Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:43 PM GMT

PDB ID	:	4D83
Title	:	Crystal Structure of Human Beta Secretase in Complex with NVP-BUR436, derived from a co-crystallization experiment
Authors	:	Rondeau, J.M.; Bourgier, E.
Deposited on	:	2012-01-10
Resolution	:	2.40 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:

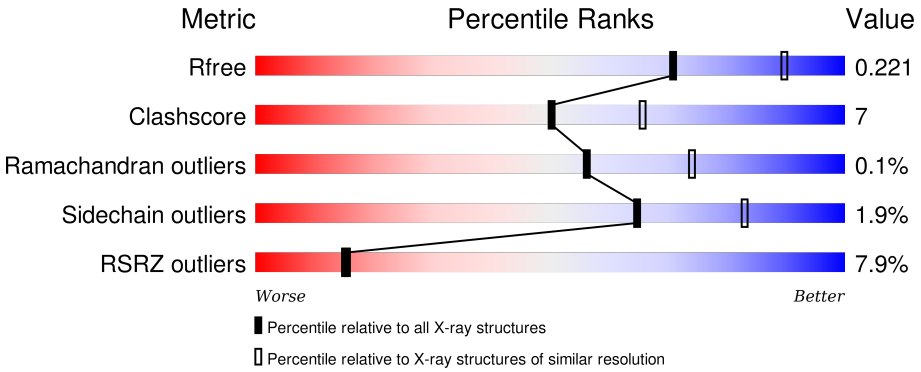
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	402	6% 79% 13% • 6%
1	B	402	9% 80% 13% • 6%
1	C	402	7% 78% 15% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9477 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.

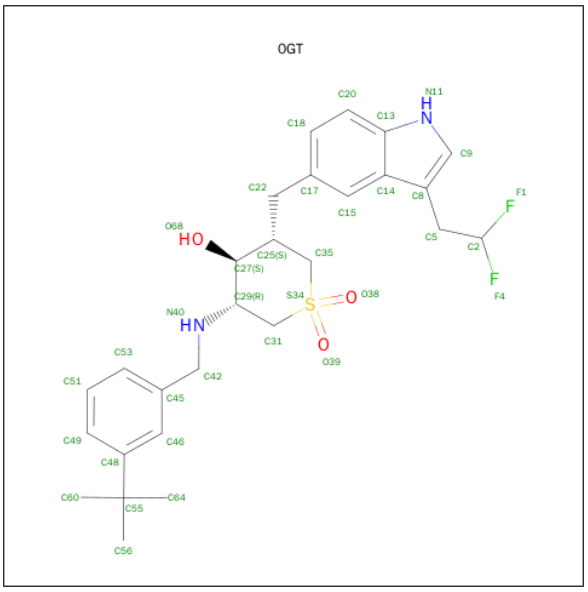
- Molecule 1 is a protein called Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	1	0
			2974	1903	496	561	14			
1	B	377	Total	C	N	O	S	0	1	0
			2974	1903	496	561	14			
1	C	377	Total	C	N	O	S	0	1	0
			2974	1903	496	561	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	EXPRESSION TAG	UNP P56817
A	-14	PRO	-	EXPRESSION TAG	UNP P56817
B	-15	GLY	-	EXPRESSION TAG	UNP P56817
B	-14	PRO	-	EXPRESSION TAG	UNP P56817
C	-15	GLY	-	EXPRESSION TAG	UNP P56817
C	-14	PRO	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is (3R,4S,5S)-3-[(3-TERT-BUTYLBENZYL)AMINO]-5-{[3-(2,2-DIFLUOROETHYL)-1H-INDOL-5-YL]METHYL}TETRAHYDRO-2H-THIOPYRAN-4-OL 1,1-DIOXIDE (three-letter code: 0GT) (formula: $C_{27}H_{34}F_2N_2O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	1
			48	37	4	3	3	1		
2	B	1	Total	C	F	N	O	S	0	1
			48	37	4	3	3	1		
2	C	1	Total	C	F	N	O	S	0	1
			48	37	4	3	3	1		

- Molecule 3 is water.

