



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:48 PM GMT

PDB ID : 3APF
Title : Crystal structure of human PI3K-gamma in complex with CH5039699
Authors : Nakamura, M.; Fukami, T.A.; Miyazaki, T.; Yoshida, M.
Deposited on : 2010-10-14
Resolution : 2.82 Å(reported)

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

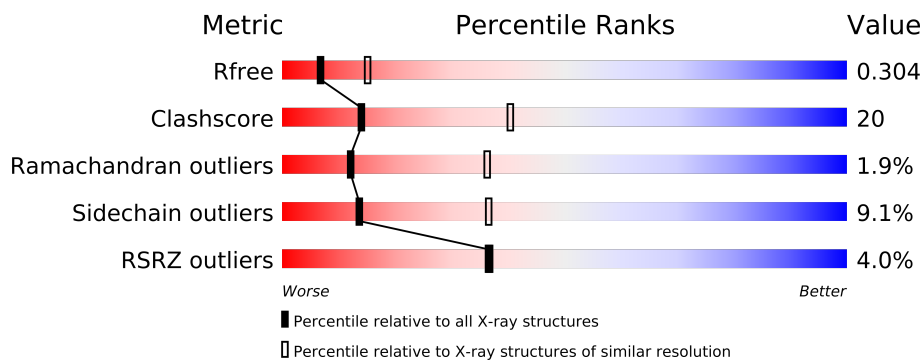
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.82 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	1963 (2.84-2.80)
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 4 unique types of molecules in this entry. The entry contains 6611 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.

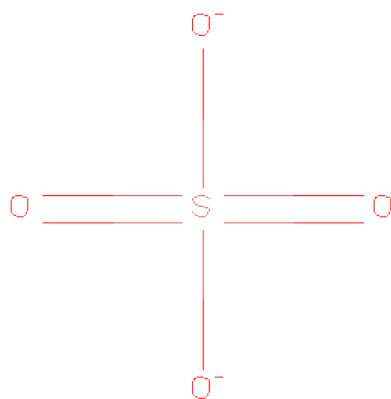
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	0
			6567	4211	1116	1206	34			

There are 7 discrepancies between the modelled and reference sequences:

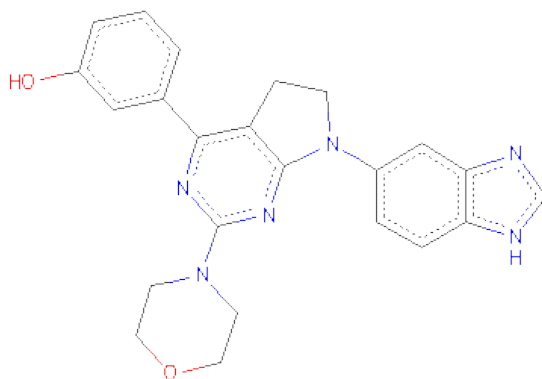
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	EXPRESSION TAG	UNP P48736
A	138	PRO	-	EXPRESSION TAG	UNP P48736
A	139	LEU	-	EXPRESSION TAG	UNP P48736
A	140	HIS	-	EXPRESSION TAG	UNP P48736
A	141	MET	-	EXPRESSION TAG	UNP P48736
A	142	GLY	-	EXPRESSION TAG	UNP P48736
A	143	SER	-	EXPRESSION TAG	UNP P48736

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is 3-[7-(1H-BENZIMIDAZOL-5-YL)-2-(MORPHOLIN-4-YL)-6,7-DIHYDRO-5H-PYRROLO[2,3-D]PYRIMIDIN-4-YL]PHENOL (three-letter code: BMW) (formula: C₂₃H₂₂N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	23	6	2		

- Molecule 4 is water.

