Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:02 PM GMT

PDB ID	:	4WOT
Title	:	ROCK2 IN COMPLEX WITH 1426382-07-1
Authors	:	Augustin, M.; Krapp, S.; Boland, S.; Defert, O.; Bourin, A.; Alen, J.; Leysen, D.
Deposited on	:	2014-10-16
Resolution	:	2.93 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:

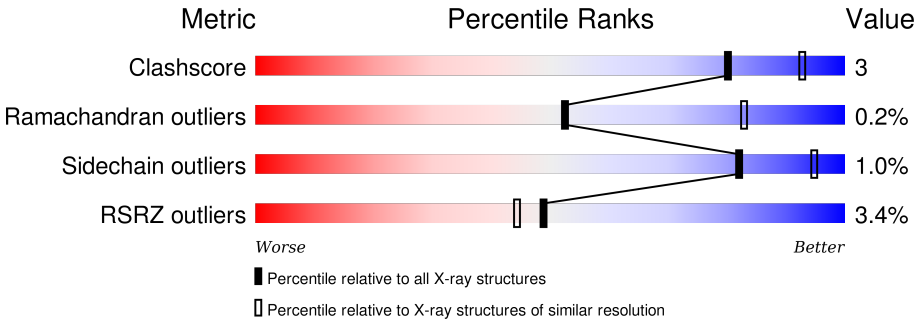
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.93 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))
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	396	3% 89% 9%
1	B	396	4% 89% 10%
1	C	396	5% 90% 9%
1	D	396	2% 91% 8%

2 Entry composition

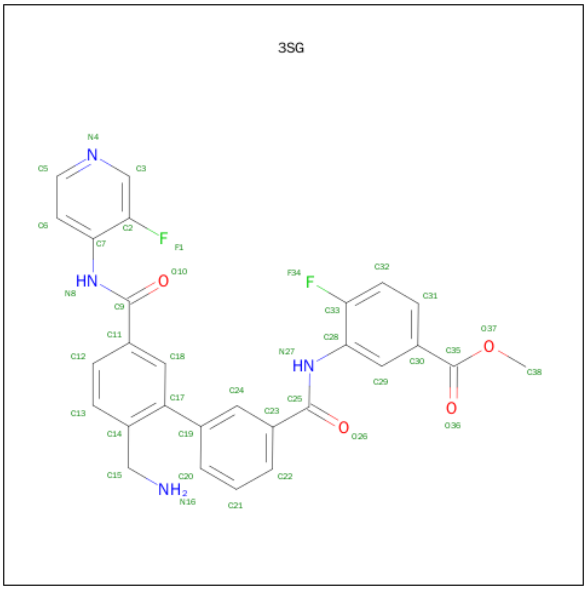
There are 3 unique types of molecules in this entry. The entry contains 12816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Rho-associated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	217	0	0
			3149	2019	529	581	20			
1	B	394	Total	C	N	O	S	171	0	0
			3181	2036	534	591	20			
1	C	392	Total	C	N	O	S	260	0	0
			3169	2030	532	587	20			
1	D	389	Total	C	N	O	S	133	0	0
			3149	2019	529	581	20			

- Molecule 2 is methyl 3-[({2'-(aminomethyl)-5'-[(3-fluoropyridin-4-yl)carbamoyl]biphenyl-3-yl}carbonyl)amino]-4-fluorobenzoate (three-letter code: 3SG) (formula: $C_{28}H_{22}F_2N_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	1	0
			38	28	2	4	4		
2	B	1	Total	C	F	N	O	1	0
			38	28	2	4	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	1	0
			38	28	2	4	4		
2	D	1	Total	C	F	N	O	1	0
			38	28	2	4	4		

- Molecule 3 is water.

