Full wwPDB X-ray Structure Validation Report (i)

Feb 9, 2017 – 10:32 AM EST

PDB ID	:	5SWP
Title	:	Crystal Structure of PI3Kalpha in complex with fragments 6 and 24
Authors	:	Gabelli, S.B.; Vogelstein, B.; Miller, M.S.; Amzel, L.M.
Deposited on	:	2016-08-08
Resolution	:	3.41 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:

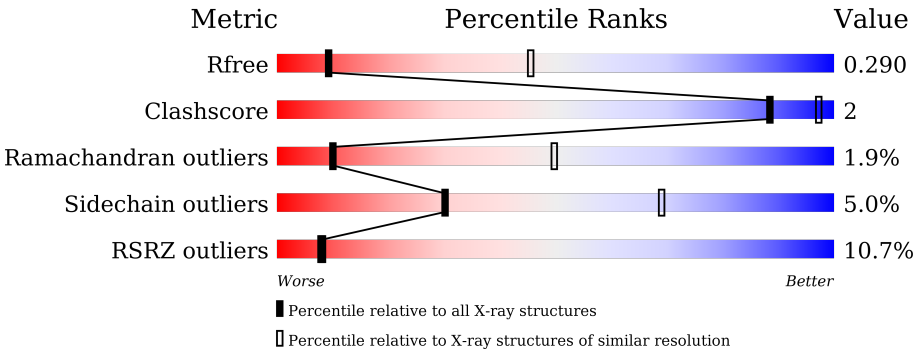
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 3.41 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	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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	1096	7% 85% 11%
2	B	279	22% 79% 13% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	70W	A	1101	-	-	-	X
3	70W	A	1102	-	-	-	X
4	70V	B	701	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10919 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 alpha isoform.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	1060	8667	5532	1485	1578	2	70	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	initiating methionine	UNP P42336
A	-26	SER	-	expression tag	UNP P42336
A	-25	TYR	-	expression tag	UNP P42336
A	-24	TYR	-	expression tag	UNP P42336
A	-23	HIS	-	expression tag	UNP P42336
A	-22	HIS	-	expression tag	UNP P42336
A	-21	HIS	-	expression tag	UNP P42336
A	-20	HIS	-	expression tag	UNP P42336
A	-19	HIS	-	expression tag	UNP P42336
A	-18	HIS	-	expression tag	UNP P42336
A	-17	ASP	-	expression tag	UNP P42336
A	-16	TYR	-	expression tag	UNP P42336
A	-15	ASP	-	expression tag	UNP P42336
A	-14	ILE	-	expression tag	UNP P42336
A	-13	PRO	-	expression tag	UNP P42336
A	-12	THR	-	expression tag	UNP P42336
A	-11	THR	-	expression tag	UNP P42336
A	-10	GLU	-	expression tag	UNP P42336
A	-9	ASN	-	expression tag	UNP P42336
A	-8	LEU	-	expression tag	UNP P42336
A	-7	TYR	-	expression tag	UNP P42336
A	-6	PHE	-	expression tag	UNP P42336
A	-5	GLN	-	expression tag	UNP P42336
A	-4	GLY	-	expression tag	UNP P42336
A	-3	ALA	-	expression tag	UNP P42336
A	-2	MET	-	expression tag	UNP P42336

Continued on next page...

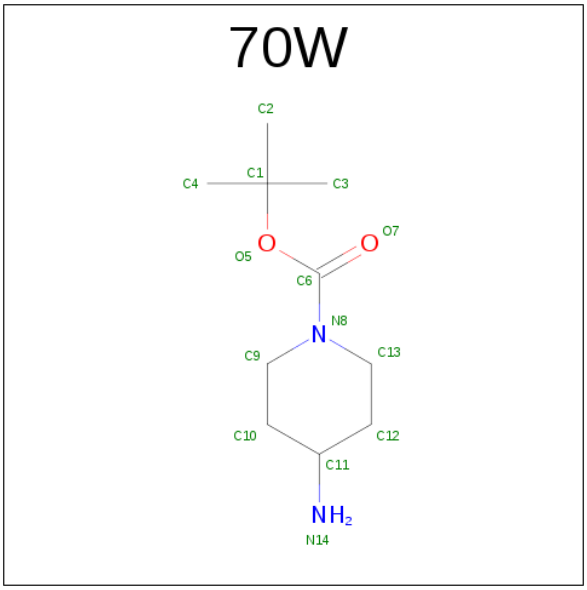
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P42336
A	0	SER	-	expression tag	UNP P42336