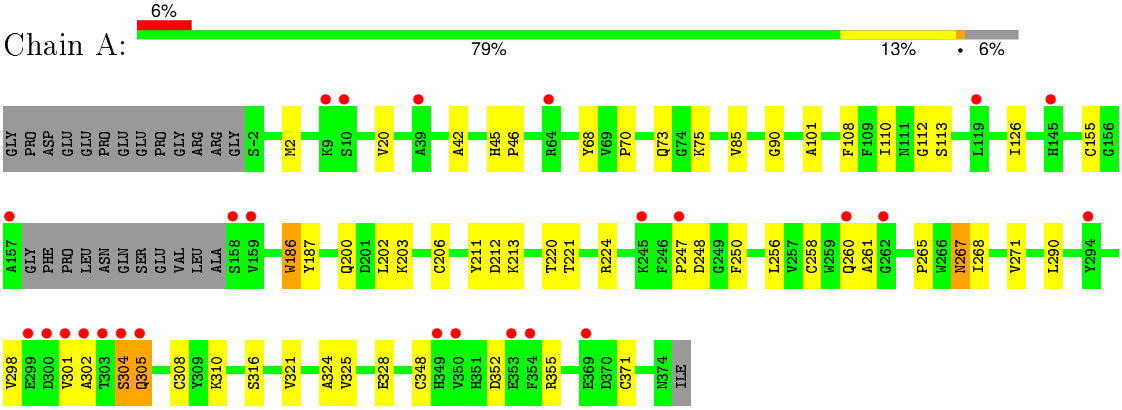
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	141	Total	O	0	0
			141	141		
3	B	120	Total	O	0	0
			120	120		
3	C	150	Total	O	0	0
			150	150		

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.

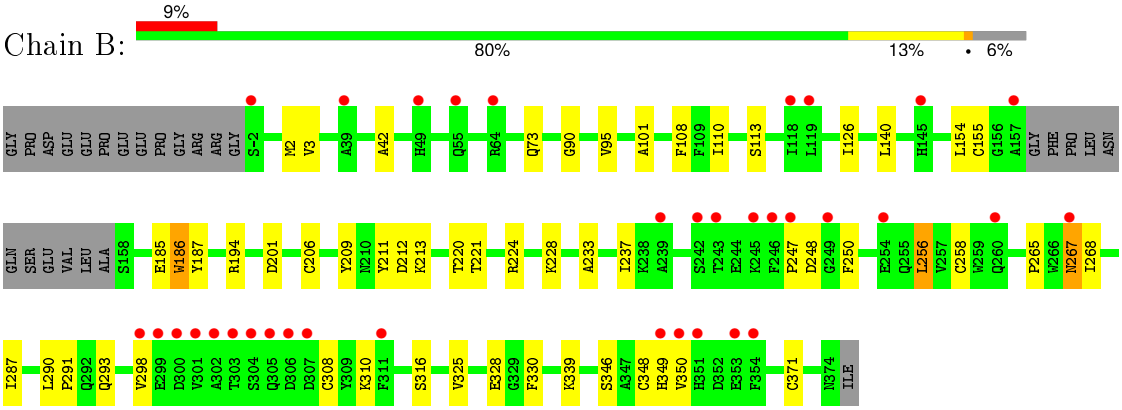
- Molecule 1: Beta-secretase 1

Chain A:



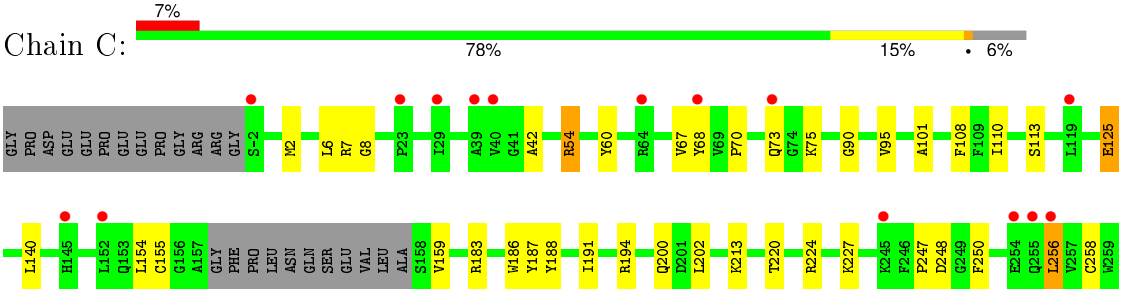
- Molecule 1: Beta-secretase 1

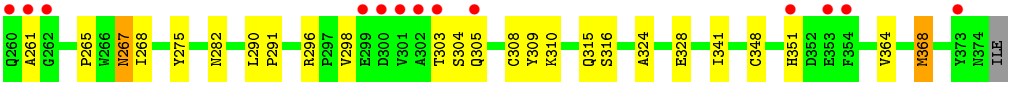
Chain B:



- Molecule 1: Beta-secretase 1

Chain C:




Q260
A261
G262
P265
W266
N267
I268
Y275
N282
L290
P291
R296
P297
V298
E299
D300
V301
A302
T303
S304
Q305
C308
Y309
K310
Q315
S316
A324
E328
I341
C348
H351
D352
E353
F354
V364
N368
Y373
N374
IIE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	81.95Å 102.89Å 100.20Å 90.00° 103.99° 90.00°	Depositor
Resolution (Å)	22.83 – 2.40 22.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (22.83-2.40) 97.7 (22.83-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.41Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.196 , 0.226 0.192 , 0.221	Depositor DCC
R_{free} test set	3109 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 61642 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9477	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: 0GT

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	0.32	0/3052	0.48	0/4147
1	B	0.33	0/3052	0.49	0/4147
1	C	0.32	0/3052	0.51	2/4147 (0.0%)
All	All	0.32	0/9156	0.49	2/12441 (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	C	54	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	C	54	ARG	NE-CZ-NH2	6.20	123.40	120.30

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	2974	0	2897	38	0
1	B	2974	0	2897	37	0
1	C	2974	0	2897	44	0
2	A	48	0	20	3	0
2	B	48	0	20	3	0
2	C	48	0	20	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	141	0	0	2	0
3	B	120	0	0	0	0
3	C	150	0	0	2	0
All	All	9477	0	8751	118	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 7.