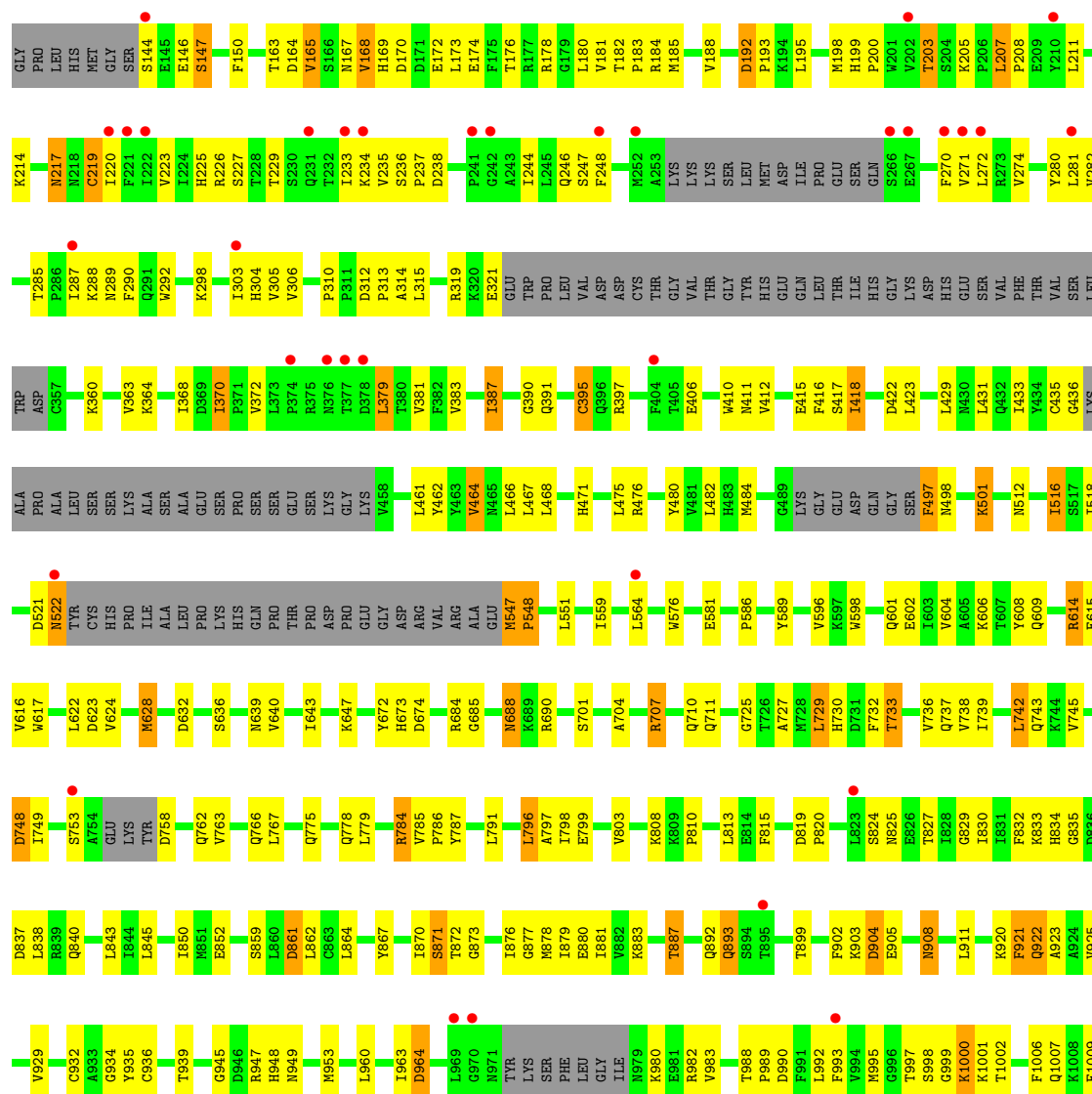
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	O	0	0
			3	3		

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

Chain A: 



Q1010	D1011	I1012	F1013	V1014	K1015	A1016	L1020	L1027	I1028	I1029	F1031	S1032	M1033	M1034	L1035	M1036	M1039	P1040	Q1041	K1045	I1048	F1049	Y1050	R1051	R1052	T1056	M1060	E1061	E1062	D1063	L1069	I1072	E1073	V1074	C1075	R1076	D1077	K1078	G1079	Q1083	W1086	F1087	L1088	H1089	L1090	V1091	L1092
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

