Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:43 PM GMT

PDB ID	:	4PS3
Title	:	Structure of PI3K gamma in complex with 1-[6-(5-methoxypyridin-3-yl)-1,3-benzothiazol-2-yl]-3-[2-(1-propyl-1H-imidazol-4-yl)ethyl]urea
Authors	:	Griffith, J.P.
Deposited on	:	2014-03-06
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

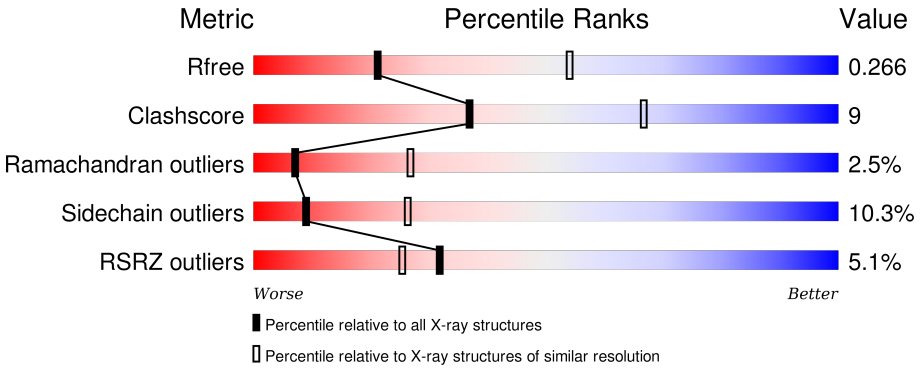
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	966	4% 62% 21% • 13%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6881 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.

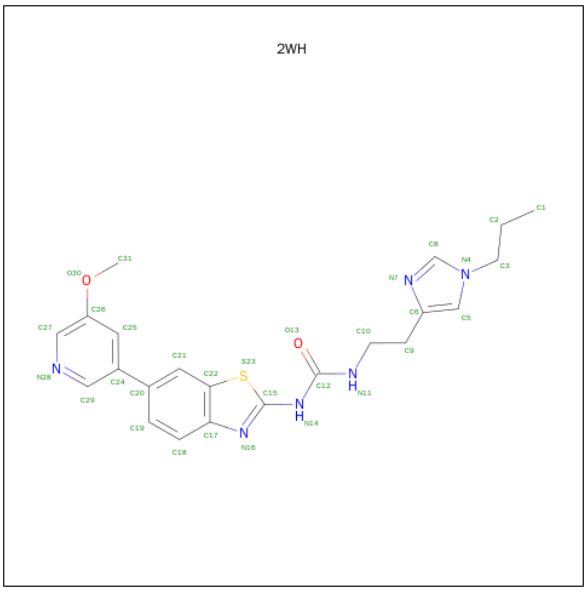
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	843	6844	4395	1170	1244	35	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	MET	-	INITIATING METHIONINE	UNP P48736
A	459	ARG	GLN	CONFLICT	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 1-[6-(5-METHOXYPYRIDIN-3-YL)-1,3-BENZOTHIAZOL-2-YL]-3-[2-(1-PROPYL-1H-IMIDAZOL-4-YL)ETHYL]UREA (three-letter code: 2WH) (formula: $C_{22}H_{24}N_6O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	22	6	2	1		

- Molecule 3 is water.

