Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:46 PM GMT

PDB ID	:	1YM2
Title	:	Crystal structure of human beta secretase complexed with NVP-AUR200
Authors	:	Hanessian, S.; Yun, H.; Hou, Y.; Yang, G.; Bayrakdarian, M.; Therrien, E.; Moitessier, N.; Roggo, S.; Veenstra, S.
Deposited on	:	2005-01-20
Resolution	:	2.05 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:

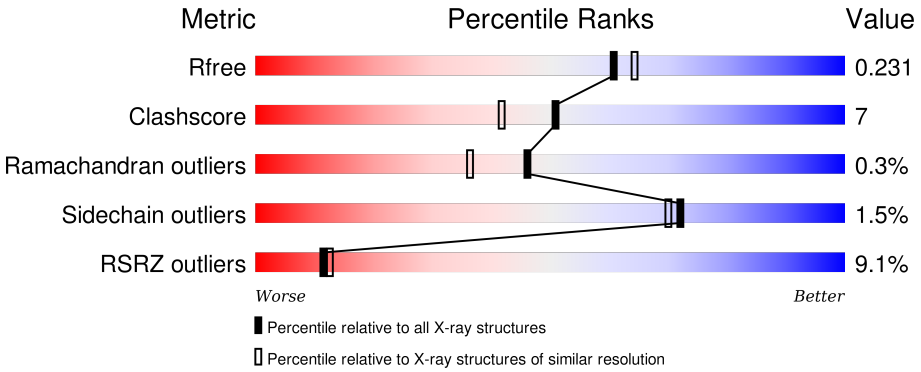
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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	8% 77% 17% 6%
1	B	402	12% 77% 14% • 6%
1	C	402	6% 79% 14% 6%
2	X	6	67% 33%
2	Y	6	67% 33%

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Mol	Chain	Length	Quality of chain
2	Z	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9605 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	376	Total	C	N	O	S	0	0	0
			2960	1895	492	559	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	376	Total	C	N	O	S	0	0	0
			2960	1895	492	559	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 a protein called NVP-AUR200 INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	6	Total	C	N	O	S	0	0	0
			47	34	5	7	1			
2	Y	6	Total	C	N	O	S	0	0	0
			47	34	5	7	1			
2	Z	6	Total	C	N	O	S	0	0	0
			47	34	5	7	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		

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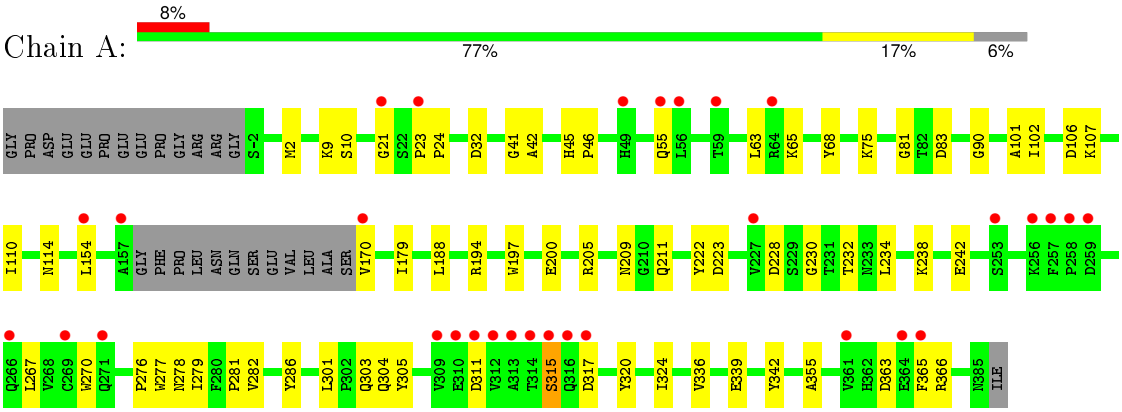
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	162	Total O 162 162	0	0
3	C	203	Total O 203 203	0	0
3	X	4	Total O 4 4	0	0
3	Y	3	Total O 3 3	0	0
3	Z	4	Total O 4 4	0	0

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.

