WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:17 AM GMT

PDB ID : 3DPD
Title : Achieving multi-isoform PI3K inhibition in a series of substituted 3,4-Dihydro-2H-benzo[1,4]oxazines
Authors : Ceska, T.A.
Deposited on : 2008-07-08
Resolution : 2.85 Å(reported)

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 2.85 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		26
Ramachandran outliers		3.0%
Sidechain outliers		8.8%
RSRZ outliers		8.0%

Worse ——— *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
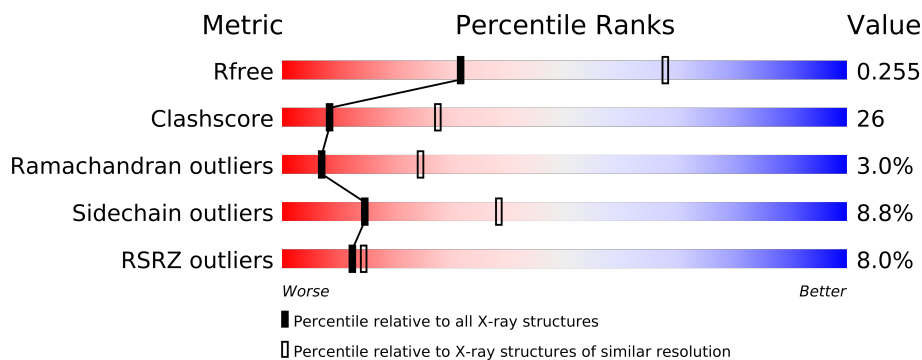
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. 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	966	

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 6879 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
			Total	C	N	O	S			
1	A	846	6861	4412	1168	1245	36	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736
A	1103	HIS	-	EXPRESSION TAG	UNP P48736
A	1104	HIS	-	EXPRESSION TAG	UNP P48736
A	1105	HIS	-	EXPRESSION TAG	UNP P48736
A	1106	HIS	-	EXPRESSION TAG	UNP P48736
A	1107	HIS	-	EXPRESSION TAG	UNP P48736