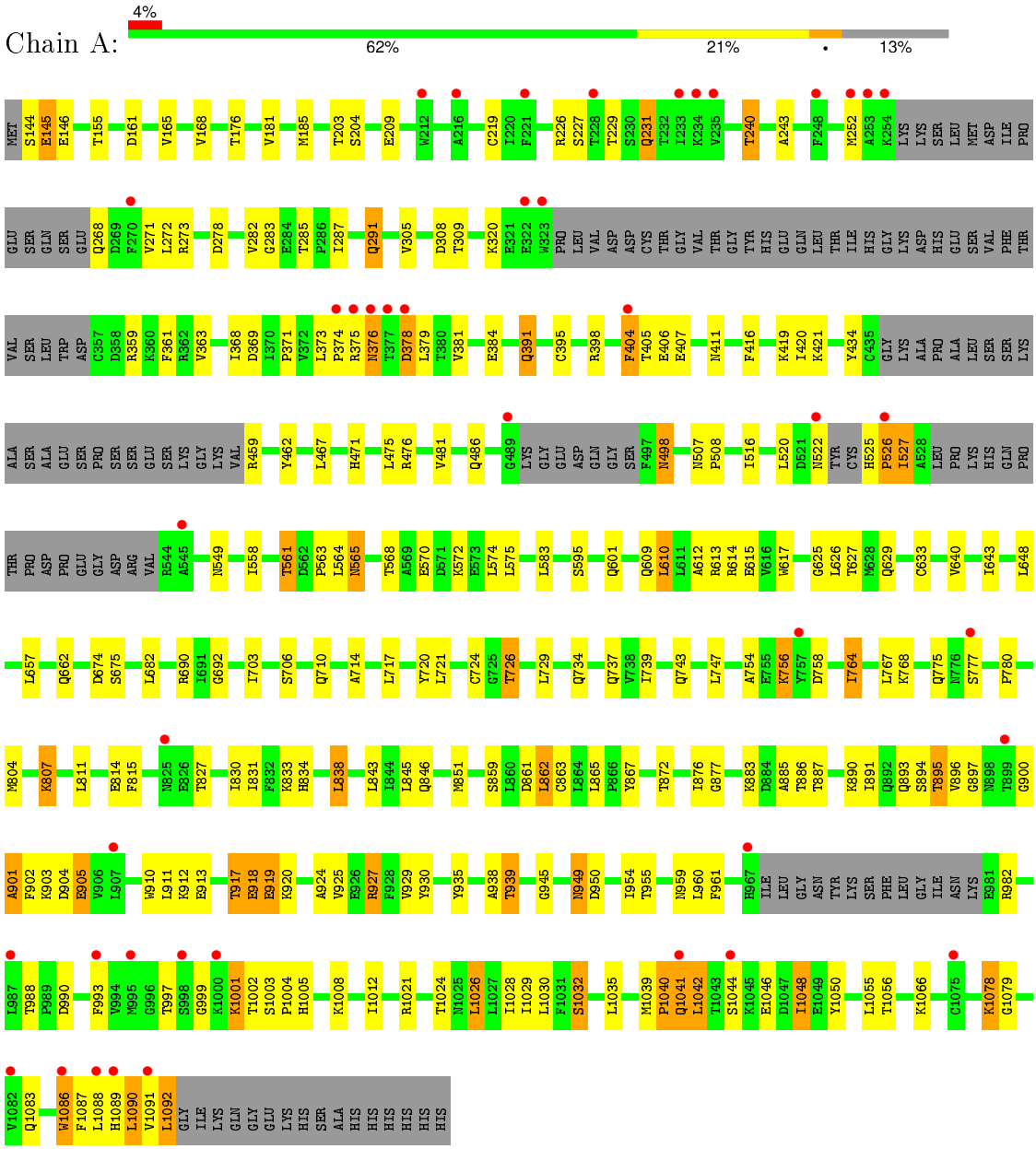
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	O	0	0
			6	6		

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 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-bisphosphate 3-kinase catalytic subunit gamma isoform

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.69Å 67.79Å 106.12Å 90.00° 96.16° 90.00°	Depositor
Resolution (Å)	105.51 – 2.90 40.91 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (105.51-2.90) 99.8 (40.91-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.39 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.211 , 0.259 0.224 , 0.266	Depositor DCC
R_{free} test set	1164 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 69.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 22751 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6881	wwPDB-VP
Average B, all atoms (Å^2)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2WH

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	0.63	4/6992 (0.1%)	0.79	0/9457

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	ASP	CB-CG	9.67	1.72	1.51
1	A	1078	LYS	C-O	7.38	1.37	1.23
1	A	918	GLU	CG-CD	6.33	1.61	1.51
1	A	1086	TRP	CB-CG	5.29	1.59	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6844	0	6886	129	0
2	A	31	0	24	8	0
3	A	6	0	0	3	0
All	All	6881	0	6910	130	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 9.