GLY
ILE
LYS
GLN
GLY
GLU
LYS
HIS
SER
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.22Å 67.87Å 106.60Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	62.23 – 2.82 57.03 – 2.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.23-2.82) 99.4 (57.03-2.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.241 , 0.315 0.232 , 0.304	Depositor DCC
R_{free} test set	1271 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 39.7	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 24972 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6611	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: SO4, BMW

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	0.60	0/6707	0.72	0/9111

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	6567	0	6378	257	0
2	A	10	0	0	1	0
3	A	31	0	22	3	0
4	A	3	0	0	0	0
All	All	6611	0	6400	258	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 (258) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:729:LEU:O	1:A:733:THR:HG23	1.62	0.99
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.49	0.94
1:A:861:ASP:C	1:A:862:LEU:HD23	1.89	0.94
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.57	0.87
1:A:482:LEU:HB2	1:A:516:ILE:HD12	1.57	0.85
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.59	0.84
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.60	0.83
1:A:167:ASN:HD22	1:A:711:GLN:HE22	1.28	0.81
1:A:922:GLN:HA	1:A:922:GLN:HE21	1.46	0.80
1:A:168:VAL:HG13	1:A:170:ASP:H	1.46	0.80
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.13	0.79
1:A:464:VAL:HG11	1:A:516:ILE:HD11	1.66	0.77
1:A:861:ASP:O	1:A:862:LEU:HD23	1.84	0.77
1:A:167:ASN:ND2	1:A:711:GLN:HE22	1.83	0.76
1:A:829:GLY:C	1:A:881:ILE:HD12	2.06	0.75
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.01	0.75
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.16	0.75
1:A:892:GLN:OE1	1:A:902:PHE:CB	2.33	0.75
1:A:729:LEU:O	1:A:733:THR:CG2	2.34	0.74
1:A:180:LEU:O	1:A:183:PRO:HD2	1.86	0.74
1:A:271:VAL:HG22	1:A:310:PRO:HG3	1.68	0.74
1:A:167:ASN:HD22	1:A:711:GLN:NE2	1.86	0.73
1:A:1074:VAL:O	1:A:1078:LYS:HG2	1.88	0.73
1:A:840:GLN:HG2	1:A:1039:MET:HE2	1.69	0.73
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.88	0.73
1:A:1088:LEU:O	1:A:1092:LEU:HB2	1.88	0.72
1:A:244:ILE:HG23	1:A:247:SER:HB2	1.71	0.72
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.73	0.71
1:A:203:THR:OG1	1:A:205:LYS:HG3	1.92	0.69
1:A:379:LEU:HB3	1:A:436:GLY:O	1.93	0.69
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.22	0.69
1:A:935:TYR:O	1:A:939:THR:HG23	1.92	0.69
1:A:233:ILE:HG22	1:A:234:LYS:O	1.95	0.67
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.76	0.67
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.77	0.67
1:A:732:PHE:O	1:A:736:VAL:HG23	1.96	0.66
1:A:762:GLN:O	1:A:766:GLN:N	2.22	0.66
1:A:464:VAL:CG1	1:A:516:ILE:HD11	2.26	0.65
1:A:707:ARG:HA	1:A:710:GLN:OE1	1.96	0.65
1:A:482:LEU:HB2	1:A:516:ILE:CD1	2.27	0.65
1:A:368:ILE:HG22	1:A:516:ILE:HG23	1.79	0.64
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.33	0.63
1:A:207:LEU:HD13	1:A:288:LYS:HB2	1.78	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.26	0.63
1:A:1013:CYS:O	1:A:1016:ALA:N	2.31	0.63
1:A:223:VAL:O	1:A:225:HIS:CD2	2.52	0.63
1:A:908:ASN:HD21	1:A:921:PHE:HZ	1.47	0.62
1:A:397:ARG:HD2	1:A:415:GLU:O	1.98	0.62
1:A:305:VAL:HG23	1:A:306:VAL:N	2.13	0.62
1:A:749:ILE:HD13	1:A:749:ILE:N	2.15	0.62
1:A:226:ARG:HB3	1:A:229:THR:OG1	2.00	0.61
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.81	0.61
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.83	0.61
1:A:725:GLY:O	1:A:729:LEU:HD12	2.00	0.61
1:A:1032:SER:O	1:A:1036:MET:HE2	2.01	0.60
1:A:219:CYS:HA	1:A:235:VAL:O	2.01	0.60
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.83	0.60
1:A:559:ILE:O	1:A:559:ILE:HG22	2.00	0.60
1:A:608:TYR:CE2	1:A:639:ASN:ND2	2.69	0.59
1:A:272:LEU:N	1:A:272:LEU:HD23	2.17	0.59
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.33	0.59
1:A:998:SER:O	1:A:1000:LYS:N	2.35	0.59
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.71	0.58
1:A:168:VAL:HG13	1:A:170:ASP:N	2.17	0.58
1:A:547:MET:CE	1:A:581:GLU:HG3	2.33	0.57
1:A:920:LYS:O	1:A:923:ALA:N	2.36	0.57
1:A:467:LEU:HD13	1:A:672:TYR:CE1	2.39	0.57
1:A:223:VAL:O	1:A:225:HIS:HD2	1.87	0.57
1:A:922:GLN:HE21	1:A:922:GLN:CA	2.18	0.57
1:A:893:GLN:HE21	1:A:893:GLN:C	2.10	0.56
1:A:192:ASP:OD1	1:A:192:ASP:C	2.44	0.56
1:A:997:THR:HG23	1:A:1001:LYS:CB	2.36	0.55
3:A:1103:BMW:H13A	3:A:1103:BMW:H28	1.87	0.55