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

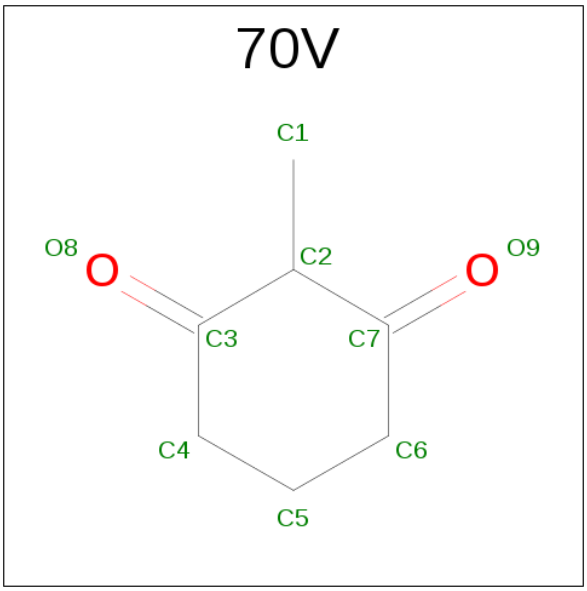
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2205	1383	396	420	6			

- Molecule 3 is tert-butyl 4-aminopiperidine-1-carboxylate (three-letter code: 70W) (formula: $C_{10}H_{20}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	10	2	2		
3	A	1	Total	C	N	O	0	0
			14	10	2	2		

- Molecule 4 is 2-methylcyclohexane-1,3-dione (three-letter code: 70V) (formula: $C_7H_{10}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 7 2	0	0
4	B	1	Total C O 9 7 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

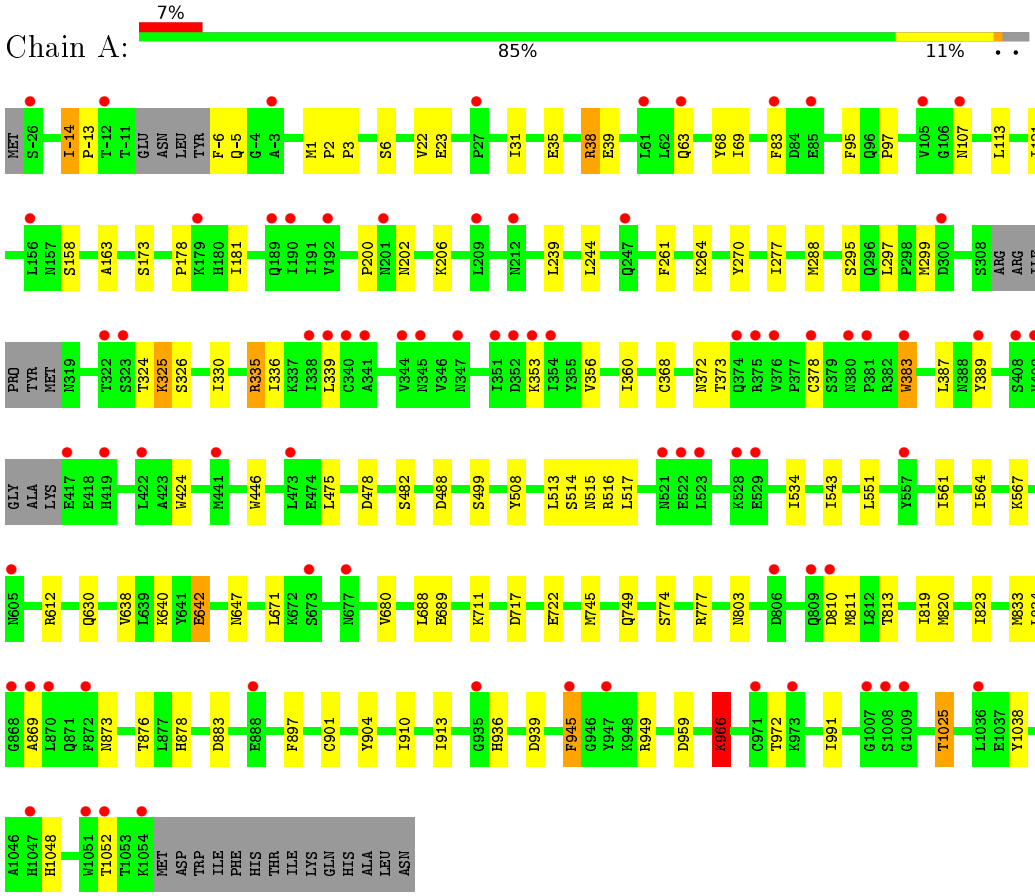
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