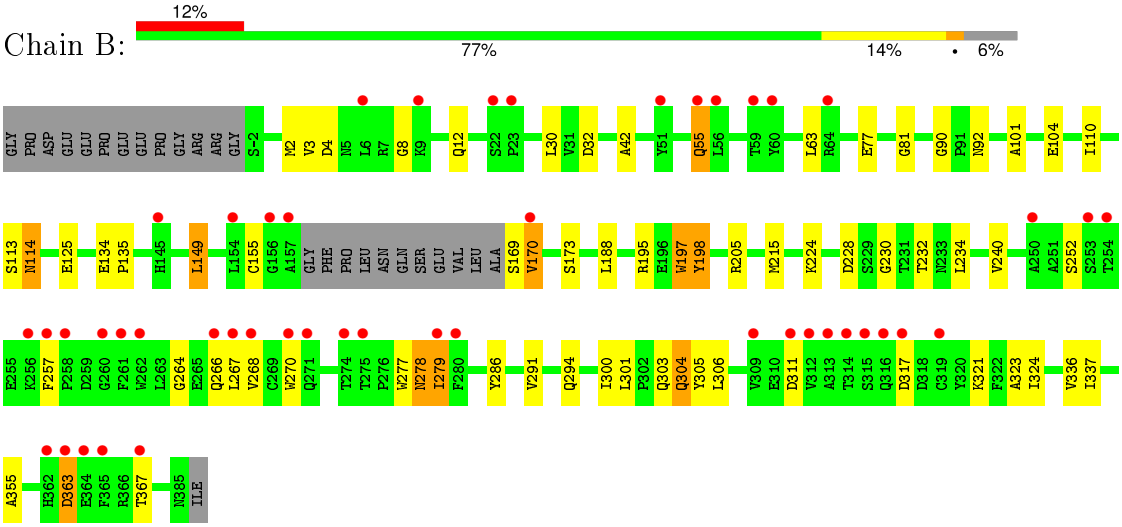
- Molecule 1: Beta-secretase 1

Chain A:



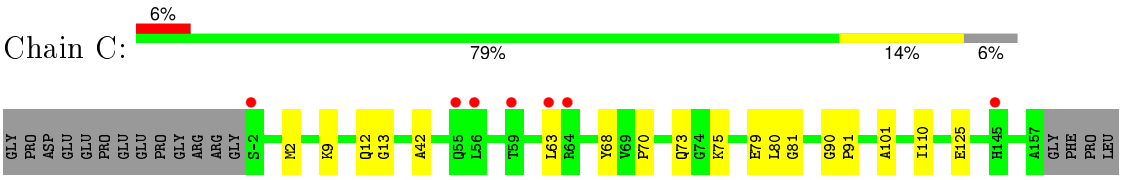
- Molecule 1: Beta-secretase 1

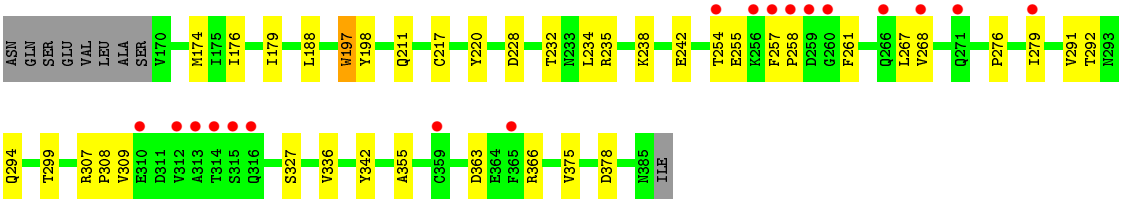
Chain B:



- Molecule 1: Beta-secretase 1

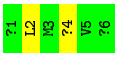
Chain C:





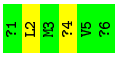
- Molecule 2: NVP-AUR200 INHIBITOR

Chain X:



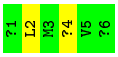
- Molecule 2: NVP-AUR200 INHIBITOR

Chain Y:



- Molecule 2: NVP-AUR200 INHIBITOR

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.26Å 103.26Å 100.62Å 90.00° 104.12° 90.00°	Depositor
Resolution (Å)	47.05 – 2.05 47.04 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.05-2.05) 99.9 (47.04-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.87 (at 2.05Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.212 , 0.237 0.208 , 0.231	Depositor DCC
R_{free} test set	10253 reflections (11.16%)	DCC
Wilson B-factor (Å^2)	43.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.6	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 102108 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9605	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: LYT, 24O, ACE