A	1108	HIS	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is 5,5-DIMETHYL-2-MORPHOLIN-4-YL-5,6-DIHYDRO-1,3-BENZOTHIAZOL-7(4H)-ONE (three-letter code: 41A) (formula: $C_{13}H_{18}N_2O_2S$).
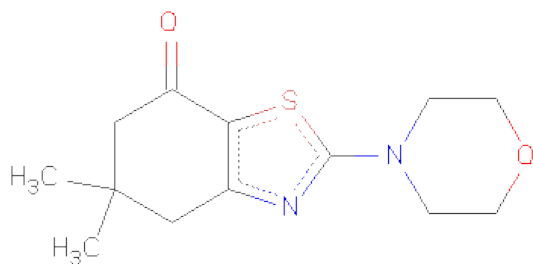
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	18	13	2	2	1	0	0

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
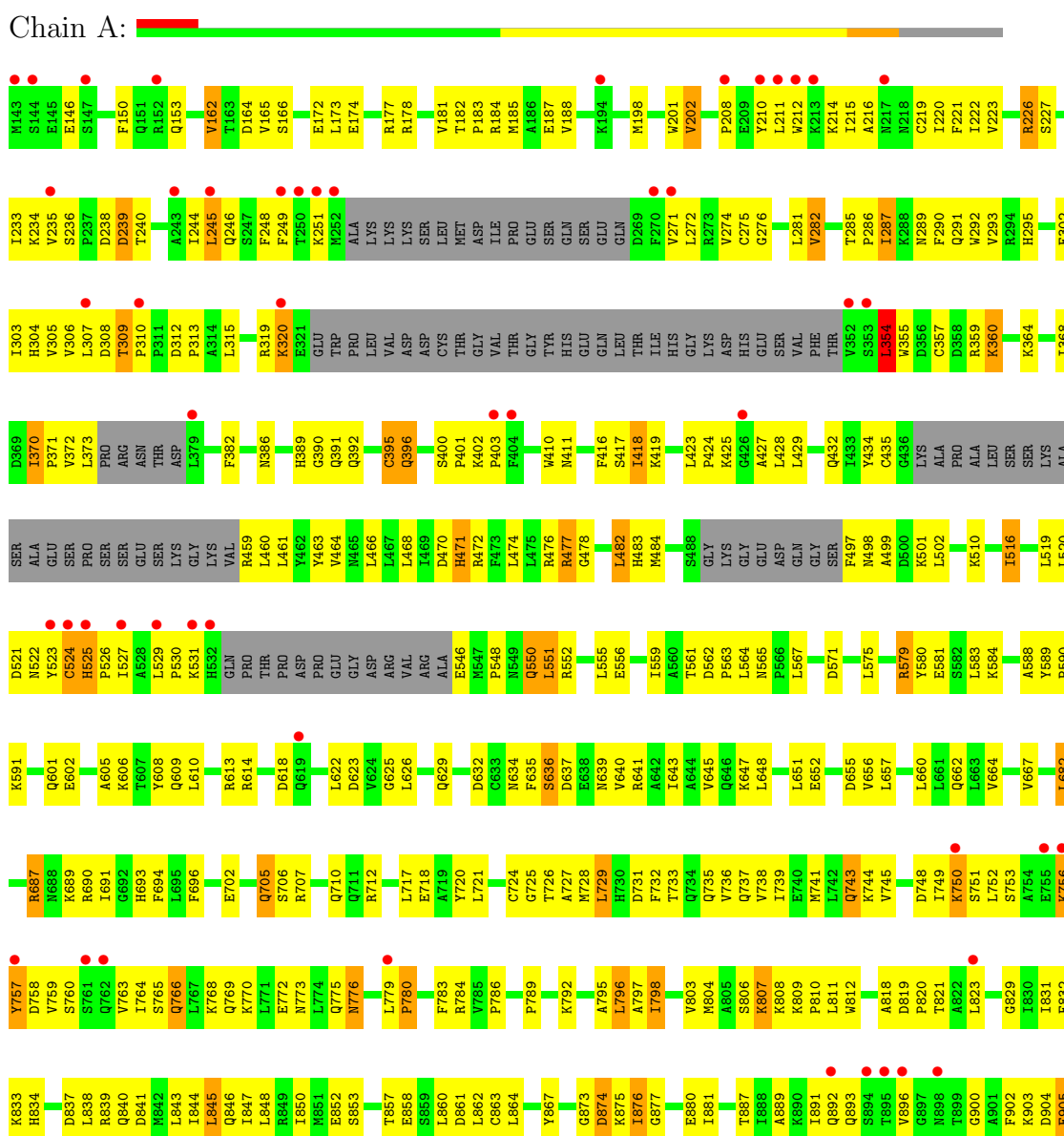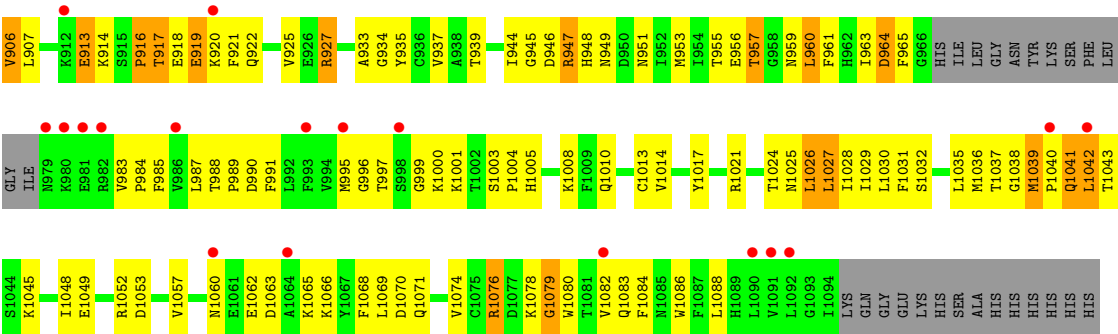
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.23Å 67.77Å 105.87Å 90.00° 95.96° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.56 – 2.84	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.85) 96.4 (30.56-2.84)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.85Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.242 , 0.318 0.245 , 0.255	Depositor DCC
R_{free} test set	1175 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	64.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	1 of 22970 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6879	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] 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: 41A