All (118) 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:258:CYS:HG	1:A:308:CYS:HG	1.09	0.96
1:B:256:LEU:HD22	1:B:298:VAL:HG21	1.50	0.93
1:C:258:CYS:HG	1:C:308:CYS:HG	0.93	0.90
1:B:258:CYS:HG	1:B:308:CYS:HG	0.87	0.85
1:C:261:ALA:HB2	1:C:305:GLN:O	1.79	0.82
1:A:256:LEU:HD22	1:A:298:VAL:HG21	1.62	0.81
1:C:256:LEU:HD22	1:C:298:VAL:HG21	1.62	0.79
1:C:200:GLN:HB2	3:C:683:HOH:O	1.89	0.72
1:B:221:THR:O	1:B:325:VAL:HG13	1.90	0.72
1:B:228:LYS:HB2	1:B:228:LYS:NZ	2.14	0.63
1:C:324:ALA:O	1:C:328:GLU:HG3	2.00	0.62
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.81	0.61
1:C:110:ILE:HD11	2:C:501[B]:0GT:H4	1.83	0.59
1:A:265:PRO:O	1:A:268:ILE:HG12	2.04	0.58
1:A:110:ILE:HD11	2:A:401[B]:0GT:H4	1.85	0.58
1:B:110:ILE:HD11	2:B:501[B]:0GT:H4	1.84	0.57
1:C:8:GLY:O	1:C:159:VAL:HG22	2.05	0.57
1:C:125:GLU:HG3	1:C:125:GLU:O	2.04	0.57
1:B:265:PRO:O	1:B:268:ILE:HG12	2.04	0.56
1:C:54:ARG:HD3	3:C:690:HOH:O	2.06	0.56
1:C:6:LEU:O	1:C:7:ARG:HD2	2.06	0.55
1:C:265:PRO:O	1:C:268:ILE:HG12	2.08	0.54
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.89	0.54
1:A:155:CYS:CB	1:A:348:CYS:HG	2.20	0.54
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.90	0.53
1:B:185:GLU:OE2	1:B:339:LYS:HE3	2.09	0.53
1:C:247:PRO:O	1:C:250:PHE:HB3	2.09	0.52
1:C:305:GLN:HA	1:C:305:GLN:HE21	1.75	0.52
1:B:154:LEU:O	1:B:328:GLU:HA	2.10	0.52
1:A:206:CYS:CB	1:A:371:CYS:HG	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HD11	2:A:401[A]:0GT:H4	1.92	0.51
1:C:54:ARG:HG2	1:C:60:TYR:CE1	2.46	0.51
1:A:221:THR:O	1:A:325:VAL:HG13	2.09	0.51
1:A:224[A]:ARG:HD2	3:A:599:HOH:O	2.10	0.51
1:C:68:TYR:OH	1:C:70:PRO:HB3	2.11	0.51
1:B:247:PRO:O	1:B:250:PHE:HB3	2.11	0.51
1:B:110:ILE:HB	1:B:113:SER:HB3	1.92	0.50
1:B:155:CYS:CB	1:B:348:CYS:HG	2.23	0.50
1:B:194:ARG:NH2	1:B:201:ASP:HB2	2.26	0.50
1:A:267:ASN:H	1:A:267:ASN:HD22	1.58	0.50
1:B:110:ILE:HD11	2:B:501[A]:0GT:H4	1.93	0.50
1:C:110:ILE:HB	1:C:113:SER:HB3	1.94	0.50
1:C:267:ASN:HD22	1:C:267:ASN:H	1.58	0.49
1:A:110:ILE:HB	1:A:113:SER:HB3	1.93	0.49
1:A:68:TYR:CD1	1:B:3:VAL:HG11	2.48	0.49
1:C:224[B]:ARG:NH2	1:C:315:GLN:O	2.46	0.49
1:C:194:ARG:HB3	1:C:275:TYR:HB2	1.94	0.49
1:B:267:ASN:H	1:B:267:ASN:HD22	1.60	0.49
1:C:303:THR:O	1:C:304:SER:HB2	2.13	0.48
1:C:110:ILE:HD11	2:C:501[A]:0GT:H4	1.95	0.48
1:A:247:PRO:O	1:A:250:PHE:HB3	2.12	0.48
1:B:256:LEU:CD2	1:B:310:LYS:HE3	2.44	0.48
1:C:282:ASN:HA	1:C:364:VAL:HA	1.96	0.48
1:C:256:LEU:CD2	1:C:310:LYS:HE3	2.44	0.48
1:A:224[A]:ARG:HB2	1:A:321:VAL:HB	1.96	0.48
1:A:302:ALA:C	1:A:304:SER:H	2.17	0.48
1:B:287:ILE:HB	1:B:330:PHE:CZ	2.49	0.47
1:C:183:ARG:HG3	1:C:368:MET:SD	2.55	0.47
1:C:154:LEU:O	1:C:328:GLU:HA	2.15	0.46
1:B:211:TYR:HA	1:B:212:ASP:HA	1.71	0.46