1:A:471:HIS:H	1:A:471:HIS:CD2	2.23	0.55
1:A:1002:THR:HG22	1:A:1007:GLN:HE21	1.71	0.55
1:A:182:THR:HB	1:A:183:PRO:HD3	1.89	0.54
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.89	0.54
1:A:745:VAL:O	1:A:749:ILE:HG12	2.06	0.54
1:A:870:ILE:HG22	1:A:871:SER:O	2.07	0.54
1:A:1006:PHE:O	1:A:1007:GLN:C	2.46	0.54
1:A:435:CYS:O	1:A:435:CYS:SG	2.66	0.54
1:A:887:THR:HG22	1:A:953:MET:CE	2.39	0.53
1:A:1006:PHE:O	1:A:1009:PHE:N	2.41	0.53
1:A:370:ILE:HD12	1:A:370:ILE:H	1.73	0.53
1:A:198:MET:HG2	1:A:280:TYR:CG	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:416:PHE:HB3	1:A:418:ILE:HD12	1.91	0.53
1:A:876:ILE:O	1:A:876:ILE:HG23	2.08	0.53
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.44	0.53
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.74	0.53
1:A:861:ASP:C	1:A:861:ASP:OD1	2.47	0.52
1:A:370:ILE:CD1	1:A:406:GLU:HA	2.39	0.52
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.10	0.52
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.91	0.52
1:A:829:GLY:O	1:A:881:ILE:HB	2.09	0.52
1:A:905:GLU:HA	1:A:993:PHE:CD2	2.44	0.52
1:A:387:ILE:HD13	1:A:468:LEU:HD11	1.92	0.52
1:A:312:ASP:HB3	1:A:315:LEU:HG	1.91	0.52
1:A:785:VAL:HG23	1:A:791:LEU:O	2.09	0.52
1:A:163:THR:O	1:A:165:VAL:HG23	2.09	0.52
1:A:988:THR:HG22	1:A:1079:GLY:O	2.10	0.52
1:A:808:LYS:O	1:A:810:PRO:HD3	2.10	0.51
1:A:168:VAL:CG1	1:A:169:HIS:N	2.73	0.51
1:A:1040:PRO:O	1:A:1041:GLN:CB	2.58	0.51
1:A:360:LYS:HB3	1:A:416:PHE:O	2.11	0.51
1:A:925:VAL:O	1:A:929:VAL:HG23	2.11	0.51
1:A:739:ILE:HG21	1:A:878:MET:HE1	1.92	0.51
1:A:862:LEU:N	1:A:862:LEU:HD23	2.19	0.51
1:A:862:LEU:HD12	1:A:934:GLY:HA2	1.93	0.51
1:A:640:VAL:O	1:A:643:ILE:HG12	2.11	0.51
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.93	0.51
1:A:211:LEU:HD21	1:A:298:LYS:HA	1.93	0.51
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.93	0.51
1:A:992:LEU:O	1:A:995:MET:N	2.44	0.50
1:A:431:LEU:HD13	1:A:516:ILE:HD13	1.92	0.50
1:A:939:THR:HB	1:A:945:GLY:HA2	1.93	0.50
1:A:181:VAL:CG1	1:A:185:MET:SD	3.00	0.50
1:A:852:GLU:HG2	1:A:864:LEU:HD12	1.93	0.49
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.47	0.49
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.48	0.49
1:A:368:ILE:CG2	1:A:516:ILE:HG23	2.43	0.49
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.31	0.49
1:A:1007:GLN:O	1:A:1011:ASP:N	2.45	0.49
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.92	0.49
1:A:980:LYS:O	1:A:982:ARG:HG2	2.13	0.49
1:A:949:ASN:HB3	1:A:1083:GLN:HE22	1.76	0.49
1:A:632:ASP:C	1:A:632:ASP:OD1	2.51	0.49
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:624:VAL:O	1:A:628:MET:HB2	2.13	0.49
1:A:843:LEU:HD13	1:A:1034:MET:HG3	1.95	0.49
1:A:908:ASN:HA	1:A:911:LEU:HD12	1.95	0.49
1:A:963:ILE:HD12	3:A:1103:BMW:C14	2.43	0.49
1:A:602:GLU:N	1:A:602:GLU:OE1	2.41	0.48
1:A:236:SER:O	1:A:238:ASP:N	2.45	0.48
1:A:521:ASP:OD1	1:A:522:ASN:N	2.46	0.48
1:A:983:VAL:HG13	1:A:983:VAL:O	2.13	0.48
1:A:144:SER:HA	1:A:147:SER:HB3	1.95	0.48
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.94	0.48
1:A:1089:HIS:HA	1:A:1092:LEU:HB2	1.95	0.48
1:A:305:VAL:CG2	1:A:306:VAL:N	2.77	0.48
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.43	0.48
1:A:383:VAL:HG22	1:A:433:ILE:HD13	1.97	0.47
1:A:997:THR:HG22	1:A:998:SER:N	2.28	0.47
1:A:303:ILE:CG2	1:A:304:HIS:N	2.77	0.47
1:A:480:TYR:HB2	1:A:518:ILE:HG13	1.96	0.47
1:A:725:GLY:C	1:A:729:LEU:HD12	2.33	0.47
1:A:784:ARG:O	1:A:786:PRO:HD3	2.15	0.47
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.49	0.47
1:A:270:PHE:HA	1:A:310:PRO:HD3	1.96	0.47
1:A:997:THR:CG2	1:A:998:SER:N	2.78	0.47
1:A:303:ILE:HG22	1:A:304:HIS:N	2.30	0.47
1:A:948:HIS:N	2:A:2:SO4:O1	2.44	0.47
1:A:990:ASP:OD1	1:A:990:ASP:N	2.48	0.47
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.47
1:A:1074:VAL:O	1:A:1078:LYS:CG	2.60	0.46
1:A:622:LEU:HD12	1:A:623:ASP:N	2.29	0.46
1:A:165:VAL:O	1:A:165:VAL:HG12	2.15	0.46
1:A:282:VAL:O	1:A:290:PHE:HZ	1.97	0.46
1:A:381:VAL:HG12	1:A:435:CYS:HB2	1.96	0.46
1:A:220:ILE:N	1:A:235:VAL:O	2.46	0.46
1:A:303:ILE:O	1:A:304:HIS:CD2	2.69	0.46
1:A:285:THR:HG22	1:A:289:ASN:CB	2.44	0.46
1:A:908:ASN:C	1:A:908:ASN:HD22	2.18	0.46
1:A:748:ASP:HB2	1:A:749:ILE:HD13	1.97	0.46
1:A:422:ASP:HA	1:A:601:GLN:HB2	1.96	0.46
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.98	0.46
1:A:181:VAL:HG12	1:A:185:MET:SD	2.56	0.46
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.98	0.46
1:A:381:VAL:HG12	1:A:435:CYS:CB	2.46	0.46
1:A:576:TRP:CZ3	1:A:596:VAL:HG22	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.51	0.46