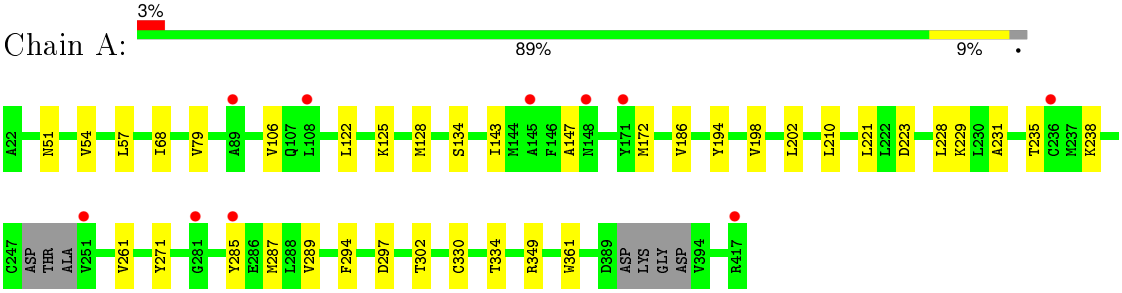
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		
3	C	4	Total	O	0	0
			4	4		
3	D	5	Total	O	0	0
			5	5		

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.

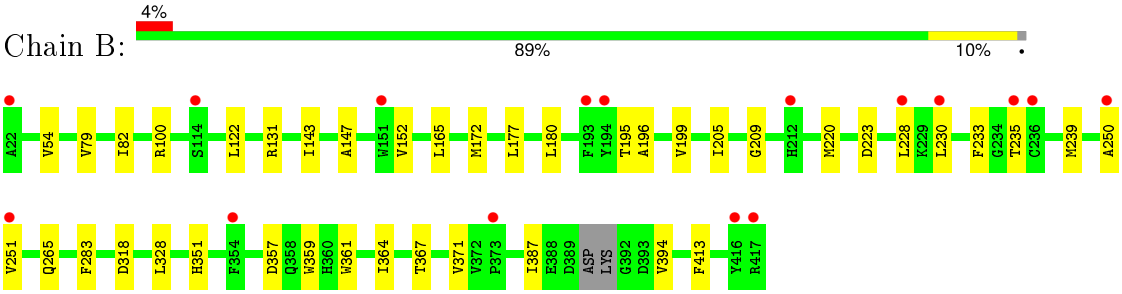
- Molecule 1: Rho-associated protein kinase 2

Chain A:



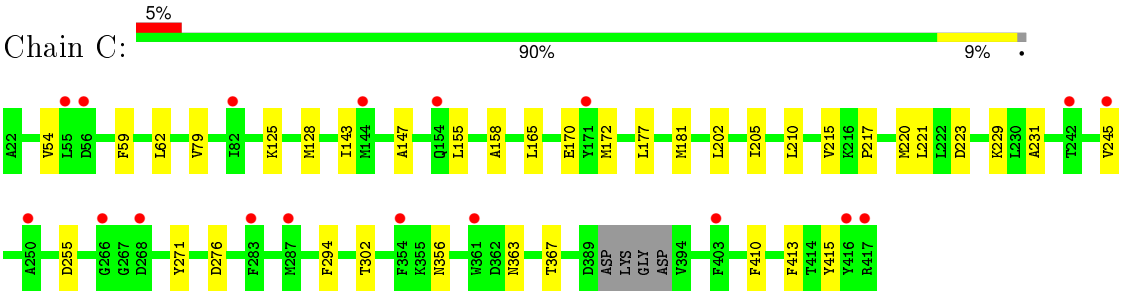
- Molecule 1: Rho-associated protein kinase 2

Chain B:



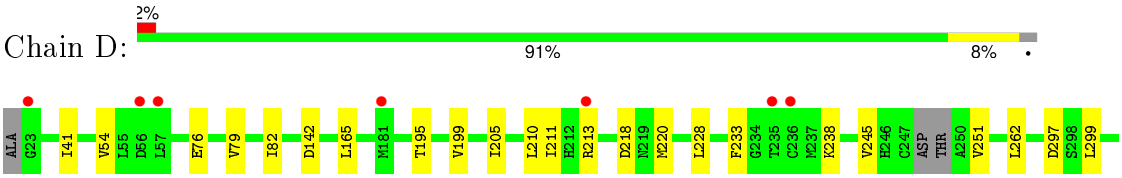
- Molecule 1: Rho-associated protein kinase 2