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	0.40	0/7010	0.58	0/9483

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	6861	0	6909	362	0
2	A	18	0	18	0	0
All	All	6879	0	6927	362	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 26.

All (362) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:629:GLN:HG2	1:A:1029:ILE:HG13	1.46	0.98
1:A:497:PHE:HB2	1:A:1042:LEU:HD22	1.45	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1039:MET:HB3	1:A:1041:GLN:HE22	1.26	0.95
1:A:418:ILE:HG12	1:A:419:LYS:H	1.34	0.93
1:A:1045:LYS:HD2	1:A:1045:LYS:H	1.35	0.90
1:A:221:PHE:HE1	1:A:234:LYS:HG2	1.36	0.90
1:A:689:LYS:HD2	1:A:728:MET:SD	2.17	0.83
1:A:949:ASN:HB2	1:A:1083:GLN:NE2	1.93	0.83
1:A:798:ILE:HD12	1:A:798:ILE:H	1.44	0.81
1:A:629:GLN:HG2	1:A:1029:ILE:CG1	2.13	0.79
1:A:497:PHE:HD1	1:A:1042:LEU:HB3	1.47	0.79
1:A:477:ARG:NE	1:A:522:ASN:HA	1.98	0.78
1:A:302:GLU:HB2	1:A:304:HIS:CE1	2.18	0.77
1:A:477:ARG:HE	1:A:522:ASN:HA	1.48	0.76
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.68	0.75
1:A:949:ASN:HB2	1:A:1083:GLN:HE22	1.48	0.74
1:A:222:ILE:HG22	1:A:303:ILE:HB	1.69	0.73
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.51	0.73
1:A:1014:VAL:HG11	1:A:1065:LYS:HG3	1.70	0.73
1:A:482:LEU:H	1:A:482:LEU:HD12	1.55	0.72
1:A:172:GLU:HG3	1:A:471:HIS:ND1	2.04	0.72
1:A:921:PHE:O	1:A:925:VAL:HG23	1.90	0.72
1:A:948:HIS:ND1	1:A:1086:TRP:HB3	2.07	0.70
1:A:202:VAL:HG12	1:A:290:PHE:HA	1.72	0.70
1:A:951:ASN:HA	1:A:963:ILE:HD11	1.73	0.70
1:A:531:LYS:HD2	1:A:608:TYR:HD1	1.57	0.70
1:A:579:ARG:HG2	1:A:610:LEU:HD11	1.73	0.69
1:A:499:ALA:HA	1:A:502:LEU:HD12	1.74	0.69
1:A:173:LEU:O	1:A:177:ARG:HG3	1.92	0.69
1:A:561:THR:HG21	1:A:565:ASN:ND2	2.07	0.68
1:A:1076:ARG:HH11	1:A:1076:ARG:HB3	1.57	0.68
1:A:772:GLU:HG2	1:A:798:ILE:HG12	1.75	0.68
1:A:198:MET:SD	1:A:282:VAL:HG21	2.34	0.68
1:A:818:ALA:O	1:A:820:PRO:HD3	1.94	0.68
1:A:364:LYS:HB3	1:A:519:LEU:HB3	1.76	0.68
1:A:645:VAL:HA	1:A:648:LEU:HD12	1.75	0.68
1:A:274:VAL:HA	1:A:305:VAL:HG12	1.76	0.67
1:A:432:GLN:HB3	1:A:460:LEU:HD11	1.75	0.67
1:A:579:ARG:HB3	1:A:610:LEU:HD21	1.76	0.67
1:A:293:VAL:HG13	1:A:303:ILE:HD13	1.76	0.66
1:A:690:ARG:HE	1:A:694:PHE:HE1	1.42	0.66
1:A:983:VAL:CG2	1:A:984:PRO:HD2	2.25	0.66
1:A:395:CYS:HB3	1:A:416:PHE:HD2	1.60	0.66
1:A:629:GLN:HG2	1:A:1029:ILE:CD1	2.26	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:757:TYR:HA	1:A:809:LYS:NZ	2.11	0.65
1:A:927:ARG:HE	1:A:959:ASN:HD22	1.42	0.65
1:A:947:ARG:HH11	1:A:947:ARG:HB3	1.62	0.65
1:A:983:VAL:HG22	1:A:984:PRO:HD2	1.76	0.65
1:A:418:ILE:HG12	1:A:419:LYS:N	2.07	0.65
1:A:201:TRP:NE1	1:A:291:GLN:HG3	2.11	0.65
1:A:354:LEU:HA	1:A:527:ILE:O	1.96	0.64
1:A:625:GLY:O	1:A:629:GLN:HG3	1.97	0.64
1:A:629:GLN:CG	1:A:1029:ILE:HG13	2.25	0.64
1:A:360:LYS:HE2	1:A:419:LYS:HG2	1.80	0.64
1:A:852:GLU:HG3	1:A:864:LEU:HD12	1.79	0.64
1:A:687:ARG:HH11	1:A:687:ARG:HG3	1.61	0.64
1:A:995:MET:O	1:A:1005:HIS:HB2	1.98	0.63
1:A:315:LEU:O	1:A:726:THR:HG22	1.97	0.63
1:A:606:LYS:O	1:A:609:GLN:HB2	1.98	0.62
1:A:1060:ASN:ND2	1:A:1063:ASP:H	1.98	0.62
1:A:660:LEU:O	1:A:664:VAL:HG23	1.99	0.62
1:A:756:LYS:HA	1:A:756:LYS:HZ2	1.64	0.62
1:A:955:THR:C	1:A:957:THR:H	2.01	0.61
1:A:880:GLU:HG2	1:A:881:ILE:N	2.14	0.61
1:A:271:VAL:HB	1:A:310:PRO:HG3	1.83	0.61
1:A:424:PRO:HD2	1:A:427:ALA:HB2	1.82	0.61