1:A:824:SER:OG	1:A:825:ASN:N	2.49	0.45
1:A:850:ILE:HD13	1:A:1030:LEU:CD1	2.46	0.45
1:A:964:ASP:C	1:A:964:ASP:OD1	2.54	0.45
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.16	0.45
1:A:168:VAL:HG13	1:A:169:HIS:N	2.31	0.45
1:A:935:TYR:O	1:A:939:THR:CG2	2.64	0.45
1:A:614:ARG:O	1:A:614:ARG:CG	2.65	0.45
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.99	0.45
1:A:168:VAL:HG13	1:A:170:ASP:O	2.17	0.45
1:A:207:LEU:CD1	1:A:288:LYS:HB2	2.44	0.45
1:A:390:GLY:O	1:A:391:GLN:HB2	2.17	0.45
1:A:704:ALA:CB	1:A:873:GLY:HA2	2.46	0.45
1:A:684:ARG:O	1:A:685:GLY:C	2.52	0.45
1:A:1013:CYS:O	1:A:1015:LYS:N	2.50	0.45
1:A:614:ARG:O	1:A:614:ARG:HG3	2.17	0.45
1:A:1073:GLU:O	1:A:1074:VAL:C	2.54	0.44
1:A:303:ILE:O	1:A:304:HIS:CG	2.70	0.44
1:A:1089:HIS:C	1:A:1091:VAL:N	2.71	0.44
1:A:893:GLN:NE2	1:A:893:GLN:C	2.71	0.44
1:A:164:ASP:C	1:A:164:ASP:OD1	2.54	0.44
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.00	0.44
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.52	0.44
1:A:947:ARG:NH2	1:A:963:ILE:O	2.50	0.44
1:A:748:ASP:OD1	1:A:748:ASP:N	2.51	0.44
1:A:879:ILE:HD12	1:A:879:ILE:N	2.33	0.43
1:A:983:VAL:CG2	1:A:1075:CYS:SG	3.06	0.43
1:A:778:GLN:N	1:A:778:GLN:OE1	2.52	0.43
1:A:767:LEU:HD22	1:A:803:VAL:HG22	1.98	0.43
1:A:271:VAL:CG2	1:A:310:PRO:HG3	2.45	0.43
1:A:236:SER:C	1:A:238:ASP:H	2.22	0.43
1:A:796:LEU:HG	1:A:815:PHE:CE1	2.53	0.43
1:A:1060:ASN:HD21	1:A:1063:ASP:HB2	1.84	0.43
1:A:198:MET:O	1:A:199:HIS:C	2.57	0.43
1:A:211:LEU:HD11	1:A:298:LYS:HB2	2.01	0.43
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.53	0.43
1:A:397:ARG:HH21	1:A:416:PHE:HA	1.82	0.43
1:A:497:PHE:HB3	1:A:498:ASN:H	1.67	0.43
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.92	0.43
1:A:737:GLN:O	1:A:738:VAL:C	2.56	0.43
1:A:953:MET:HE3	3:A:1103:BMW:N16	2.34	0.42
1:A:688:ASN:C	1:A:688:ASN:OD1	2.56	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:606:LYS:O	1:A:609:GLN:HG2	2.18	0.42
1:A:833:LYS:O	1:A:876:ILE:HA	2.18	0.42
1:A:1052:ARG:O	1:A:1056:THR:N	2.52	0.42
1:A:738:VAL:CG1	1:A:742:LEU:HD12	2.50	0.42
1:A:1069:LEU:O	1:A:1072:ILE:HG12	2.18	0.42
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.42
1:A:220:ILE:HD12	1:A:237:PRO:HB3	2.01	0.42
1:A:879:ILE:HG22	1:A:880:GLU:N	2.34	0.42
1:A:830:ILE:N	1:A:881:ILE:HD12	2.34	0.42
1:A:199:HIS:O	1:A:200:PRO:C	2.56	0.42
1:A:173:LEU:CD2	1:A:673:HIS:CD2	3.02	0.42
1:A:850:ILE:HD13	1:A:1030:LEU:HD13	2.02	0.42
1:A:1086:TRP:HA	1:A:1086:TRP:CE3	2.55	0.42
1:A:808:LYS:HG2	1:A:835:GLY:HA3	2.02	0.42
1:A:303:ILE:HD12	1:A:303:ILE:N	2.35	0.42
1:A:796:LEU:O	1:A:798:ILE:N	2.53	0.41
1:A:482:LEU:HD12	1:A:516:ILE:CD1	2.50	0.41
1:A:168:VAL:CG1	1:A:170:ASP:O	2.69	0.41
1:A:363:VAL:O	1:A:363:VAL:HG13	2.19	0.41
1:A:920:LYS:O	1:A:922:GLN:N	2.54	0.41
1:A:1029:ILE:HA	1:A:1029:ILE:HD13	1.79	0.41
1:A:602:GLU:N	1:A:602:GLU:CD	2.73	0.41
1:A:423:LEU:HA	1:A:423:LEU:HD23	1.72	0.41
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.99	0.41
1:A:887:THR:HG22	1:A:953:MET:HE2	2.02	0.41
1:A:903:LYS:O	1:A:905:GLU:N	2.54	0.41
1:A:185:MET:CE	1:A:321:GLU:HG3	2.50	0.41
1:A:244:ILE:O	1:A:244:ILE:HG22	2.21	0.41
1:A:908:ASN:HA	1:A:911:LEU:HB2	2.03	0.41
1:A:192:ASP:OD2	1:A:195:LEU:HD12	2.21	0.41
1:A:1076:ARG:C	1:A:1078:LYS:H	2.24	0.41
1:A:462:TYR:HB3	1:A:484:MET:HE2	2.03	0.41
1:A:614:ARG:HB2	1:A:617:TRP:HB3	2.03	0.41
1:A:688:ASN:OD1	1:A:690:ARG:N	2.54	0.41
1:A:184:ARG:O	1:A:188:VAL:HG23	2.21	0.41
1:A:904:ASP:O	1:A:993:PHE:HB3	2.21	0.40
1:A:497:PHE:HE1	1:A:501:LYS:HE3	1.87	0.40
1:A:287:ILE:HA	1:A:287:ILE:HD12	1.91	0.40
1:A:932:CYS:O	1:A:936:CYS:SG	2.66	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.88	0.40
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.61	0.40
1:A:185:MET:HE2	1:A:321:GLU:HG3	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:704:ALA:HB1	1:A:873:GLY:HA2	2.03	0.40
1:A:845:LEU:HD23	1:A:845:LEU:HA	1.96	0.40
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.57	0.40
1:A:707:ARG:NH1	1:A:707:ARG:H	2.20	0.40
1:A:827:THR:OG1	1:A:883:LYS:NZ	2.54	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	824/966 (85%)	713 (86%)	95 (12%)	16 (2%)	12	36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	859	SER
1	A	921	PHE
1	A	1000	LYS
1	A	1014	VAL
1	A	797	ALA
1	A	904	ASP
1	A	964	ASP
1	A	999	GLY
1	A	1013	CYS
1	A	1077	ASP
1	A	1061	GLU
1	A	165	VAL
1	A	217	ASN
1	A	1079	GLY
1	A	548	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	694/862 (80%)	631 (91%)	63 (9%)	14	36