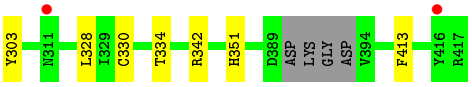
Chain C:



- Molecule 1: Rho-associated protein kinase 2

Chain D:




Y303
N311
L328
T329
C330
T334
R342
H351
D389
ASP
LYS
GLY
ASP
V394
F413
Y416
R417

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.19Å 148.23Å 117.38Å 90.00° 118.65° 90.00°	Depositor
Resolution (Å)	103.01 – 2.93 48.88 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (103.01-2.93) 99.9 (48.88-2.93)	Depositor EDS
R_{merge}	5.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.223 , 0.268 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	96.9	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 120.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 47740 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12816	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.55 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.8582e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: 3SG

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	0.46	0/3226	0.58	0/4356
1	B	0.46	0/3259	0.58	0/4403
1	C	0.49	0/3247	0.58	0/4387
1	D	0.47	0/3226	0.61	2/4356 (0.0%)
All	All	0.47	0/12958	0.59	2/17502 (0.0%)

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	B	0	1

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	D	299	LEU	CB-CG-CD2	5.15	119.76	111.00
1	D	251	VAL	CA-CB-CG2	5.11	118.56	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ARG	Peptide

5.2 Too-close contacts (i)

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	3149	0	3074	23	0
1	B	3181	0	3098	20	0
1	C	3169	0	3091	23	0
1	D	3149	0	3074	13	0
2	A	38	0	22	1	0
2	B	38	0	22	0	0
2	C	38	0	22	0	0
2	D	38	0	22	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	5	0	0	0	0
All	All	12816	0	12425	78	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 3.