1:A:946:ASP:HB2	1:A:983:VAL:O	2.00	0.61
1:A:760:SER:O	1:A:763:VAL:HG12	2.01	0.61
1:A:531:LYS:HE2	1:A:605:ALA:HB2	1.83	0.60
1:A:775:GLN:NE2	1:A:795:ALA:HB1	2.15	0.60
1:A:370:ILE:HD13	1:A:371:PRO:N	2.15	0.60
1:A:784:ARG:HD3	1:A:789:PRO:O	2.02	0.60
1:A:806:SER:HB3	1:A:810:PRO:HD3	1.84	0.60
1:A:201:TRP:CE2	1:A:291:GLN:HG3	2.37	0.59
1:A:355:TRP:HH2	1:A:531:LYS:HG2	1.67	0.59
1:A:561:THR:O	1:A:591:LYS:NZ	2.35	0.59
1:A:1010:GLN:HB3	1:A:1069:LEU:HD21	1.84	0.59
1:A:162:VAL:HG21	1:A:718:GLU:OE2	2.03	0.59
1:A:567:LEU:HD22	1:A:571:ASP:HB3	1.85	0.59
1:A:876:ILE:N	1:A:876:ILE:HD13	2.16	0.59
1:A:287:ILE:O	1:A:287:ILE:HD13	2.03	0.59
1:A:757:TYR:HA	1:A:809:LYS:HZ1	1.68	0.59
1:A:743:GLN:HG2	1:A:876:ILE:HG21	1.85	0.59
1:A:319:ARG:HG2	1:A:320:LYS:H	1.68	0.58
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.86	0.58
1:A:784:ARG:CZ	1:A:792:LYS:HE3	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:905:GLU:CD	1:A:905:GLU:H	2.06	0.58
1:A:389:HIS:O	1:A:392:GLN:HB3	2.04	0.58
1:A:359:ARG:HD2	1:A:360:LYS:H	1.69	0.58
1:A:181:VAL:HG12	1:A:185:MET:CE	2.34	0.57
1:A:402:LYS:HB3	1:A:403:PRO:HD2	1.86	0.57
1:A:208:PRO:HD2	1:A:211:LEU:HD12	1.85	0.57
1:A:432:GLN:HB3	1:A:460:LEU:CD1	2.34	0.57
1:A:750:LYS:HD3	1:A:751:SER:N	2.20	0.57
1:A:763:VAL:HA	1:A:766:GLN:HG3	1.85	0.57
1:A:602:GLU:H	1:A:602:GLU:CD	2.06	0.57
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.87	0.57
1:A:622:LEU:HD12	1:A:623:ASP:N	2.20	0.56
1:A:738:VAL:HG21	1:A:783:PHE:HB3	1.87	0.56
1:A:174:GLU:O	1:A:178:ARG:HG3	2.05	0.56
1:A:914:LYS:O	1:A:916:PRO:HD3	2.06	0.56
1:A:497:PHE:CD1	1:A:1042:LEU:HB3	2.34	0.56
1:A:784:ARG:O	1:A:786:PRO:HD3	2.06	0.56
1:A:775:GLN:HE22	1:A:795:ALA:HB1	1.69	0.56
1:A:1013:CYS:HB3	1:A:1068:PHE:CE2	2.41	0.56
1:A:181:VAL:HG12	1:A:185:MET:HE1	1.88	0.56
1:A:564:LEU:HD13	1:A:1049:GLU:HA	1.87	0.56
1:A:687:ARG:HG3	1:A:687:ARG:NH1	2.21	0.55
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	1.87	0.55
1:A:563:PRO:HD3	1:A:1025:ASN:ND2	2.20	0.55
1:A:724:CYS:SG	1:A:729:LEU:HD13	2.47	0.55
1:A:1084:PHE:CE2	1:A:1088:LEU:HD11	2.41	0.55
1:A:1063:ASP:HA	1:A:1066:LYS:HE2	1.88	0.55
1:A:210:TYR:CE1	1:A:211:LEU:HG	2.42	0.54
1:A:1014:VAL:HG11	1:A:1065:LYS:CG	2.38	0.54
1:A:731:ASP:O	1:A:735:GLN:HG3	2.08	0.54
1:A:960:LEU:HG	1:A:961:PHE:N	2.22	0.54
1:A:1045:LYS:H	1:A:1045:LYS:CD	2.12	0.54
1:A:847:ILE:O	1:A:850:ILE:HB	2.08	0.54
1:A:464:VAL:HB	1:A:484:MET:HG2	1.90	0.54
1:A:735:GLN:O	1:A:739:ILE:HG12	2.08	0.54
1:A:834:HIS:HA	1:A:875:LYS:O	2.07	0.54
1:A:223:VAL:O	1:A:304:HIS:HA	2.07	0.54
1:A:913:GLU:HG3	1:A:914:LYS:N	2.22	0.54
1:A:386:ASN:OD1	1:A:396:GLN:HB2	2.08	0.54
1:A:861:ASP:C	1:A:862:LEU:HD22	2.28	0.54
1:A:364:LYS:NZ	1:A:411:ASN:O	2.41	0.53
1:A:953:MET:O	1:A:960:LEU:HD12	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:693:HIS:CD2	1:A:789:PRO:HB3	2.43	0.53
1:A:999:GLY:O	1:A:1000:LYS:HD3	2.08	0.53
1:A:635:PHE:O	1:A:641:ARG:HD2	2.09	0.53
1:A:846:GLN:O	1:A:850:ILE:HG12	2.09	0.53
1:A:306:VAL:HG13	1:A:308:ASP:OD1	2.08	0.52
1:A:955:THR:C	1:A:957:THR:N	2.63	0.52
1:A:732:PHE:O	1:A:736:VAL:HG23	2.09	0.52
1:A:903:LYS:HB2	1:A:906:VAL:HG23	1.90	0.52
1:A:1035:LEU:HB3	1:A:1043:THR:HG21	1.92	0.52
1:A:806:SER:C	1:A:808:LYS:H	2.13	0.52
1:A:182:THR:HB	1:A:183:PRO:HD3	1.92	0.52
1:A:360:LYS:CE	1:A:419:LYS:HG2	2.40	0.52
1:A:368:ILE:HG13	1:A:368:ILE:O	2.10	0.51