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	147	SER
1	A	150	PHE
1	A	168	VAL
1	A	192	ASP
1	A	203	THR
1	A	207	LEU
1	A	208	PRO
1	A	214	LYS
1	A	217	ASN
1	A	219	CYS
1	A	246	GLN
1	A	319	ARG
1	A	370	ILE
1	A	372	VAL
1	A	379	LEU
1	A	387	ILE
1	A	395	CYS
1	A	417	SER
1	A	418	ILE
1	A	464	VAL
1	A	475	LEU
1	A	497	PHE
1	A	501	LYS
1	A	512	ASN
1	A	516	ILE
1	A	522	ASN
1	A	547	MET
1	A	614	ARG
1	A	615	GLU
1	A	616	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	628	MET
1	A	636	SER
1	A	688	ASN
1	A	701	SER
1	A	707	ARG
1	A	729	LEU
1	A	733	THR
1	A	742	LEU
1	A	743	GLN
1	A	748	ASP
1	A	753	SER
1	A	758	ASP
1	A	763	VAL
1	A	775	GLN
1	A	779	LEU
1	A	784	ARG
1	A	796	LEU
1	A	799	GLU
1	A	832	PHE
1	A	861	ASP
1	A	871	SER
1	A	887	THR
1	A	893	GLN
1	A	899	THR
1	A	908	ASN
1	A	922	GLN
1	A	960	LEU
1	A	1045	LYS
1	A	1051	ILE
1	A	1061	GLU
1	A	1072	ILE
1	A	1091	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	HIS
1	A	391	GLN
1	A	471	HIS
1	A	512	ASN
1	A	554	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	585	HIS
1	A	601	GLN
1	A	705	GLN
1	A	734	GLN
1	A	775	GLN
1	A	840	GLN
1	A	893	GLN
1	A	922	GLN
1	A	1007	GLN
1	A	1023	HIS
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 ⓘ