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	0.26	0/3035	0.59	1/4125 (0.0%)
1	B	0.26	0/3041	0.57	2/4133 (0.0%)
1	C	0.26	0/3035	0.59	1/4125 (0.0%)
2	X	1.17	0/22	1.63	0/27
2	Y	0.80	0/22	1.64	0/27
2	Z	0.84	0/22	1.61	0/27
All	All	0.27	0/9177	0.60	4/12464 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	LEU	N-CA-C	-5.45	96.28	111.00
1	B	234	LEU	N-CA-C	-5.31	96.67	111.00
1	C	234	LEU	N-CA-C	-5.29	96.73	111.00
1	B	198	TYR	N-CA-C	-5.11	97.20	111.00

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	2960	0	2873	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2966	0	2878	45	0
1	C	2960	0	2873	39	0
2	X	47	0	58	4	0
2	Y	47	0	58	2	0
2	Z	47	0	58	3	0
3	A	202	0	0	5	0
3	B	162	0	0	2	0
3	C	203	0	0	2	0
3	X	4	0	0	0	0
3	Y	3	0	0	0	0
3	Z	4	0	0	0	0
All	All	9605	0	8798	123	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 (123) 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:C:258:PRO:HD2	1:C:268:VAL:HG12	1.55	0.88
1:A:110:ILE:HD11	2:X:2:LEU:HD13	1.56	0.85
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.60	0.84
1:A:366:ARG:HA	1:C:211:GLN:HE22	1.45	0.81
1:B:252:SER:HA	1:B:279:ILE:HD12	1.67	0.77
1:A:2:MET:HG2	1:A:90:GLY:HA2	1.71	0.72
1:A:110:ILE:HD11	2:X:2:LEU:CD1	2.22	0.69
1:B:267:LEU:HD23	1:B:267:LEU:H	1.59	0.66
1:B:169:SER:HB3	3:B:2141:HOH:O	1.96	0.65
1:B:4:ASP:H	1:B:173:SER:HB3	1.61	0.65
1:A:276:PRO:O	1:A:279:ILE:HG12	1.97	0.64
1:B:155:CYS:O	1:B:170:VAL:HG22	1.98	0.64
1:C:276:PRO:O	1:C:279:ILE:HG12	1.98	0.63
1:A:9:LYS:HG2	3:A:1191:HOH:O	1.98	0.62
1:B:270:TRP:O	1:B:317:ASP:HB3	1.99	0.61
1:B:77:GLU:HG2	1:B:104:GLU:HB2	1.84	0.60
1:B:278:ASN:HD22	1:B:279:ILE:N	1.98	0.59
1:A:110:ILE:CD1	2:X:2:LEU:HD13	2.30	0.59
1:B:300:ILE:HG21	1:B:337:ILE:HD13	1.85	0.59
1:A:270:TRP:O	1:A:317:ASP:HB3	2.03	0.57
1:B:149:LEU:HD12	1:B:149:LEU:C	2.24	0.57
1:B:12:GLN:NE2	1:B:113:SER:HA	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.86	0.56
1:C:267:LEU:HD22	1:C:309:VAL:HG21	1.86	0.56
1:B:301:LEU:HD11	1:B:367:THR:HA	1.86	0.56
1:C:363:ASP:HB3	1:C:366:ARG:O	2.06	0.55
1:C:254:THR:HG21	1:C:279:ILE:HG21	1.88	0.55
1:B:303:GLN:NE2	1:B:363:ASP:HB3	2.21	0.55
1:C:238:LYS:O	1:C:242:GLU:HG3	2.08	0.54
1:A:10:SER:HB3	1:A:339:GLU:OE1	2.07	0.53
1:B:215:MET:HE1	1:B:240:VAL:HA	1.91	0.53
1:C:257:PHE:HD2	1:C:268:VAL:HG11	1.73	0.52
1:A:65:LYS:HB3	1:A:65:LYS:NZ	2.23	0.52