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.

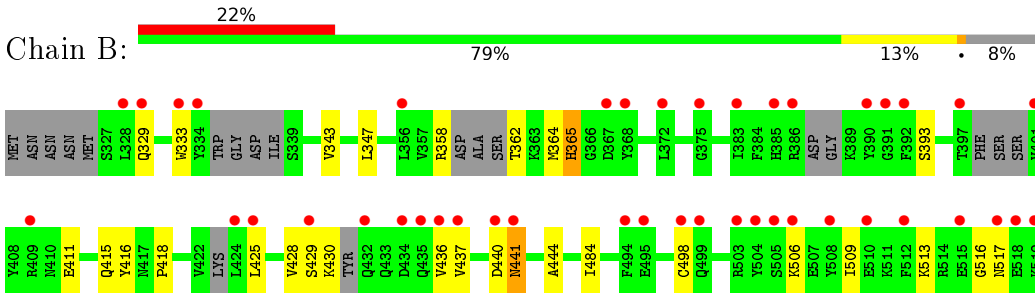
• Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform

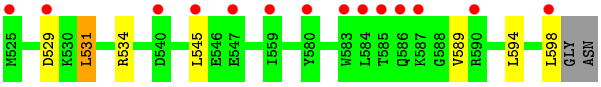
Chain A:



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha

Chain B:




M525
D529
K530
L531
R534
D540
L545
E546
E547
T559
Y580
W583
L584
T585
Q586
K587
G588
V589
R590
L594
L598
GLY
ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.12Å 116.13Å 148.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.41 48.86 – 3.41	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-3.41) 99.2 (48.86-3.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 3.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.216 , 0.296 0.216 , 0.290	Depositor DCC
R_{free} test set	1386 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	99.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 79.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10919	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 70V, 70W, CL, SEP

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	0.45	0/8847	0.69	0/11956
2	B	0.44	0/2235	0.66	0/2983
All	All	0.45	0/11082	0.69	0/14939

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	LYS	Peptide

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	8667	0	8627	43	0
2	B	2205	0	2198	14	0
3	A	28	0	0	0	0
4	A	9	0	0	0	0
4	B	9	0	0	0	0
5	A	1	0	0	0	0
All	All	10919	0	10825	54	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 2.