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.11	0
3	BMW	A	1103	-	36,36,36	1.72	4 (11%)	52,52,52	2.20	13 (25%)
2	SO4	A	2	-	4,4,4	0.13	0	6,6,6	0.19	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
2	SO4	A	1	-	-	0/0/0/0	0/0/0/0
3	BMW	A	1103	-	-	0/12/29/29	0/2/6/6
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	BMW	C26-C25	-7.53	1.40	1.48
3	A	1103	BMW	C10-N11	-3.66	1.33	1.42
3	A	1103	BMW	C14-C15	-3.00	1.40	1.46
3	A	1103	BMW	C15-N11	-2.79	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	BMW	C14-C15-N16	-7.44	117.71	127.23
3	A	1103	BMW	N16-C15-N11	6.31	133.10	126.14
3	A	1103	BMW	N16-C17-N18	4.79	122.56	117.11
3	A	1103	BMW	C25-N24-C17	4.53	121.81	115.92
3	A	1103	BMW	C14-C25-N24	-3.81	117.93	122.89
3	A	1103	BMW	O21-C22-C23	-3.52	103.55	111.89
3	A	1103	BMW	C23-N18-C19	3.15	118.15	111.67
3	A	1103	BMW	N24-C17-N16	-3.00	121.11	126.28
3	A	1103	BMW	C17-N16-C15	2.91	120.88	114.89
3	A	1103	BMW	C25-C14-C15	2.85	120.55	115.68
3	A	1103	BMW	C26-C25-N24	2.65	118.85	115.42
3	A	1103	BMW	C12-N11-C15	2.62	112.32	109.36
3	A	1103	BMW	C2-C7-N6	2.04	107.63	106.01