1:A:184:ARG:O	1:A:188:VAL:HG23	2.09	0.51
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.92	0.51
1:A:370:ILE:C	1:A:370:ILE:HD13	2.29	0.51
1:A:1045:LYS:O	1:A:1049:GLU:HG3	2.10	0.51
1:A:833:LYS:HG2	1:A:834:HIS:N	2.26	0.51
1:A:201:TRP:CZ3	1:A:690:ARG:NH1	2.79	0.51
1:A:470:ASP:HB3	1:A:476:ARG:NH2	2.25	0.51
1:A:892:GLN:HE22	1:A:902:PHE:HA	1.75	0.51
1:A:996:GLY:O	1:A:1001:LYS:HE3	2.10	0.51
1:A:690:ARG:NE	1:A:694:PHE:HE1	2.06	0.51
1:A:319:ARG:HG2	1:A:320:LYS:HG3	1.93	0.51
1:A:651:LEU:HD22	1:A:655:ASP:HB3	1.93	0.51
1:A:702:GLU:O	1:A:706:SER:HB3	2.10	0.51
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.40	0.51
1:A:470:ASP:OD1	1:A:472:ARG:N	2.40	0.51
1:A:464:VAL:HG11	1:A:516:ILE:HG21	1.93	0.51
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.92	0.50
1:A:955:THR:O	1:A:957:THR:N	2.44	0.50
1:A:434:TYR:HA	1:A:459:ARG:O	2.10	0.50
1:A:939:THR:OG1	1:A:945:GLY:HA2	2.10	0.50
1:A:744:LYS:HE2	1:A:748:ASP:OD1	2.12	0.50
1:A:770:LYS:O	1:A:773:ASN:HB2	2.12	0.50
1:A:640:VAL:O	1:A:643:ILE:HG12	2.12	0.50
1:A:215:ILE:HG23	1:A:220:ILE:HG22	1.93	0.50
1:A:622:LEU:HD12	1:A:623:ASP:H	1.76	0.50
1:A:997:THR:O	1:A:997:THR:HG22	2.11	0.50
1:A:772:GLU:CG	1:A:798:ILE:HG12	2.42	0.50
1:A:756:LYS:C	1:A:758:ASP:H	2.15	0.50
1:A:435:CYS:HB3	1:A:461:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:935:TYR:O	1:A:939:THR:HG22	2.12	0.49
1:A:223:VAL:HB	1:A:304:HIS:CD2	2.47	0.49
1:A:614:ARG:HG3	1:A:618:ASP:OD2	2.13	0.49
1:A:1038:GLY:O	1:A:1040:PRO:HD3	2.12	0.49
1:A:900:GLY:HA2	1:A:902:PHE:CE2	2.47	0.49
1:A:652:GLU:HG2	1:A:655:ASP:OD2	2.13	0.49
1:A:233:ILE:N	1:A:233:ILE:HD12	2.27	0.49
1:A:951:ASN:HA	1:A:963:ILE:CD1	2.40	0.49
1:A:271:VAL:HG22	1:A:272:LEU:N	2.28	0.49
1:A:435:CYS:SG	1:A:459:ARG:HG2	2.52	0.49
1:A:917:THR:HG23	1:A:920:LYS:HB2	1.93	0.49
1:A:226:ARG:HD3	1:A:307:LEU:HB3	1.95	0.49
1:A:887:THR:HG22	1:A:889:ALA:H	1.77	0.49
1:A:276:GLY:HA2	1:A:819:ASP:HB3	1.94	0.49
1:A:364:LYS:HD3	1:A:519:LEU:HD23	1.94	0.49
1:A:1074:VAL:O	1:A:1078:LYS:HG3	2.13	0.48
1:A:240:THR:O	1:A:244:ILE:HG13	2.12	0.48
1:A:873:GLY:HA3	1:A:876:ILE:HG12	1.94	0.48
1:A:807:LYS:HD2	1:A:807:LYS:N	2.28	0.48
1:A:757:TYR:HB3	1:A:807:LYS:HG3	1.95	0.48
1:A:803:VAL:HG22	1:A:811:LEU:CD2	2.43	0.48
1:A:705:GLN:OE1	1:A:839:ARG:NE	2.46	0.48
1:A:738:VAL:HG22	1:A:780:PRO:HD2	1.96	0.47
1:A:219:CYS:HA	1:A:236:SER:HA	1.95	0.47
1:A:625:GLY:HA2	1:A:1026:LEU:HD23	1.96	0.47
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.42	0.47
1:A:927:ARG:HE	1:A:959:ASN:ND2	2.11	0.47
1:A:222:ILE:O	1:A:222:ILE:HG13	2.15	0.47
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.49	0.47
1:A:483:HIS:CD2	1:A:510:LYS:HG2	2.50	0.47
1:A:477:ARG:HD3	1:A:521:ASP:O	2.15	0.47
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.97	0.47
1:A:810:PRO:O	1:A:811:LEU:HD23	2.14	0.47
1:A:474:LEU:HD22	1:A:527:ILE:HG12	1.96	0.47
1:A:652:GLU:O	1:A:656:VAL:HG23	2.15	0.47
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.15	0.46
1:A:477:ARG:HD2	1:A:478:GLY:H	1.80	0.46
1:A:292:TRP:O	1:A:295:HIS:HB3	2.14	0.46
1:A:552:ARG:O	1:A:556:GLU:HG3	2.15	0.46
1:A:308:ASP:N	1:A:308:ASP:OD1	2.48	0.46
1:A:662:GLN:NE2	1:A:1030:LEU:HD22	2.31	0.46
1:A:997:THR:HG21	1:A:1076:ARG:NH2	2.30	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:987:LEU:HD11	1:A:995:MET:CE	2.46	0.46