1:A:256:LEU:CD2	1:A:310:LYS:HE3	2.45	0.46
1:A:248:ASP:O	1:A:248:ASP:OD1	2.34	0.46
1:A:211:TYR:HA	1:A:212:ASP:HA	1.72	0.46
1:B:206:CYS:HG	1:B:371:CYS:CB	2.24	0.45
1:A:126:ILE:HG23	1:A:186:TRP:HB2	1.98	0.45
1:B:293:GLN:OE1	1:B:350:VAL:HG21	2.17	0.45
1:B:108:PHE:CD1	2:B:501[B]:0GT:H8	2.52	0.45
1:A:352:ASP:HB3	1:A:355:ARG:O	2.17	0.44
1:B:95:VAL:HG11	1:B:140:LEU:HA	1.99	0.44
1:C:248:ASP:O	1:C:248:ASP:OD1	2.35	0.44
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PRO:HA	1:A:75:LYS:HB3	1.99	0.44
1:B:187:TYR:CE2	1:B:213:LYS:HE3	2.53	0.44
1:A:305:GLN:H	1:A:305:GLN:CD	2.20	0.44
1:C:191:ILE:HD11	1:C:368:MET:SD	2.58	0.43
1:C:298:VAL:O	1:C:308:CYS:HB2	2.18	0.43
1:B:293:GLN:CD	1:B:350:VAL:HG21	2.38	0.43
1:A:108:PHE:CD1	2:A:401[B]:0GT:H8	2.53	0.43
1:C:296:ARG:O	1:C:309:TYR:HA	2.18	0.43
1:C:256:LEU:HD13	1:C:298:VAL:HG23	1.99	0.43
1:C:8:GLY:C	1:C:159:VAL:HG22	2.38	0.43
1:A:224[A]:ARG:HB3	1:A:316:SER:HB2	2.00	0.43
1:B:346:SER:O	1:B:349:HIS:HB3	2.19	0.43
1:C:227:LYS:HG3	1:C:315:GLN:OE1	2.19	0.43
1:C:155:CYS:HG	1:C:348:CYS:CB	2.30	0.43
1:C:95:VAL:HG11	1:C:140:LEU:HA	2.00	0.43
1:A:256:LEU:HD23	1:A:310:LYS:HE3	2.02	0.42
1:B:233:ALA:O	1:B:237:ILE:HG13	2.19	0.42
1:B:256:LEU:HD23	1:B:310:LYS:HE3	2.01	0.42
1:C:67:VAL:HG22	1:C:68:TYR:N	2.35	0.42
1:B:290:LEU:HB3	1:B:291:PRO:HD2	2.01	0.42
1:C:290:LEU:HB3	1:C:291:PRO:HD2	2.02	0.42
1:B:228:LYS:HB2	1:B:228:LYS:HZ3	1.84	0.42
1:C:187:TYR:CE2	1:C:213:LYS:HE3	2.55	0.42
1:B:206:CYS:HA	1:B:209:TYR:CD1	2.55	0.42
1:C:108:PHE:CD1	2:C:501[B]:0GT:H8	2.53	0.42
1:A:298:VAL:HG11	1:A:310:LYS:HG3	2.01	0.42
1:B:224[A]:ARG:HB3	1:B:316:SER:HB2	2.00	0.41
1:C:202:LEU:HD23	1:C:202:LEU:HA	1.88	0.41
1:A:20:VAL:HG12	1:A:85:VAL:HG22	2.02	0.41
1:B:126:ILE:HG23	1:B:186:TRP:HB2	2.01	0.41
1:A:202:LEU:O	1:A:203:LYS:HB2	2.18	0.41
1:A:224[B]:ARG:HB2	1:A:321:VAL:HB	2.01	0.41
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.51	0.41
1:A:260:GLN:O	1:A:261:ALA:C	2.59	0.41
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.56	0.41
1:A:271:VAL:HG12	1:A:290:LEU:HD23	2.02	0.41
1:A:112:GLY:HA2	3:A:622:HOH:O	2.20	0.41
1:C:224[A]:ARG:HB3	1:C:316:SER:HB2	2.02	0.41
1:B:224[B]:ARG:HB3	1:B:316:SER:HB2	2.01	0.41
1:B:248:ASP:OD1	1:B:248:ASP:O	2.38	0.41
1:A:187:TYR:CE2	1:A:213:LYS:HE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.50	0.40
1:A:324:ALA:O	1:A:328:GLU:HG3	2.21	0.40
1:C:188:TYR:HB3	1:C:341:ILE:HD11	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	374/402 (93%)	360 (96%)	13 (4%)	1 (0%)	46 63
1	B	374/402 (93%)	360 (96%)	14 (4%)	0	100 100
1	C	374/402 (93%)	362 (97%)	12 (3%)	0	100 100
All	All	1122/1206 (93%)	1082 (96%)	39 (4%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	VAL