All (130) 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:893:GLN:HA	1:A:897:GLY:HA2	1.35	1.03
1:A:851:MET:HE1	1:A:938:ALA:HA	1.62	0.80
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.64	0.79
1:A:893:GLN:HA	1:A:897:GLY:CA	2.16	0.74
1:A:883:LYS:NZ	2:A:1201:2WH:H4	2.03	0.73
1:A:935:TYR:O	1:A:939:THR:HB	1.90	0.71
1:A:525:HIS:HB2	1:A:526:PRO:HD3	1.73	0.69
1:A:883:LYS:HZ3	2:A:1201:2WH:H4	1.56	0.67
1:A:1086:TRP:CE3	1:A:1087:PHE:HA	2.30	0.66
1:A:867:TYR:OH	3:A:1302:HOH:O	2.13	0.66
1:A:1041:GLN:HA	1:A:1041:GLN:HE21	1.61	0.64
1:A:1035:LEU:HA	1:A:1039:MET:HG2	1.80	0.63
1:A:583:LEU:HD22	1:A:610:LEU:HD22	1.81	0.63
1:A:919:GLU:OE2	1:A:920:LYS:N	2.33	0.62
1:A:949:ASN:H	1:A:1083:GLN:HE22	1.46	0.62
1:A:525:HIS:CB	1:A:526:PRO:HD3	2.32	0.58
1:A:918:GLU:OE1	1:A:918:GLU:O	2.22	0.58
1:A:893:GLN:CA	1:A:897:GLY:HA2	2.24	0.57
1:A:925:VAL:O	1:A:929:VAL:HG23	2.05	0.57
1:A:1021:ARG:O	1:A:1024:THR:OG1	2.17	0.56
1:A:1086:TRP:CH2	1:A:1090:LEU:HD21	2.41	0.55
1:A:863:CYS:SG	1:A:927:ARG:NH1	2.80	0.55
1:A:814:GLU:OE2	2:A:1201:2WH:H7	2.05	0.55
1:A:381:VAL:HG21	1:A:404:PHE:CD2	2.42	0.54
1:A:291:GLN:HA	1:A:291:GLN:HE21	1.72	0.54
1:A:308:ASP:OD1	1:A:308:ASP:N	2.41	0.54
1:A:807:LYS:NZ	3:A:1305:HOH:O	2.41	0.54
1:A:614:ARG:HG2	1:A:617:TRP:HB3	1.89	0.54
1:A:405:THR:O	1:A:407:GLU:N	2.41	0.53
1:A:1024:THR:HG22	1:A:1028:ILE:HD12	1.89	0.53
1:A:905:GLU:HG3	1:A:993:PHE:CE2	2.44	0.53
1:A:743:GLN:O	1:A:747:LEU:HD12	2.09	0.53
1:A:726:THR:HA	1:A:729:LEU:HD12	1.91	0.52
1:A:1005:HIS:O	1:A:1008:LYS:HB3	2.09	0.52
1:A:583:LEU:HD22	1:A:610:LEU:CD2	2.39	0.52
1:A:827:THR:O	1:A:883:LYS:NZ	2.43	0.52
1:A:271:VAL:HG23	1:A:282:VAL:CG1	2.40	0.52
1:A:997:THR:HG23	1:A:1001:LYS:HG3	1.91	0.52
1:A:434:TYR:HA	1:A:459:ARG:O	2.10	0.51
1:A:764:ILE:O	1:A:768:LYS:HG2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:GLN:OE1	1:A:633:CYS:HB2	2.10	0.51
1:A:1089:HIS:C	1:A:1091:VAL:N	2.63	0.51
1:A:378:ASP:OD1	1:A:378:ASP:N	2.44	0.51
1:A:692:GLY:HA3	1:A:720:TYR:OH	2.10	0.51
1:A:240:THR:HG22	1:A:243:ALA:H	1.76	0.50
1:A:181:VAL:O	1:A:185:MET:HG3	2.11	0.50
1:A:363:VAL:HG13	1:A:363:VAL:O	2.11	0.50
1:A:272:LEU:HB3	1:A:305:VAL:HG11	1.94	0.50
1:A:814:GLU:OE2	2:A:1201:2WH:C3	2.60	0.49
1:A:231:GLN:HA	1:A:231:GLN:HE21	1.77	0.49
1:A:1086:TRP:CZ3	1:A:1090:LEU:HD21	2.47	0.49
1:A:384:GLU:OE2	1:A:398:ARG:NH1	2.46	0.49
1:A:1026:LEU:O	1:A:1030:LEU:HG	2.13	0.49
1:A:498:ASN:C	1:A:498:ASN:OD1	2.50	0.49
2:A:1201:2WH:S23	2:A:1201:2WH:O13	2.70	0.49
1:A:887:THR:CG2	1:A:950:ASP:HA	2.44	0.48
1:A:475:LEU:HD21	1:A:522:ASN:HB2	1.95	0.48
1:A:883:LYS:NZ	2:A:1201:2WH:C2	2.75	0.48
1:A:861:ASP:C	1:A:862:LEU:HD22	2.34	0.48
1:A:939:THR:HG23	1:A:945:GLY:CA	2.44	0.48
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.95	0.48
1:A:885:ALA:H	2:A:1201:2WH:H10	1.79	0.47
1:A:935:TYR:CE2	1:A:961:PHE:HA	2.50	0.47
1:A:911:LEU:HD22	1:A:924:ALA:HB1	1.96	0.47
1:A:558:ILE:O	1:A:561:THR:HB	2.13	0.47
1:A:614:ARG:O	1:A:615:GLU:C	2.52	0.47
1:A:703:ILE:HD11	1:A:714:ALA:HA	1.96	0.47
1:A:734:GLN:NE2	1:A:780:PRO:HB3	2.30	0.47