1:A:181:VAL:O	1:A:185:MET:HE2	2.15	0.46
1:A:418:ILE:HD13	1:A:423:LEU:HD23	1.98	0.46
1:A:1040:PRO:O	1:A:1041:GLN:C	2.54	0.46
1:A:984:PRO:HB2	1:A:985:PHE:CD2	2.50	0.46
1:A:807:LYS:HD2	1:A:807:LYS:H	1.80	0.46
1:A:428:LEU:C	1:A:428:LEU:HD23	2.36	0.46
1:A:988:THR:O	1:A:991:PHE:HB2	2.15	0.46
1:A:1052:ARG:HH11	1:A:1052:ARG:HG2	1.80	0.46
1:A:226:ARG:HG3	1:A:227:SER:H	1.80	0.46
1:A:1041:GLN:O	1:A:1043:THR:N	2.49	0.46
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.50	0.46
1:A:581:GLU:OE2	1:A:584:LYS:HD2	2.16	0.45
1:A:707:ARG:HD2	1:A:710:GLN:OE1	2.16	0.45
1:A:1041:GLN:N	1:A:1041:GLN:HE21	2.14	0.45
1:A:725:GLY:O	1:A:729:LEU:HB2	2.15	0.45
1:A:622:LEU:HD21	1:A:651:LEU:HG	1.98	0.45
1:A:235:VAL:HG11	1:A:244:ILE:CD1	2.47	0.45
1:A:523:TYR:HB3	1:A:524:CYS:H	1.48	0.45
1:A:983:VAL:HB	1:A:1082:VAL:HG21	1.99	0.45
1:A:775:GLN:OE1	1:A:779:LEU:HD23	2.16	0.45
1:A:484:MET:HE3	1:A:516:ILE:HG21	1.98	0.45
1:A:212:TRP:CE3	1:A:212:TRP:HA	2.51	0.45
1:A:548:PRO:HB2	1:A:551:LEU:HB2	1.99	0.45
1:A:1031:PHE:HE2	1:A:1048:ILE:HA	1.80	0.45
1:A:696:PHE:CE1	1:A:721:LEU:HD21	2.51	0.45
1:A:319:ARG:HG2	1:A:320:LYS:N	2.29	0.45
1:A:751:SER:C	1:A:753:SER:H	2.20	0.45
1:A:729:LEU:HD12	1:A:729:LEU:HA	1.67	0.45
1:A:1052:ARG:HD3	1:A:1057:VAL:HG21	1.99	0.45
1:A:1017:TYR:O	1:A:1021:ARG:HG3	2.17	0.45
1:A:559:ILE:HD13	1:A:588:ALA:HB2	1.97	0.45
1:A:779:LEU:HD12	1:A:780:PRO:HD2	1.98	0.45
1:A:498:ASN:OD1	1:A:498:ASN:C	2.56	0.45
1:A:1060:ASN:HD22	1:A:1062:GLU:HB2	1.81	0.45
1:A:862:LEU:HB3	1:A:934:GLY:HA3	1.98	0.45
1:A:989:PRO:HD2	1:A:1080:TRP:CE2	2.51	0.45
1:A:907:LEU:HD12	1:A:990:ASP:OD2	2.17	0.45
1:A:555:LEU:O	1:A:559:ILE:HG13	2.17	0.44
1:A:174:GLU:HA	1:A:177:ARG:HD3	1.99	0.44
1:A:803:VAL:HG13	1:A:810:PRO:O	2.17	0.44
1:A:1076:ARG:HB3	1:A:1076:ARG:NH1	2.28	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:212:TRP:HE3	1:A:212:TRP:HA	1.83	0.44
1:A:293:VAL:HG13	1:A:303:ILE:CD1	2.44	0.44
1:A:198:MET:HE3	1:A:282:VAL:HG21	1.99	0.44
1:A:947:ARG:CB	1:A:947:ARG:HH11	2.29	0.44
1:A:589:TYR:HB2	1:A:590:PRO:HD3	2.00	0.44
1:A:667:VAL:O	1:A:712:ARG:NH1	2.51	0.44
1:A:838:LEU:CD1	1:A:877:GLY:HA3	2.43	0.44
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.53	0.44
1:A:745:VAL:O	1:A:749:ILE:HG12	2.18	0.44
1:A:244:ILE:HG22	1:A:245:LEU:H	1.83	0.44
1:A:281:LEU:HD22	1:A:290:PHE:CD2	2.53	0.43
1:A:862:LEU:HD12	1:A:934:GLY:N	2.33	0.43
1:A:933:ALA:O	1:A:937:VAL:HG23	2.19	0.43
1:A:733:THR:HG22	1:A:737:GLN:HE21	1.83	0.43
1:A:1024:THR:O	1:A:1028:ILE:HG13	2.18	0.43
1:A:360:LYS:HE2	1:A:419:LYS:HE2	1.99	0.43
1:A:946:ASP:OD1	1:A:983:VAL:HG12	2.18	0.43
1:A:657:LEU:HG	1:A:691:ILE:HG12	2.00	0.43
1:A:765:SER:O	1:A:769:GLN:HB2	2.19	0.43
1:A:988:THR:HG21	1:A:1083:GLN:HG3	2.00	0.43
1:A:561:THR:HG22	1:A:562:ASP:N	2.33	0.43
1:A:863:CYS:HB3	1:A:959:ASN:HD21	1.82	0.43
1:A:784:ARG:NH2	1:A:792:LYS:HE3	2.32	0.43
1:A:887:THR:O	1:A:891:ILE:HG13	2.18	0.43
1:A:271:VAL:HG23	1:A:282:VAL:HG13	2.01	0.43
1:A:892:GLN:NE2	1:A:902:PHE:HA	2.33	0.43
1:A:1070:ASP:O	1:A:1074:VAL:HG23	2.19	0.43
1:A:221:PHE:CE1	1:A:234:LYS:HG2	2.29	0.43
1:A:1013:CYS:HB3	1:A:1068:PHE:HE2	1.82	0.43
1:A:917:THR:OG1	1:A:919:GLU:HB3	2.19	0.43
1:A:853:SER:O	1:A:857:THR:HG23	2.19	0.43
1:A:463:TYR:CE1	1:A:501:LYS:HA	2.53	0.43
1:A:497:PHE:CB	1:A:1042:LEU:HD22	2.33	0.43
1:A:187:GLU:CD	1:A:687:ARG:HG2	2.39	0.43