All (78) 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:B:82:ILE:HD11	1:D:41:ILE:HD13	1.56	0.85
1:B:54:VAL:HG21	1:B:79:VAL:HG21	1.61	0.81
1:A:54:VAL:HG21	1:A:79:VAL:HG21	1.61	0.81
1:A:221:LEU:HD23	1:A:231:ALA:HB3	1.74	0.68
1:C:54:VAL:HG21	1:C:79:VAL:HG21	1.76	0.67
1:C:221:LEU:HD23	1:C:231:ALA:HB3	1.83	0.60
1:A:57:LEU:HD22	1:A:68:ILE:HD13	1.86	0.57
1:D:330:CYS:O	1:D:334:THR:HG23	2.04	0.57
1:A:221:LEU:HD23	1:A:231:ALA:CB	2.35	0.57
1:A:143:ILE:O	1:A:147:ALA:HB2	2.03	0.57
1:D:205:ILE:HD11	1:D:233:PHE:HE1	1.72	0.54
1:C:177:LEU:HD13	1:C:220:MET:CB	2.38	0.54
1:B:165:LEU:HD22	1:B:413:PHE:CD2	2.44	0.53
1:A:261:VAL:HG22	1:A:271:TYR:CE2	2.45	0.52
1:C:158:ALA:HB3	1:C:415:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:MET:HE1	1:C:217:PRO:HG3	1.93	0.51
1:B:152:VAL:HG13	1:B:233:PHE:CZ	2.46	0.50
1:A:349:ARG:HB2	1:A:361:TRP:CE2	2.46	0.50
1:D:262:LEU:HD13	1:D:303:TYR:CD1	2.47	0.50
1:A:210:LEU:HD23	1:A:238:LYS:HA	1.93	0.50
1:C:125:LYS:HA	1:C:128:MET:HE3	1.93	0.50
1:D:195:THR:O	1:D:199:VAL:HG23	2.12	0.50
1:C:177:LEU:HD13	1:C:220:MET:HB2	1.94	0.49
1:C:245:VAL:HG12	1:C:271:TYR:O	2.13	0.48
1:B:250:ALA:HB2	1:B:265:GLN:HB2	1.96	0.48
1:B:209:GLY:HA2	1:B:239:MET:HE3	1.96	0.48
1:D:211:ILE:HD12	1:D:245:VAL:CG1	2.45	0.47
1:D:165:LEU:HD22	1:D:413:PHE:CD2	2.49	0.47
1:B:328:LEU:HD13	1:B:351:HIS:CG	2.49	0.47
1:A:194:TYR:O	1:A:198:VAL:HG23	2.13	0.47
1:B:122:LEU:HD12	1:B:122:LEU:N	2.29	0.47
1:D:328:LEU:HD13	1:D:351:HIS:CG	2.50	0.46
1:A:125:LYS:HA	1:A:128:MET:HE2	1.97	0.46
1:A:186:VAL:HG11	1:A:287:MET:CE	2.45	0.46
1:A:330:CYS:O	1:A:334:THR:HG23	2.16	0.46
1:A:172:MET:HE1	1:A:223:ASP:HB3	1.96	0.45
1:B:177:LEU:HD23	1:B:283:PHE:CZ	2.52	0.45
1:A:172:MET:HE2	1:A:229:LYS:HB2	1.98	0.45
1:C:205:ILE:HG22	1:C:210:LEU:O	2.16	0.44
1:A:106:VAL:HG23	2:A:501:3SG:H20	2.00	0.44
1:D:220:MET:HB3	1:D:228:LEU:HD11	1.99	0.44
1:A:285:TYR:CE1	1:A:289:VAL:HG21	2.52	0.44
1:C:143:ILE:O	1:C:147:ALA:HB2	2.17	0.43
1:A:198:VAL:HG12	1:A:202:LEU:HD12	2.01	0.43
1:B:195:THR:O	1:B:199:VAL:HG23	2.18	0.43
1:A:285:TYR:CZ	1:A:289:VAL:HG21	2.53	0.43
1:C:177:LEU:HD13	1:C:220:MET:HB3	2.00	0.43
1:C:155:LEU:HD21	1:C:158:ALA:HB2	2.00	0.43
1:D:211:ILE:HD12	1:D:245:VAL:HG12	1.99	0.43
1:C:165:LEU:HD22	1:C:413:PHE:CD2	2.53	0.43
1:D:210:LEU:HD23	1:D:238:LYS:HA	2.01	0.43
1:B:196:ALA:HB1	1:B:361:TRP:CZ3	2.54	0.43
1:B:235:THR:HG23	1:B:251:VAL:HB	2.01	0.43
1:C:363:ASN:O	1:C:367:THR:HG23	2.18	0.42
1:D:54:VAL:HG21	1:D:79:VAL:HG21	2.01	0.42
1:A:261:VAL:HG22	1:A:271:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:O	1:B:147:ALA:HB2	2.19	0.42
1:B:100:ARG:NH2	1:B:387:ILE:HG22	2.34	0.42
1:C:170:GLU:OE2	1:C:229:LYS:NZ	2.43	0.42
1:B:359:TRP:CD2	1:B:364:ILE:HD12	2.55	0.42
1:B:394:VAL:HG13	1:B:394:VAL:O	2.19	0.42
1:A:294:PHE:O	1:A:302:THR:HG23	2.20	0.42
1:C:165:LEU:HD11	1:C:410:PHE:CD1	2.55	0.41
1:A:228:LEU:HD23	1:A:229:LYS:N	2.34	0.41
1:C:294:PHE:O	1:C:302:THR:HG23	2.20	0.41
1:C:172:MET:HE1	1:C:223:ASP:HB3	2.02	0.41
1:B:180:LEU:HD11	1:B:371:VAL:HG21	2.01	0.41
1:A:186:VAL:HG11	1:A:287:MET:HE1	2.02	0.41
1:B:172:MET:HE1	1:B:223:ASP:HB3	2.03	0.41
1:D:245:VAL:HG13	1:D:245:VAL:O	2.21	0.41
1:B:177:LEU:HD13	1:B:220:MET:O	2.21	0.41
1:C:172:MET:HE2	1:C:229:LYS:HB2	2.02	0.41
1:C:202:LEU:HD13	1:C:276:ASP:HB3	2.02	0.41
1:A:122:LEU:HD12	1:A:122:LEU:N	2.36	0.40
1:C:202:LEU:HD21	1:C:215:VAL:HG22	2.01	0.40
1:C:165:LEU:HD11	1:C:410:PHE:HD1	1.87	0.40
1:C:59:PHE:HB2	1:C:62:LEU:HD13	2.03	0.40
1:B:205:ILE:HD11	1:B:230:LEU:HD12	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	383/396 (97%)	364 (95%)	18 (5%)	1 (0%)	46 78
1	B	390/396 (98%)	374 (96%)	15 (4%)	1 (0%)	46 78
1	C	388/396 (98%)	369 (95%)	19 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	383/396 (97%)	368 (96%)	14 (4%)	1 (0%)	46 78
All	All	1544/1584 (98%)	1475 (96%)	66 (4%)	3 (0%)	52 83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	76	GLU
1	B	318	ASP
1	A	134	SER