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, 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	840/966 (86%)	0.13	34 (4%) 36 37	24, 64, 109, 126	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	SER	7.1
1	A	376	ASN	6.7
1	A	222	ILE	5.2
1	A	221	PHE	5.2
1	A	241	PRO	5.0
1	A	267	GLU	4.7
1	A	970	GLY	4.1
1	A	374	PRO	3.9
1	A	377	THR	3.9
1	A	823	LEU	3.4
1	A	287	ILE	3.4
1	A	271	VAL	3.3
1	A	281	LEU	3.2
1	A	252	MET	3.1
1	A	270	PHE	3.1
1	A	242	GLY	2.9
1	A	564	LEU	2.9
1	A	231	GLN	2.8
1	A	248	PHE	2.8
1	A	272	LEU	2.8
1	A	220	ILE	2.8
1	A	234	LYS	2.7
1	A	895	THR	2.6
1	A	202	VAL	2.4
1	A	969	LEU	2.3
1	A	522	ASN	2.3
1	A	378	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	303	ILE	2.2
1	A	993	PHE	2.2
1	A	210	TYR	2.2
1	A	753	SER	2.1
1	A	144	SER	2.0
1	A	233	ILE	2.0
1	A	404	PHE	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
3	BMW	A	1103	31/31	0.19	-0.21	53,70,87,90	0
2	SO4	A	1	5/5	0.19	-0.42	98,101,104,108	0
2	SO4	A	2	5/5	0.17	-0.84	94,103,106,106	0

6.5 Other polymers ⓘ

There are no such residues in this entry.