1:A:988:THR:OG1	1:A:990:ASP:OD1	2.30	0.47
1:A:395:CYS:HG	1:A:416:PHE:HD1	1.62	0.47
1:A:1021:ARG:HE	1:A:1056:THR:HG22	1.79	0.47
1:A:565:ASN:C	1:A:565:ASN:ND2	2.69	0.47
1:A:901:ALA:O	1:A:902:PHE:CG	2.68	0.46
1:A:361:PHE:HB2	1:A:420:ILE:HD13	1.97	0.46
1:A:939:THR:HG23	1:A:945:GLY:HA2	1.96	0.46
1:A:706:SER:O	1:A:710:GLN:HB3	2.16	0.46
1:A:609:GLN:O	1:A:612:ALA:HB3	2.16	0.46
1:A:1055:LEU:O	1:A:1056:THR:HG22	2.16	0.46
1:A:917:THR:OG1	1:A:919:GLU:OE2	2.34	0.46
1:A:1042:LEU:O	1:A:1042:LEU:HD22	2.16	0.46
1:A:1092:LEU:O	1:A:1092:LEU:HD13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:838:LEU:HD23	1:A:877:GLY:HA3	1.97	0.45
1:A:411:ASN:O	1:A:411:ASN:ND2	2.50	0.45
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.88	0.45
1:A:421:LYS:HE3	1:A:527:ILE:HD12	1.98	0.45
1:A:954:ILE:HA	1:A:960:LEU:HA	1.98	0.45
1:A:674:ASP:C	1:A:674:ASP:OD1	2.55	0.45
1:A:155:THR:HG23	1:A:161:ASP:HA	1.99	0.45
1:A:930:TYR:CE2	1:A:1012:ILE:HD13	2.52	0.44
1:A:883:LYS:HD3	2:A:1201:2WH:H4	1.99	0.44
1:A:568:THR:HG22	1:A:570:GLU:H	1.82	0.44
1:A:507:ASN:HA	1:A:508:PRO:HD2	1.86	0.44
1:A:756:LYS:O	1:A:758:ASP:O	2.36	0.44
1:A:419:LYS:O	1:A:420:ILE:C	2.56	0.44
1:A:891:ILE:HG12	1:A:910:TRP:CD1	2.53	0.44
1:A:368:ILE:HG22	1:A:516:ILE:HB	1.99	0.44
1:A:1089:HIS:O	1:A:1091:VAL:N	2.51	0.44
1:A:572:LYS:HD3	1:A:595:SER:HA	1.99	0.44
1:A:165:VAL:HG12	1:A:165:VAL:O	2.18	0.44
1:A:955:THR:OG1	1:A:959:ASN:N	2.41	0.43
1:A:283:GLY:O	1:A:285:THR:N	2.50	0.43
1:A:862:LEU:N	1:A:862:LEU:CD2	2.81	0.43
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.19	0.43
1:A:481:VAL:O	1:A:481:VAL:HG12	2.17	0.43
1:A:811:LEU:O	1:A:831:ILE:HA	2.18	0.43
1:A:627:THR:HG21	1:A:648:LEU:CD2	2.48	0.43
1:A:657:LEU:HD11	1:A:690:ARG:HD3	2.01	0.43
1:A:144:SER:OG	1:A:145:GLU:N	2.50	0.43
1:A:756:LYS:NZ	1:A:756:LYS:HA	2.34	0.42
1:A:894:SER:OG	1:A:895:THR:N	2.52	0.42
1:A:625:GLY:O	1:A:629:GLN:HG3	2.18	0.42
1:A:1003:SER:HB2	1:A:1004:PRO:HD2	2.00	0.42
1:A:1039:MET:HB3	1:A:1040:PRO:HD2	2.01	0.42
1:A:834:HIS:HB2	1:A:876:ILE:HD12	2.01	0.42
1:A:851:MET:HE1	1:A:938:ALA:CA	2.39	0.42
1:A:462:TYR:CD1	1:A:486:GLN:HA	2.53	0.42
1:A:640:VAL:O	1:A:643:ILE:HG12	2.20	0.42
1:A:721:LEU:HA	1:A:724:CYS:SG	2.60	0.42
1:A:734:GLN:HE22	1:A:780:PRO:HB3	1.85	0.41
1:A:949:ASN:H	1:A:1083:GLN:NE2	2.17	0.41
1:A:833:LYS:CE	3:A:1304:HOH:O	2.69	0.41
1:A:563:PRO:HD2	1:A:1028:ILE:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:SER:HB2	1:A:1048:ILE:HG21	2.02	0.41
1:A:527:ILE:HD11	1:A:601:GLN:OE1	2.21	0.41
1:A:815:PHE:CE1	1:A:830:ILE:HD12	2.56	0.41
1:A:918:GLU:O	1:A:918:GLU:CD	2.59	0.41
1:A:273:ARG:O	1:A:305:VAL:HG13	2.20	0.41
1:A:467:LEU:O	1:A:476:ARG:NH1	2.54	0.40
1:A:614:ARG:NH1	1:A:643:ILE:HG22	2.36	0.40
1:A:209:GLU:HB2	1:A:859:SER:HB3	2.03	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	827/966 (86%)	737 (89%)	69 (8%)	21 (2%)	7 27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	374	PRO
1	A	406	GLU
1	A	527	ILE
1	A	754	ALA
1	A	949	ASN
1	A	376	ASN
1	A	471	HIS
1	A	726	THR
1	A	756	LYS
1	A	1090	LEU
1	A	900	GLY
1	A	1040	PRO