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	323/342 (94%)	317 (98%)	6 (2%)	65 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	323/342 (94%)	319 (99%)	4 (1%)	78 90
1	C	323/342 (94%)	315 (98%)	8 (2%)	55 76
All	All	969/1026 (94%)	951 (98%)	18 (2%)	65 83

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	186	TRP
1	A	200	GLN
1	A	267	ASN
1	A	304	SER
1	A	305	GLN
1	B	73	GLN
1	B	186	TRP
1	B	256	LEU
1	B	267	ASN
1	C	73	GLN
1	C	75	LYS
1	C	125	GLU
1	C	186	TRP
1	C	256	LEU
1	C	267	ASN
1	C	351	HIS
1	C	368	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	267	ASN
1	A	305	GLN
1	A	315	GLN
1	A	351	HIS
1	B	114	ASN
1	B	267	ASN
1	B	282	ASN
1	B	315	GLN
1	C	114	ASN
1	C	267	ASN

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Mol	Chain	Res	Type
1	C	305	GLN
1	C	349	HIS

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

6 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	0GT	A	401[A]	-	35,38,38	1.84	10 (28%)	38,57,57	1.22	3 (7%)
2	0GT	A	401[B]	-	35,38,38	1.85	9 (25%)	38,57,57	1.11	3 (7%)
2	0GT	B	501[A]	-	35,38,38	1.80	10 (28%)	38,57,57	1.24	3 (7%)
2	0GT	B	501[B]	-	35,38,38	1.81	10 (28%)	38,57,57	1.14	3 (7%)
2	0GT	C	501[A]	-	35,38,38	1.80	9 (25%)	38,57,57	1.26	4 (10%)
2	0GT	C	501[B]	-	35,38,38	1.80	8 (22%)	38,57,57	1.15	4 (10%)

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	0GT	A	401[A]	-	-	0/16/37/37	0/4/4/4
2	0GT	A	401[B]	-	-	0/16/37/37	0/4/4/4
2	0GT	B	501[A]	-	-	0/16/37/37	0/4/4/4
2	0GT	B	501[B]	-	-	0/16/37/37	0/4/4/4
2	0GT	C	501[A]	-	-	0/16/37/37	0/4/4/4
2	0GT	C	501[B]	-	-	0/16/37/37	0/4/4/4

