2.08	120.82	124.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	833/980 (85%)	0.29	46 (5%) 24 27	39, 70, 106, 120	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	6.8
1	A	900	GLY	5.8
1	A	896	VAL	5.7
1	A	376	ASN	5.2
1	A	375	ARG	5.0
1	A	1044	SER	5.0
1	A	252	MET	4.9
1	A	901	ALA	4.5
1	A	895	THR	4.5
1	A	404	PHE	4.3
1	A	143	SER	4.1
1	A	823	LEU	4.0
1	A	212	TRP	3.9
1	A	377	THR	3.8
1	A	147	SER	3.1
1	A	899	THR	3.0
1	A	233	ILE	3.0
1	A	754	ALA	2.9
1	A	226	ARG	2.8
1	A	489	GLY	2.7
1	A	250	THR	2.6
1	A	757	TYR	2.6
1	A	758	ASP	2.6
1	A	488	SER	2.6
1	A	756	LYS	2.5
1	A	403	PRO	2.5
1	A	545	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	248	PHE	2.4
1	A	898	ASN	2.4
1	A	1041	GLN	2.4
1	A	148	GLN	2.3
1	A	550	GLN	2.3
1	A	213	LYS	2.3
1	A	374	PRO	2.3
1	A	461	LEU	2.3
1	A	231	GLN	2.2
1	A	460	LEU	2.2
1	A	232	THR	2.2
1	A	671	PRO	2.2
1	A	914	LYS	2.2
1	A	380	THR	2.1
1	A	145	GLU	2.1
1	A	803	VAL	2.0
1	A	910	TRP	2.0
1	A	1045	LYS	2.0
1	A	216	ALA	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	534	A	2088	37/37	0.14	-1.07	61,66,70,71	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.