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	341/346 (99%)	338 (99%)	3 (1%)	84 95
1	B	344/346 (99%)	341 (99%)	3 (1%)	84 95
1	C	343/346 (99%)	341 (99%)	2 (1%)	90 97
1	D	341/346 (99%)	335 (98%)	6 (2%)	66 89
All	All	1369/1384 (99%)	1355 (99%)	14 (1%)	82 95

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	235	THR
1	A	297	ASP
1	B	228	LEU
1	B	357	ASP
1	B	367	THR
1	C	255	ASP
1	C	356	ASN
1	D	82	ILE
1	D	142	ASP
1	D	213	ARG

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Mol	Chain	Res	Type
1	D	218	ASP
1	D	297	ASP
1	D	342	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	154	GLN
1	B	70	ASN
1	B	383	ASN
1	C	70	ASN

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

4 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	3SG	A	501	-	40,41,41	0.69	0	54,57,57	1.45	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	3SG	B	501	-	40,41,41	0.82	1 (2%)	54,57,57	1.45	7 (12%)
2	3SG	C	501	-	40,41,41	0.78	1 (2%)	54,57,57	1.50	10 (18%)
2	3SG	D	501	-	40,41,41	0.75	1 (2%)	54,57,57	1.58	12 (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
2	3SG	A	501	-	-	0/28/28/28	0/4/4/4
2	3SG	B	501	-	-	0/28/28/28	0/4/4/4
2	3SG	C	501	-	-	0/28/28/28	0/4/4/4
2	3SG	D	501	-	-	0/28/28/28	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	3SG	O37-C38	-3.71	1.36	1.45
2	C	501	3SG	O37-C38	-3.07	1.37	1.45
2	D	501	3SG	O37-C38	2.19	1.50	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	3SG	C3-C2-C7	-3.57	119.90	123.41
2	D	501	3SG	C3-C2-C7	-3.55	119.92	123.41
2	C	501	3SG	C3-C2-C7	-3.49	119.98	123.41
2	D	501	3SG	F34-C33-C28	-3.16	114.32	117.50
2	D	501	3SG	C15-C14-C13	-3.15	114.00	120.16
2	B	501	3SG	C3-C2-C7	-3.13	120.33	123.41
2	A	501	3SG	C15-C14-C13	-2.84	114.59	120.16
2	B	501	3SG	C15-C14-C13	-2.70	114.88	120.16
2	A	501	3SG	O26-C25-C23	-2.48	116.74	120.97
2	C	501	3SG	C15-C14-C13	-2.26	115.74	120.16
2	A	501	3SG	O26-C25-N27	-2.06	119.16	123.68
2	C	501	3SG	C32-C33-C28	-2.02	121.19	123.36
2	D	501	3SG	O26-C25-N27	-2.02	119.24	123.68
2	C	501	3SG	O26-C25-N27	-2.00	119.28	123.68
2	D	501	3SG	C29-C28-C33	2.00	119.24	117.84
2	A	501	3SG	F1-C2-C7	2.12	119.62	117.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	3SG	C19-C17-C14	2.33	126.36	122.89
2	D	501	3SG	F34-C33-C32	2.40	123.91	118.47
2	C	501	3SG	C15-C14-C17	2.41	125.23	121.44
2	D	501	3SG	F1-C2-C7	2.43	119.94	117.50
2	B	501	3SG	C15-C14-C17	2.61	125.55	121.44
2	A	501	3SG	C5-N4-C3	2.68	121.77	116.84