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[B]	0GT	C9-N11	-2.65	1.31	1.36
2	A	401[A]	0GT	C9-N11	-2.64	1.31	1.36
2	B	501[A]	0GT	C9-N11	-2.57	1.31	1.36
2	C	501[A]	0GT	C9-N11	-2.57	1.31	1.36
2	C	501[B]	0GT	C9-N11	-2.46	1.31	1.36
2	B	501[B]	0GT	C9-N11	-2.46	1.31	1.36
2	C	501[A]	0GT	C9-C8	-2.05	1.34	1.38
2	A	401[A]	0GT	C9-C8	-2.05	1.34	1.38
2	B	501[A]	0GT	C9-C8	-2.04	1.34	1.38
2	A	401[B]	0GT	C9-C8	-2.04	1.34	1.38
2	B	501[B]	0GT	C9-C8	-2.01	1.34	1.38
2	B	501[B]	0GT	C18-C17	2.00	1.43	1.38
2	A	401[A]	0GT	C18-C17	2.00	1.43	1.38
2	B	501[B]	0GT	C22-C25	2.02	1.57	1.53
2	B	501[A]	0GT	C22-C25	2.02	1.57	1.53
2	C	501[A]	0GT	C15-C17	2.07	1.42	1.37
2	B	501[A]	0GT	C18-C17	2.08	1.43	1.38
2	B	501[A]	0GT	C15-C17	2.11	1.42	1.37
2	A	401[A]	0GT	C15-C17	2.12	1.42	1.37
2	C	501[A]	0GT	C22-C25	2.22	1.57	1.53
2	C	501[B]	0GT	C22-C25	2.22	1.57	1.53
2	C	501[B]	0GT	C15-C17	2.26	1.42	1.37
2	A	401[B]	0GT	C22-C25	2.26	1.57	1.53
2	A	401[A]	0GT	C22-C25	2.26	1.57	1.53
2	A	401[B]	0GT	C15-C17	2.29	1.43	1.37
2	B	501[B]	0GT	C15-C17	2.32	1.43	1.37
2	A	401[B]	0GT	C49-C48	2.47	1.43	1.39
2	A	401[A]	0GT	C49-C48	2.47	1.43	1.39
2	C	501[A]	0GT	C49-C48	2.62	1.43	1.39
2	C	501[B]	0GT	C49-C48	2.62	1.43	1.39
2	B	501[B]	0GT	C49-C48	2.63	1.43	1.39
2	B	501[A]	0GT	C49-C48	2.63	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501[B]	0GT	C20-C18	2.70	1.42	1.36
2	C	501[A]	0GT	C20-C18	2.73	1.42	1.36
2	A	401[A]	0GT	C20-C18	2.73	1.42	1.36
2	B	501[A]	0GT	C20-C18	2.74	1.42	1.36
2	A	401[B]	0GT	C25-C27	2.76	1.56	1.53
2	A	401[A]	0GT	C25-C27	2.76	1.56	1.53
2	B	501[B]	0GT	C20-C18	2.78	1.42	1.36
2	A	401[B]	0GT	C20-C18	2.79	1.42	1.36
2	B	501[B]	0GT	C25-C27	3.04	1.57	1.53
2	B	501[A]	0GT	C25-C27	3.04	1.57	1.53
2	C	501[A]	0GT	C25-C27	3.14	1.57	1.53
2	C	501[B]	0GT	C25-C27	3.14	1.57	1.53
2	B	501[B]	0GT	C35-S34	3.78	1.79	1.76
2	B	501[A]	0GT	C35-S34	3.78	1.79	1.76
2	C	501[A]	0GT	C35-S34	3.78	1.79	1.76
2	C	501[B]	0GT	C35-S34	3.78	1.79	1.76
2	C	501[A]	0GT	C31-S34	4.23	1.80	1.76
2	C	501[B]	0GT	C31-S34	4.23	1.80	1.76
2	A	401[B]	0GT	C35-S34	4.28	1.80	1.76
2	A	401[A]	0GT	C35-S34	4.28	1.80	1.76
2	B	501[B]	0GT	C31-S34	4.45	1.80	1.76
2	B	501[A]	0GT	C31-S34	4.45	1.80	1.76
2	A	401[B]	0GT	C31-S34	4.67	1.80	1.76
2	A	401[A]	0GT	C31-S34	4.67	1.80	1.76