All (54) 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)
2:B:407:HIS:HE1	2:B:411:GLU:OE1	1.47	0.97
2:B:407:HIS:CE1	2:B:411:GLU:OE1	2.19	0.94
1:A:745:MET:SD	1:A:749:GLN:NE2	2.68	0.66
1:A:163:ALA:HB2	1:A:297:LEU:HD11	1.81	0.61
2:B:429:SER:O	2:B:430:LYS:C	2.43	0.57
2:B:333:TRP:HA	2:B:429:SER:HB2	1.86	0.56
1:A:31:ILE:HD11	2:B:531:LEU:HD13	1.87	0.56
1:A:372:ASN:HB3	1:A:387:LEU:HD21	1.88	0.56
1:A:339:LEU:O	1:A:383:TRP:O	2.26	0.54
1:A:325:LYS:HG2	1:A:330:ILE:HD11	1.90	0.53
1:A:602:LEU:O	1:A:612:ARG:NH2	2.41	0.53
1:A:640:LYS:HE2	1:A:680:VAL:HG11	1.91	0.53
1:A:261:PHE:HA	1:A:270:TYR:CE2	2.45	0.52
1:A:910:ILE:O	1:A:1025:THR:HG21	2.10	0.51
1:A:873:ASN:HB3	1:A:876:THR:HG23	1.93	0.51
1:A:945:PHE:CG	2:B:598:LEU:HB3	2.47	0.49
1:A:717:ASP:OD1	1:A:803:ASN:ND2	2.46	0.49
2:B:506:LYS:HA	2:B:509:ILE:HG22	1.96	0.48
2:B:362:THR:HG22	2:B:364:MET:N	2.29	0.47
1:A:819:ILE:HG22	1:A:823:ILE:HD12	1.96	0.47
2:B:516:GLY:O	2:B:520:GLU:N	2.48	0.47
1:A:534:ILE:HG21	1:A:551:LEU:HD11	1.97	0.46
1:A:774:SER:O	1:A:777:ARG:NH1	2.47	0.46
1:A:335:ARG:NE	1:A:478:ASP:OD2	2.48	0.45
1:A:864:GLY:O	1:A:876:THR:HG21	2.16	0.45
1:A:878:HIS:CE1	1:A:966:LYS:O	2.70	0.45
1:A:1038:TYR:O	1:A:1042:GLN:HG2	2.17	0.45
1:A:-14:ILE:HD13	1:A:-13:PRO:HD3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:TRP:CE2	1:A:446:TRP:HB2	2.51	0.45
1:A:878:HIS:NE2	1:A:966:LYS:O	2.49	0.45
1:A:63:GLN:HB2	1:A:68:TYR:CE2	2.51	0.45
1:A:23:GLU:OE1	2:B:534:ARG:NE	2.48	0.44
1:A:121:ILE:HD11	1:A:689:GLU:HA	2.00	0.44
1:A:939:ASP:OD1	1:A:949:ARG:NH2	2.51	0.43
1:A:897:PHE:O	1:A:901:CYS:HB2	2.18	0.43
1:A:336:ILE:HD12	1:A:389:TYR:CE1	2.53	0.43
1:A:181:ILE:HG23	1:A:277:ILE:HG21	1.99	0.43
1:A:561:ILE:O	1:A:564:ILE:HG22	2.18	0.43
2:B:343:VAL:HG12	2:B:347:LEU:HD12	2.01	0.43
1:A:642:GLU:HG2	1:A:647:ASN:CG	2.38	0.43
1:A:810:ASP:HA	1:A:813:THR:HG22	2.01	0.43
1:A:833:MET:HE1	1:A:904:TYR:HA	2.01	0.43
2:B:484:ILE:HG13	2:B:545:LEU:HD23	2.01	0.42
1:A:22:VAL:HG12	1:A:97:PRO:HB2	2.01	0.42
1:A:820:MET:HG2	1:A:991:ILE:HD12	2.03	0.41
1:A:69:ILE:HD11	1:A:83:PHE:HA	2.03	0.41
1:A:356:VAL:HG23	1:A:383:TRP:CH2	2.55	0.41
1:A:360:ILE:N	1:A:360:ILE:HD12	2.36	0.41
1:A:671:LEU:HB2	1:A:688:LEU:HD21	2.03	0.40
1:A:178:PRO:HD2	1:A:181:ILE:HD12	2.02	0.40
2:B:362:THR:HG22	2:B:364:MET:H	1.86	0.40
2:B:441:ASN:HB3	2:B:444:ALA:HB3	2.03	0.40
1:A:1044:ASN:O	1:A:1048:HIS:N	2.53	0.40
1:A:543:ILE:HD11	1:A:567:LYS:HD3	2.04	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	1050/1096 (96%)	937 (89%)	95 (9%)	18 (2%)	11 52
2	B	244/279 (88%)	220 (90%)	17 (7%)	7 (3%)	6 41
All	All	1294/1375 (94%)	1157 (89%)	112 (9%)	25 (2%)	10 50