1:A:150:PHE:O	1:A:153:GLN:HB3	2.19	0.43
1:A:531:LYS:HE2	1:A:605:ALA:CB	2.49	0.43
1:A:390:GLY:N	1:A:636:SER:HB3	2.34	0.43
1:A:287:ILE:C	1:A:287:ILE:HD13	2.40	0.42
1:A:525:HIS:N	1:A:526:PRO:HD3	2.35	0.42
1:A:198:MET:CE	1:A:282:VAL:HG21	2.48	0.42
1:A:382:PHE:CE1	1:A:434:TYR:HB2	2.55	0.42
1:A:1014:VAL:HG13	1:A:1065:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:863:CYS:SG	1:A:927:ARG:HD3	2.59	0.42
1:A:309:THR:HG22	1:A:310:PRO:HD2	2.02	0.42
1:A:501:LYS:HB3	1:A:501:LYS:HE2	1.83	0.42
1:A:997:THR:HG23	1:A:1001:LYS:HG3	2.00	0.42
1:A:983:VAL:HG22	1:A:984:PRO:CD	2.45	0.42
1:A:370:ILE:O	1:A:370:ILE:HG23	2.19	0.42
1:A:918:GLU:O	1:A:922:GLN:HG2	2.19	0.42
1:A:831:ILE:CG2	1:A:832:PHE:N	2.83	0.42
1:A:162:VAL:O	1:A:177:ARG:NH1	2.53	0.42
1:A:947:ARG:CB	1:A:947:ARG:NH1	2.83	0.42
1:A:806:SER:C	1:A:808:LYS:N	2.73	0.42
1:A:804:MET:CE	1:A:812:TRP:HB2	2.49	0.42
1:A:275:CYS:SG	1:A:821:THR:HG22	2.60	0.42
1:A:390:GLY:C	1:A:392:GLN:H	2.23	0.42
1:A:382:PHE:CZ	1:A:434:TYR:HB2	2.55	0.42
1:A:829:GLY:HA3	1:A:881:ILE:HB	2.03	0.41
1:A:766:GLN:HE21	1:A:766:GLN:HB3	1.56	0.41
1:A:682:LEU:HD21	1:A:720:TYR:HA	2.02	0.41
1:A:531:LYS:HD2	1:A:608:TYR:CD1	2.46	0.41
1:A:720:TYR:CZ	1:A:724:CYS:HB3	2.55	0.41
1:A:889:ALA:O	1:A:893:GLN:HG3	2.20	0.41
1:A:844:ILE:O	1:A:848:LEU:HD13	2.21	0.41
1:A:400:SER:HA	1:A:401:PRO:HD3	1.88	0.41
1:A:164:ASP:C	1:A:166:SER:H	2.24	0.41
1:A:529:LEU:HA	1:A:530:PRO:HD3	1.95	0.41
1:A:904:ASP:OD2	1:A:904:ASP:N	2.52	0.41
1:A:775:GLN:HE22	1:A:796:LEU:H	1.68	0.41
1:A:1068:PHE:O	1:A:1071:GLN:HB2	2.20	0.41
1:A:845:LEU:HD12	1:A:845:LEU:HA	1.84	0.41
1:A:239:ASP:O	1:A:286:PRO:HA	2.20	0.41
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.51	0.41
1:A:749:ILE:HG21	1:A:803:VAL:HG21	2.03	0.41
1:A:201:TRP:CD1	1:A:291:GLN:HG3	2.55	0.41
1:A:862:LEU:HA	1:A:862:LEU:HD13	1.88	0.41
1:A:696:PHE:CD1	1:A:721:LEU:HD21	2.56	0.41
1:A:764:ILE:O	1:A:768:LYS:HG3	2.21	0.41
1:A:1035:LEU:C	1:A:1043:THR:HG21	2.41	0.41
1:A:823:LEU:HD22	1:A:823:LEU:H	1.86	0.41
1:A:632:ASP:OD1	1:A:634:ASN:HB2	2.20	0.41
1:A:418:ILE:CG1	1:A:419:LYS:H	2.16	0.41
1:A:963:ILE:O	1:A:964:ASP:C	2.59	0.41
1:A:370:ILE:HD13	1:A:372:VAL:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:643:ILE:O	1:A:647:LYS:HG2	2.21	0.41
1:A:551:LEU:HA	1:A:551:LEU:HD12	1.72	0.41
1:A:286:PRO:O	1:A:289:ASN:HB2	2.20	0.41
1:A:550:GLN:O	1:A:550:GLN:NE2	2.53	0.41
1:A:373:LEU:HA	1:A:373:LEU:HD12	1.94	0.41
1:A:520:LEU:O	1:A:521:ASP:C	2.59	0.41
1:A:945:GLY:C	1:A:985:PHE:HA	2.41	0.41
1:A:1032:SER:O	1:A:1036:MET:HG2	2.20	0.41
1:A:477:ARG:HG3	1:A:478:GLY:N	2.36	0.40
1:A:354:LEU:N	1:A:354:LEU:HD23	2.36	0.40
1:A:806:SER:HB3	1:A:810:PRO:CD	2.51	0.40
1:A:1053:ASP:N	1:A:1053:ASP:OD1	2.53	0.40
1:A:1027:LEU:HA	1:A:1027:LEU:HD12	1.78	0.40
1:A:637:ASP:OD1	1:A:639:ASN:HB2	2.21	0.40
1:A:996:GLY:O	1:A:1003:SER:HB3	2.21	0.40
1:A:796:LEU:HB3	1:A:797:ALA:H	1.65	0.40
1:A:312:ASP:HA	1:A:313:PRO:HD2	1.84	0.40
1:A:726:THR:CG2	1:A:727:ALA:N	2.85	0.40
1:A:651:LEU:HD22	1:A:655:ASP:CB	2.51	0.40
1:A:1078:LYS:O	1:A:1079:GLY:C	2.60	0.40
1:A:741:MET:O	1:A:744:LYS:HB3	2.21	0.40
1:A:773:ASN:HA	1:A:776:ASN:ND2	2.37	0.40
1:A:944:ILE:HD12	1:A:965:PHE:HD2	1.87	0.40
1:A:245:LEU:CA	1:A:248:PHE:HB3	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	830/966 (86%)	690 (83%)	115 (14%)	25 (3%)	7	24