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401[A]	0GT	C18-C20-C13	-2.96	117.67	120.88
2	C	501[A]	0GT	C18-C20-C13	-2.96	117.67	120.88
2	B	501[A]	0GT	C18-C20-C13	-2.91	117.72	120.88
2	C	501[A]	0GT	O38-S34-C35	-2.49	107.32	109.27
2	C	501[B]	0GT	O38-S34-C35	-2.49	107.32	109.27
2	B	501[B]	0GT	C18-C20-C13	-2.43	118.24	120.88
2	C	501[B]	0GT	C18-C20-C13	-2.40	118.28	120.88
2	A	401[B]	0GT	C18-C20-C13	-2.36	118.32	120.88
2	A	401[B]	0GT	C42-N40-C29	2.62	120.78	115.06
2	A	401[A]	0GT	C42-N40-C29	2.62	120.78	115.06
2	C	501[B]	0GT	C15-C14-C13	2.63	121.38	120.34
2	B	501[B]	0GT	C15-C14-C13	2.67	121.40	120.34
2	B	501[B]	0GT	C42-N40-C29	2.72	121.00	115.06
2	B	501[A]	0GT	C42-N40-C29	2.72	121.00	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501[A]	0GT	C42-N40-C29	2.90	121.38	115.06
2	C	501[B]	0GT	C42-N40-C29	2.90	121.38	115.06
2	A	401[B]	0GT	C15-C14-C13	2.94	121.50	120.34
2	B	501[A]	0GT	C15-C14-C13	3.36	121.67	120.34
2	C	501[A]	0GT	C15-C14-C13	3.37	121.67	120.34
2	A	401[A]	0GT	C15-C14-C13	3.63	121.78	120.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401[A]	0GT	1	0
2	A	401[B]	0GT	2	0
2	B	501[A]	0GT	1	0
2	B	501[B]	0GT	2	0
2	C	501[A]	0GT	1	0
2	C	501[B]	0GT	2	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	377/402 (93%)	0.26	26 (6%)	20	19	33, 49, 79, 99	0
1	B	377/402 (93%)	0.40	35 (9%)	11	10	30, 49, 83, 103	0
1	C	377/402 (93%)	0.31	28 (7%)	17	17	32, 49, 80, 99	0
All	All	1131/1206 (93%)	0.32	89 (7%)	15	15	30, 49, 81, 103	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	303	THR	10.9
1	C	301	VAL	10.0
1	B	302	ALA	9.7
1	A	303	THR	8.3
1	A	301	VAL	6.8
1	B	301	VAL	6.1
1	C	299	GLU	5.3
1	C	302	ALA	5.3
1	C	303	THR	5.2
1	C	261	ALA	5.1
1	A	300	ASP	5.0
1	B	350	VAL	5.0
1	A	159	VAL	4.9
1	A	305	GLN	4.7
1	B	298	VAL	4.6
1	B	245	LYS	4.6
1	B	305	GLN	4.5
1	B	300	ASP	4.4
1	B	299	GLU	4.3
1	B	304	SER	4.2
1	C	64	ARG	4.2
1	B	353	GLU	4.0
1	B	242	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	-2	SER	4.0
1	C	262	GLY	3.9
1	A	157	ALA	3.8
1	C	353	GLU	3.8
1	B	354	PHE	3.8
1	C	145	HIS	3.8
1	A	302	ALA	3.8
1	A	158	SER	3.5
1	B	243	THR	3.5
1	C	354	PHE	3.5
1	A	299	GLU	3.4
1	C	305	GLN	3.3
1	A	145	HIS	3.2
1	C	351	HIS	3.2
1	A	64	ARG	3.1
1	A	353	GLU	3.1
1	C	39	ALA	3.0
1	C	300	ASP	3.0
1	B	247	PRO	3.0
1	C	40	VAL	3.0
1	B	119	LEU	3.0
1	A	304	SER	2.9
1	C	23	PRO	2.9
1	A	294	TYR	2.9
1	B	254	GLU	2.8
1	B	306	ASP	2.8
1	C	245	LYS	2.8
1	A	245	LYS	2.7
1	A	350	VAL	2.7
1	A	10	SER	2.7
1	A	39	ALA	2.7
1	B	49	HIS	2.6
1	C	68	TYR	2.6
1	A	9	LYS	2.6
1	C	260	GLN	2.6
1	C	29	ILE	2.6
1	B	249	GLY	2.6
1	B	246	PHE	2.5
1	B	-2	SER	2.5
1	C	152	LEU	2.5
1	B	157	ALA	2.5
1	A	119	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	73	GLN	2.4
1	C	255	GLN	2.4
1	B	39	ALA	2.4
1	C	373	TYR	2.4
1	B	351	HIS	2.4
1	B	145	HIS	2.4
1	A	354	PHE	2.4
1	B	311	PHE	2.4
1	B	239	ALA	2.4
1	A	349	HIS	2.3
1	B	349	HIS	2.3
1	C	119	LEU	2.3
1	B	260	GLN	2.2
1	B	267	ASN	2.2
1	B	64	ARG	2.2
1	B	118	ILE	2.2
1	A	262	GLY	2.2
1	C	256	LEU	2.2
1	B	307	ASP	2.2
1	A	247	PRO	2.1
1	A	260	GLN	2.1
1	A	369	GLU	2.1
1	B	55	GLN	2.1
1	C	254	GLU	2.1

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	0GT	A	401[A]	35/35	0.95	0.16	-0.10	39,43,51,54	13
2	0GT	A	401[B]	35/35	0.95	0.16	-0.14	39,42,46,49	13
2	0GT	B	501[A]	35/35	0.96	0.13	-0.48	36,42,51,53	13
2	0GT	C	501[A]	35/35	0.96	0.13	-0.51	38,43,50,52	13
2	0GT	B	501[B]	35/35	0.96	0.13	-0.52	36,42,46,49	13
2	0GT	C	501[B]	35/35	0.96	0.13	-0.55	38,43,47,47	13

6.5 Other polymers (i)

There are no such residues in this entry.