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	3	PRO
1	A	514	SER
2	B	365	HIS
1	A	202	ASN
1	A	264	LYS
1	A	378	CYS
1	A	869	ALA
1	A	945	PHE
1	A	966	LYS
1	A	972	THR
2	B	513	LYS
1	A	95	PHE
1	A	517	LEU
1	A	508	TYR
2	B	393	SER
1	A	959	ASP
1	A	1052	THR
2	B	418	PRO
1	A	38	ARG
1	A	913	ILE
2	B	589	VAL
2	B	436	VAL
2	B	428	VAL
1	A	200	PRO

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	966/997 (97%)	919 (95%)	47 (5%)	31 70
2	B	242/259 (93%)	228 (94%)	14 (6%)	25 65
All	All	1208/1256 (96%)	1147 (95%)	61 (5%)	30 69

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-14	ILE
1	A	-6	PHE
1	A	-5	GLN
1	A	1	MET
1	A	6	SER
1	A	35	GLU
1	A	38	ARG
1	A	39	GLU
1	A	107	ASN
1	A	113	LEU
1	A	138	ASP
1	A	148	LYS
1	A	158	SER
1	A	173	SER
1	A	206	LYS
1	A	239	LEU
1	A	244	LEU
1	A	288	MET
1	A	295	SER
1	A	299	MET
1	A	324	THR
1	A	326	SER
1	A	335	ARG
1	A	353	LYS
1	A	368	CYS
1	A	373	THR
1	A	383	TRP
1	A	475	LEU
1	A	482	SER
1	A	488	ASP
1	A	499	SER
1	A	513	LEU
1	A	515	ASN
1	A	516	ARG
1	A	575	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	630	GLN
1	A	638	VAL
1	A	642	GLU
1	A	711	LYS
1	A	722	GLU
1	A	811	MET
1	A	834	LEU
1	A	883	ASP
1	A	936	HIS
1	A	966	LYS
1	A	1025	THR
1	A	1045	ASP
2	B	329	GLN
2	B	358	ARG
2	B	365	HIS
2	B	415	GLN
2	B	416	TYR
2	B	425	LEU
2	B	437	VAL
2	B	440	ASP
2	B	441	ASN
2	B	498	CYS
2	B	517	ASN
2	B	529	ASP
2	B	531	LEU
2	B	594	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	331	ASN
1	A	467	ASN
1	A	526	ASN
1	A	554	HIS
1	A	575	ASN
2	B	365	HIS
2	B	407	HIS
2	B	475	GLN
2	B	527	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	SEP	A	7	1	7,9,10	0.79	0	8,12,14	1.35	1 (12%)
1	SEP	A	790	1	7,9,10	0.68	0	8,12,14	2.21	1 (12%)