2	B	501	3SG	C5-N4-C3	2.69	121.78	116.84
2	C	501	3SG	C5-N4-C3	2.72	121.85	116.84
2	A	501	3SG	C15-C14-C17	2.73	125.74	121.44
2	B	501	3SG	C23-C25-N27	2.78	121.36	115.94
2	C	501	3SG	C29-C28-C33	2.80	119.80	117.84
2	C	501	3SG	C38-O37-C35	2.87	121.75	115.84
2	D	501	3SG	C5-N4-C3	2.92	122.21	116.84
2	C	501	3SG	C23-C25-N27	3.04	121.87	115.94
2	D	501	3SG	C23-C25-N27	3.44	122.65	115.94
2	D	501	3SG	C15-C14-C17	3.52	126.98	121.44
2	B	501	3SG	O37-C35-C30	3.98	119.10	112.36
2	C	501	3SG	O37-C35-C30	4.17	119.42	112.36
2	A	501	3SG	C23-C25-N27	4.17	124.08	115.94
2	A	501	3SG	O37-C35-C30	4.26	119.58	112.36
2	B	501	3SG	C38-O37-C35	4.44	124.97	115.84
2	D	501	3SG	O37-C35-C30	4.45	119.90	112.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	3SG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	389/396 (98%)	0.23	10 (2%)	59	56	63, 89, 134, 149	76 (19%)
1	B	394/396 (99%)	0.23	16 (4%)	41	37	56, 88, 131, 158	57 (14%)
1	C	392/396 (98%)	0.33	18 (4%)	36	32	74, 102, 141, 169	98 (25%)
1	D	389/396 (98%)	0.09	9 (2%)	64	61	57, 83, 122, 161	49 (12%)
All	All	1564/1584 (98%)	0.22	53 (3%)	49	44	56, 91, 133, 169	280 (17%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	266	GLY	4.6
1	C	354	PHE	4.3
1	A	251	VAL	3.9
1	D	23	GLY	3.6
1	B	417	ARG	3.5
1	B	235	THR	3.4
1	A	108	LEU	3.3
1	A	281	GLY	3.1
1	D	235	THR	3.1
1	C	82	ILE	3.0
1	D	57	LEU	3.0
1	B	354	PHE	2.9
1	B	250	ALA	2.9
1	C	417	ARG	2.8
1	B	236	CYS	2.8
1	A	285	TYR	2.7
1	B	22	ALA	2.7
1	B	114	SER	2.7
1	A	417	ARG	2.7
1	B	251	VAL	2.7
1	C	403	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	154	GLN	2.7
1	B	230	LEU	2.6
1	C	245	VAL	2.6
1	B	212	HIS	2.5
1	C	268	ASP	2.5
1	C	56	ASP	2.4
1	D	56	ASP	2.4
1	D	181	MET	2.4
1	A	171	TYR	2.4
1	A	148	ASN	2.3
1	C	242	THR	2.3
1	B	151	TRP	2.3
1	D	311	ASN	2.3
1	B	194	TYR	2.2
1	D	236	CYS	2.2
1	C	55	LEU	2.2
1	A	89	ALA	2.2
1	A	145	ALA	2.2
1	C	287	MET	2.2
1	C	416	TYR	2.2
1	B	193	PHE	2.2
1	D	416	TYR	2.2
1	C	283	PHE	2.1
1	C	171	TYR	2.1
1	C	250	ALA	2.1
1	D	213	ARG	2.1
1	C	144	MET	2.1
1	C	361	TRP	2.1
1	B	228	LEU	2.0
1	B	373	PRO	2.0
1	B	416	TYR	2.0
1	A	236	CYS	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	3SG	C	501	38/38	0.91	0.24	-0.21	76,83,93,96	1
2	3SG	D	501	38/38	0.93	0.19	-0.31	60,77,103,107	1
2	3SG	A	501	38/38	0.91	0.20	-0.42	68,78,105,110	1
2	3SG	B	501	38/38	0.93	0.19	-0.64	53,69,87,89	1

6.5 Other polymers (i)

There are no such residues in this entry.