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Mol	Chain	Res	Type
1	A	371	PRO
1	A	901	ALA
1	A	999	GLY
1	A	391	GLN
1	A	252	MET
1	A	526	PRO
1	A	777	SER
1	A	1079	GLY

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	757/864 (88%)	679 (90%)	78 (10%)	9 26

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	GLU
1	A	146	GLU
1	A	168	VAL
1	A	203	THR
1	A	204	SER
1	A	219	CYS
1	A	226	ARG
1	A	229	THR
1	A	231	GLN
1	A	240	THR
1	A	268	GLN
1	A	278	ASP
1	A	287	ILE
1	A	291	GLN
1	A	309	THR
1	A	320	LYS
1	A	359	ARG
1	A	369	ASP

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Mol	Chain	Res	Type
1	A	373	LEU
1	A	375	ARG
1	A	376	ASN
1	A	378	ASP
1	A	379	LEU
1	A	404	PHE
1	A	498	ASN
1	A	520	LEU
1	A	549	ASN
1	A	561	THR
1	A	565	ASN
1	A	574	LEU
1	A	575	LEU
1	A	610	LEU
1	A	613	ARG
1	A	626	LEU
1	A	662	GLN
1	A	675	SER
1	A	682	LEU
1	A	717	LEU
1	A	737	GLN
1	A	739	ILE
1	A	764	ILE
1	A	767	LEU
1	A	775	GLN
1	A	804	MET
1	A	807	LYS
1	A	838	LEU
1	A	843	LEU
1	A	845	LEU
1	A	846	GLN
1	A	862	LEU
1	A	865	LEU
1	A	886	THR
1	A	890	LYS
1	A	895	THR
1	A	896	VAL
1	A	903	LYS
1	A	905	GLU
1	A	912	LYS
1	A	913	GLU
1	A	917	THR