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
1	SEP	A	7	1	-	0/5/8/10	0/0/0/0
1	SEP	A	790	1	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	7	SEP	OG-CB-CA	-2.12	106.42	108.26
1	A	790	SEP	OG-CB-CA	5.08	112.69	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	70W	A	1101	-	14,14,14	2.29	1 (7%)	20,20,20	3.35	6 (30%)
3	70W	A	1102	-	14,14,14	2.16	2 (14%)	20,20,20	2.38	4 (20%)
4	70V	A	1103	-	9,9,9	0.66	0	9,12,12	1.79	3 (33%)
4	70V	B	701	-	9,9,9	0.54	0	9,12,12	1.78	2 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	70W	A	1101	-	-	0/9/19/19	0/1/1/1
3	70W	A	1102	-	-	0/9/19/19	1/1/1/1
4	70V	A	1103	-	-	0/0/14/14	0/1/1/1
4	70V	B	701	-	-	0/0/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	70W	O5-C1	-2.07	1.44	1.48
3	A	1102	70W	O5-C6	7.32	1.47	1.33
3	A	1101	70W	O5-C6	7.91	1.48	1.33

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	70W	O5-C6-O7	-5.06	117.83	126.21
3	A	1101	70W	C12-C11-C10	-5.01	104.74	110.27
3	A	1102	70W	O5-C6-O7	-4.35	119.02	126.21
4	A	1103	70V	O9-C7-C6	-2.04	119.21	122.13
3	A	1102	70W	C13-N8-C9	2.43	117.02	112.57
3	A	1101	70W	C10-C9-N8	2.64	114.84	110.99
4	A	1103	70V	C4-C3-C2	2.80	120.47	115.55
4	B	701	70V	C4-C3-C2	2.86	120.56	115.55
4	B	701	70V	C6-C7-C2	3.02	120.84	115.55
4	A	1103	70V	C6-C7-C2	3.14	121.06	115.55
3	A	1102	70W	C1-O5-C6	3.45	124.90	120.98
3	A	1101	70W	C13-N8-C9	3.96	119.81	112.57
3	A	1101	70W	C1-O5-C6	6.24	128.08	120.98
3	A	1102	70W	O5-C6-N8	8.04	118.77	110.91
3	A	1101	70W	O5-C6-N8	10.09	120.77	110.91

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	70W	C10-C11-C12-C13-C9-N8

No monomer is involved in short contacts.