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	916	PRO
1	A	165	VAL
1	A	214	LYS
1	A	251	LYS
1	A	776	ASN
1	A	956	GLU
1	A	1042	LEU
1	A	226	ARG
1	A	239	ASP
1	A	752	LEU
1	A	796	LEU
1	A	216	ALA
1	A	354	LEU
1	A	757	TYR
1	A	874	ASP
1	A	162	VAL
1	A	425	LYS
1	A	896	VAL
1	A	964	ASP
1	A	418	ILE
1	A	798	ILE
1	A	906	VAL
1	A	1079	GLY
1	A	759	VAL
1	A	780	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	761/864 (88%)	694 (91%)	67 (9%)	14	38

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	202	VAL
1	A	238	ASP

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Mol	Chain	Res	Type
1	A	245	LEU
1	A	246	GLN
1	A	249	PHE
1	A	282	VAL
1	A	285	THR
1	A	287	ILE
1	A	309	THR
1	A	320	LYS
1	A	354	LEU
1	A	357	CYS
1	A	360	LYS
1	A	370	ILE
1	A	391	GLN
1	A	395	CYS
1	A	396	GLN
1	A	410	TRP
1	A	417	SER
1	A	471	HIS
1	A	477	ARG
1	A	482	LEU
1	A	516	ILE
1	A	524	CYS
1	A	525	HIS
1	A	546	GLU
1	A	550	GLN
1	A	551	LEU
1	A	575	LEU
1	A	579	ARG
1	A	580	TYR
1	A	601	GLN
1	A	613	ARG
1	A	626	LEU
1	A	636	SER
1	A	682	LEU
1	A	687	ARG
1	A	705	GLN
1	A	717	LEU
1	A	729	LEU
1	A	743	GLN
1	A	750	LYS
1	A	756	LYS
1	A	766	GLN

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Mol	Chain	Res	Type
1	A	807	LYS
1	A	841	ASP
1	A	843	LEU
1	A	845	LEU
1	A	858	GLU
1	A	860	LEU
1	A	874	ASP
1	A	876	ILE
1	A	905	GLU
1	A	913	GLU
1	A	917	THR
1	A	919	GLU
1	A	927	ARG
1	A	947	ARG
1	A	957	THR
1	A	960	LEU
1	A	1026	LEU
1	A	1027	LEU
1	A	1037	THR
1	A	1039	MET
1	A	1041	GLN
1	A	1076	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	GLN
1	A	225	HIS
1	A	388	GLN
1	A	391	GLN
1	A	396	GLN
1	A	483	HIS
1	A	550	GLN
1	A	565	ASN
1	A	577	HIS
1	A	619	GLN
1	A	634	ASN
1	A	639	ASN
1	A	662	GLN
1	A	711	GLN
1	A	734	GLN
1	A	737	GLN

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Mol	Chain	Res	Type
1	A	766	GLN
1	A	776	ASN
1	A	825	ASN
1	A	840	GLN
1	A	892	GLN
1	A	893	GLN
1	A	908	ASN
1	A	951	ASN
1	A	959	ASN
1	A	1007	GLN
1	A	1023	HIS
1	A	1041	GLN
1	A	1083	GLN
1	A	1085	ASN
1	A	1089	HIS

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	41A	A	2040	-	20,20,20	1.17	2 (10%)	27,30,30	2.30	7 (25%)

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	41A	A	2040	-	-	0/2/26/26	0/1/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2040	41A	C04-C02	2.62	1.57	1.53
2	A	2040	41A	C17-N12	2.18	1.50	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2040	41A	C17-N12-C11	-6.73	112.29	121.58
2	A	2040	41A	C05-C06-C07	5.76	124.90	122.19
2	A	2040	41A	C13-N12-C11	-4.06	115.97	121.58
2	A	2040	41A	C02-C08-C07	3.90	118.32	113.59
2	A	2040	41A	C08-C02-C04	3.28	110.57	107.86
2	A	2040	41A	C06-C05-N18	2.28	115.44	110.68
2	A	2040	41A	S10-C11-N12	-2.12	120.78	123.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	846/966 (87%)	0.38	68 (8%)	12	14	14, 58, 106, 126	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	979	ASN	6.5
1	A	143	MET	5.9
1	A	895	THR	5.1
1	A	379	LEU	5.1
1	A	212	TRP	5.1
1	A	249	PHE	4.3
1	A	529	LEU	4.2
1	A	270	PHE	4.1
1	A	755	GLU	4.1
1	A	211	LEU	3.9
1	A	353	SER	3.9
1	A	252	MET	3.8
1	A	525	HIS	3.6
1	A	527	ILE	3.5
1	A	217	ASN	3.5
1	A	896	VAL	3.5
1	A	524	CYS	3.4
1	A	1042	LEU	3.3
1	A	761	SER	3.2
1	A	250	THR	3.2
1	A	1090	LEU	3.2
1	A	981	GLU	3.2
1	A	1091	VAL	3.2
1	A	892	GLN	3.1
1	A	144	SER	3.1
1	A	995	MET	3.0
1	A	762	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	986	VAL	3.0
1	A	210	TYR	3.0
1	A	757	TYR	3.0
1	A	523	TYR	2.9
1	A	251	LYS	2.9
1	A	980	LYS	2.8
1	A	245	LEU	2.8
1	A	920	LYS	2.8
1	A	403	PRO	2.8
1	A	152	ARG	2.7
1	A	1092	LEU	2.7
1	A	310	PRO	2.7
1	A	532	HIS	2.6
1	A	1060	ASN	2.6
1	A	1040	PRO	2.5
1	A	235	VAL	2.5
1	A	531	LYS	2.4
1	A	307	LEU	2.4
1	A	756	LYS	2.4
1	A	982	ARG	2.4
1	A	1082	VAL	2.3
1	A	898	ASN	2.3
1	A	998	SER	2.3
1	A	1064	ALA	2.2
1	A	426	GLY	2.2
1	A	147	SER	2.2
1	A	404	PHE	2.2
1	A	352	VAL	2.2
1	A	194	LYS	2.1
1	A	320	LYS	2.1
1	A	894	SER	2.1
1	A	750	LYS	2.1
1	A	271	VAL	2.1
1	A	912	LYS	2.1
1	A	993	PHE	2.1
1	A	823	LEU	2.1
1	A	619	GLN	2.1
1	A	213	LYS	2.1
1	A	779	LEU	2.1
1	A	208	PRO	2.1
1	A	243	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, 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	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	41A	A	2040	18/18	0.19	-0.28	49,60,66,70	0

6.5　Other polymers ⓘ

There are no such residues in this entry.