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Mol	Chain	Res	Type
1	A	919	GLU
1	A	927	ARG
1	A	939	THR
1	A	982	ARG
1	A	1001	LYS
1	A	1002	THR
1	A	1026	LEU
1	A	1029	ILE
1	A	1032	SER
1	A	1041	GLN
1	A	1042	LEU
1	A	1044	SER
1	A	1046	GLU
1	A	1048	ILE
1	A	1066	LYS
1	A	1078	LYS
1	A	1088	LEU
1	A	1092	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	GLN
1	A	153	GLN
1	A	218	ASN
1	A	225	HIS
1	A	231	GLN
1	A	291	GLN
1	A	295	HIS
1	A	304	HIS
1	A	411	ASN
1	A	565	ASN
1	A	730	HIS
1	A	734	GLN
1	A	743	GLN
1	A	766	GLN
1	A	773	ASN
1	A	776	ASN
1	A	825	ASN
1	A	1007	GLN
1	A	1041	GLN
1	A	1083	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no 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	2WH	A	1201	-	29,34,34	0.82	0	33,46,46	1.97	10 (30%)

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	2WH	A	1201	-	-	0/16/19/19	0/4/4/4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	2WH	C15-N14-C12	-6.95	121.63	130.13
2	A	1201	2WH	C26-C27-N28	-3.66	119.67	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	2WH	C9-C10-N11	-2.81	105.11	111.97
2	A	1201	2WH	C9-C6-C5	-2.63	125.48	129.55
2	A	1201	2WH	C6-C5-N4	-2.36	105.06	107.75
2	A	1201	2WH	C19-C18-C17	-2.28	118.41	120.88
2	A	1201	2WH	O13-C12-N11	-2.05	118.95	122.75
2	A	1201	2WH	C22-C17-N16	2.00	112.80	108.16
2	A	1201	2WH	N14-C12-N11	2.80	118.55	114.00
2	A	1201	2WH	C29-N28-C27	3.37	122.58	117.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	2WH	8	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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^{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	843/966 (87%)	0.20	43 (5%) 32 25	31, 75, 135, 176	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	LYS	7.1
1	A	1044	SER	7.0
1	A	1088	LEU	6.6
1	A	375	ARG	6.1
1	A	323	TRP	5.6
1	A	899	THR	5.4
1	A	377	THR	5.4
1	A	322	GLU	4.9
1	A	374	PRO	4.9
1	A	376	ASN	4.7
1	A	1089	HIS	4.5
1	A	1091	VAL	3.9
1	A	1086	TRP	3.8
1	A	489	GLY	3.6
1	A	995	MET	3.6
1	A	234	LYS	3.6
1	A	993	PHE	3.3
1	A	270	PHE	3.3
1	A	378	ASP	3.2
1	A	1075	CYS	3.0
1	A	404	PHE	2.9
1	A	216	ALA	2.8
1	A	998	SER	2.7
1	A	757	TYR	2.7
1	A	235	VAL	2.6
1	A	1082	VAL	2.6
1	A	253	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	221	PHE	2.6
1	A	522	ASN	2.5
1	A	545	ALA	2.5
1	A	1041	GLN	2.5
1	A	1000	LYS	2.4
1	A	987	LEU	2.4
1	A	967	HIS	2.4
1	A	526	PRO	2.4
1	A	233	ILE	2.4
1	A	212	TRP	2.4
1	A	228	THR	2.4
1	A	248	PHE	2.4
1	A	252	MET	2.3
1	A	777	SER	2.2
1	A	907	LEU	2.0
1	A	825	ASN	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. 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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	2WH	A	1201	31/31	0.96	0.18	-0.35	50,60,74,77	0

6.5 Other polymers (i)

There are no such residues in this entry.