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	1058/1096 (96%)	0.59	80 (7%) 17 16	56, 102, 166, 228	0
2	B	258/279 (92%)	1.19	61 (23%) 1 1	100, 154, 197, 223	0
All	All	1316/1375 (95%)	0.71	141 (10%) 8 8	56, 111, 184, 228	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	523	LEU	6.2
2	B	432	GLN	6.0
1	A	870	LEU	5.8
1	A	869	ALA	5.6
1	A	872	PHE	5.6
2	B	392	PHE	4.9
2	B	505	SER	4.8
1	A	353	LYS	4.8
1	A	-26	SER	4.7
1	A	351	ILE	4.6
1	A	947	TYR	4.5
1	A	522	GLU	4.5
1	A	409	VAL	4.5
2	B	391	GLY	4.4
1	A	408	SER	4.4
2	B	510	GLU	4.4
1	A	-3	ALA	4.4
1	A	323	SER	4.2
1	A	1054	LYS	4.2
1	A	354	ILE	4.2
1	A	557	TYR	4.2
1	A	322	THR	4.2
2	B	580	TYR	4.1
1	A	381	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	586	GLN	4.0
2	B	515	GLU	3.9
2	B	584	LEU	3.9
2	B	435	GLN	3.8
2	B	512	PHE	3.6
2	B	385	HIS	3.6
1	A	867	LYS	3.6
1	A	341	ALA	3.6
2	B	440	ASP	3.6
1	A	340	CYS	3.5
2	B	397	THR	3.5
1	A	374	GLN	3.5
1	A	201	ASN	3.5
2	B	587	LYS	3.5
1	A	189	GLN	3.4
1	A	1008	SER	3.4
2	B	498	CYS	3.4
2	B	504	TYR	3.4
2	B	508	TYR	3.4
1	A	1009	GLY	3.4
2	B	409	ARG	3.3
1	A	810	ASP	3.3
1	A	868	GLY	3.3
1	A	-12	THR	3.2
1	A	344	VAL	3.2
2	B	333	TRP	3.2
2	B	328	LEU	3.1
2	B	405	ILE	3.1
2	B	518	GLU	3.1
1	A	107	ASN	3.1
1	A	521	ASN	3.0
1	A	378	CYS	3.0
1	A	419	HIS	3.0
1	A	376	VAL	3.0
1	A	422	LEU	2.9
1	A	300	ASP	2.9
2	B	529	ASP	2.9
1	A	375	ARG	2.9
2	B	424	LEU	2.9
2	B	368	TYR	2.9
1	A	864	GLY	2.9
2	B	522	GLN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	156	LEU	2.8
2	B	390	TYR	2.8
2	B	503	ARG	2.8
2	B	519	LYS	2.8
1	A	347	ASN	2.8
2	B	437	VAL	2.7
1	A	190	ILE	2.7
1	A	247	GLN	2.7
1	A	338	ILE	2.7
1	A	809	GLN	2.6
1	A	806	ASP	2.6
1	A	61	LEU	2.6
2	B	372	LEU	2.6
1	A	971	CYS	2.5
1	A	383	TRP	2.5
2	B	434	ASP	2.5
2	B	590	ARG	2.5
2	B	429	SER	2.5
2	B	401	VAL	2.5
1	A	1052	THR	2.5
2	B	441	ASN	2.5
2	B	583	TRP	2.5
1	A	345	ASN	2.5
2	B	425	LEU	2.5
2	B	383	ILE	2.4
2	B	329	GLN	2.4
1	A	352	ASP	2.4
2	B	334	TYR	2.4
2	B	598	LEU	2.4
1	A	1036	LEU	2.4
1	A	105	VAL	2.4
2	B	375	GLY	2.4
2	B	494	PHE	2.4
2	B	525	MET	2.4
2	B	559	ILE	2.3
1	A	85	GLU	2.3
2	B	545	LEU	2.3
1	A	83	PHE	2.3
1	A	417	GLU	2.3
2	B	547	GLU	2.3
1	A	209	LEU	2.3
1	A	441	MET	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	179	LYS	2.3
2	B	356	LEU	2.3
1	A	605	ASN	2.3
2	B	436	VAL	2.3
1	A	677	ASN	2.3
2	B	367	ASP	2.3
1	A	673	SER	2.3
1	A	945	PHE	2.2
1	A	888	GLU	2.2
2	B	540	ASP	2.2
1	A	380	ASN	2.2
1	A	1051	TRP	2.2
1	A	935	GLY	2.2
1	A	473	LEU	2.2
1	A	389	TYR	2.1
1	A	529	GLU	2.1
2	B	406	ASN	2.1
1	A	1047	HIS	2.1
1	A	973	LYS	2.1
2	B	386	ARG	2.1
2	B	506	LYS	2.1
1	A	212	ASN	2.1
1	A	1007	GLY	2.1
2	B	521	ILE	2.1
2	B	499	GLN	2.0
2	B	585	THR	2.0
1	A	27	PRO	2.0
1	A	63	GLN	2.0
1	A	192	VAL	2.0
1	A	528	LYS	2.0
2	B	495	GLU	2.0
1	A	339	LEU	2.0
2	B	517	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	A	790	10/11	0.93	0.16	-	92,107,153,159	0
1	SEP	A	7	10/11	0.54	0.34	-	139,178,197,201	0

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
4	70V	B	701	9/9	0.88	1.00	11.61	150,156,161,163	0
3	70W	A	1101	14/14	0.85	0.67	5.69	100,113,125,126	0
3	70W	A	1102	14/14	0.77	0.33	3.28	144,159,175,176	0
5	CL	A	1104	1/1	0.95	0.32	0.93	78,78,78,78	0
4	70V	A	1103	9/9	0.85	0.30	-	124,139,142,143	0

6.5 Other polymers (i)

There are no such residues in this entry.