1:B:8:GLY:C	1:B:170:VAL:HG12	2.30	0.52
1:A:63:LEU:HG	1:A:81:GLY:HA2	1.91	0.52
1:C:228:ASP:OD2	2:Z:4:24O:H552	2.09	0.51
1:B:30:LEU:HD11	2:Y:2:LEU:HD21	1.92	0.51
1:B:264:GLY:O	1:B:321:LYS:HE3	2.12	0.50
1:C:179:ILE:HG23	1:C:342:TYR:HE2	1.77	0.50
1:A:363:ASP:HB3	1:A:366:ARG:O	2.12	0.50
1:C:261:PHE:CD1	1:C:268:VAL:HG13	2.47	0.50
1:C:292:THR:HG21	1:C:378:ASP:HB3	1.94	0.50
1:C:110:ILE:HD11	2:Z:2:LEU:HD13	1.93	0.49
1:C:217:CYS:HA	1:C:220:TYR:CD1	2.47	0.49
1:C:125:GLU:HG3	3:C:3114:HOH:O	2.12	0.49
1:B:277:TRP:HZ3	1:B:306:LEU:HD12	1.78	0.49
1:B:55:GLN:NE2	1:B:55:GLN:H	2.11	0.49
1:B:55:GLN:CD	1:B:55:GLN:H	2.17	0.48
1:A:232:THR:O	1:A:336:VAL:HG13	2.13	0.48
1:A:41:GLY:HA2	1:A:102:ILE:HB	1.95	0.48
1:C:91:PRO:HD3	1:C:176:ILE:HB	1.96	0.48
1:B:305:TYR:HB2	1:B:324:ILE:HG13	1.95	0.48
1:A:32:ASP:OD1	1:A:230:GLY:HA3	2.14	0.47
1:A:222:TYR:HA	1:A:223:ASP:HA	1.68	0.47
1:A:9:LYS:HD2	3:A:1154:HOH:O	2.13	0.47
1:B:2:MET:CG	1:B:90:GLY:HA2	2.38	0.47
1:A:188:LEU:HD23	1:A:355:ALA:HB2	1.97	0.47
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.96	0.47
1:C:2:MET:HG2	1:C:90:GLY:HA2	1.96	0.47
1:A:228:ASP:OD2	2:X:4:24O:H552	2.14	0.47
1:A:304:GLN:O	1:A:336:VAL:HB	2.15	0.46
1:A:55:GLN:CD	1:A:55:GLN:H	2.17	0.46
1:C:68:TYR:HE1	1:C:75:LYS:HD3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:OD2	1:A:107:LYS:HG3	2.16	0.46
1:A:311:ASP:HB3	1:A:315:SER:HA	1.97	0.46
1:A:179:ILE:HG23	1:A:342:TYR:HE2	1.81	0.45
1:B:232:THR:O	1:B:336:VAL:HG13	2.17	0.45
1:B:278:ASN:HD22	1:B:279:ILE:H	1.63	0.45
1:C:68:TYR:OH	1:C:70:PRO:HB3	2.16	0.45
1:C:73:GLN:HA	1:C:73:GLN:NE2	2.32	0.45
1:B:323:ALA:HB1	1:B:336:VAL:HG11	1.99	0.45
1:A:366:ARG:HA	1:C:211:GLN:NE2	2.25	0.44
1:C:73:GLN:HA	1:C:73:GLN:HE21	1.83	0.44
1:B:267:LEU:HD23	1:B:267:LEU:N	2.30	0.44
1:C:307:ARG:HA	1:C:308:PRO:HD3	1.84	0.44
1:A:170:VAL:HG12	3:A:1186:HOH:O	2.17	0.44
3:A:1152:HOH:O	1:C:299:THR:HG21	2.17	0.44
1:C:13:GLY:HA2	3:C:3146:HOH:O	2.18	0.44
1:C:267:LEU:HD22	1:C:309:VAL:CG2	2.47	0.43
1:B:228:ASP:OD2	2:Y:4:24O:H552	2.18	0.43
1:A:68:TYR:CG	1:B:3:VAL:HG11	2.53	0.43
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.48	0.43
1:A:282:VAL:HG12	1:A:301:LEU:HD23	2.01	0.43
1:A:209:ASN:ND2	1:A:281:PRO:HB3	2.34	0.43
1:C:174:MET:CE	1:C:176:ILE:HD11	2.48	0.43
1:C:375:VAL:O	1:C:375:VAL:HG13	2.19	0.43
1:C:291:VAL:HB	1:C:294:GLN:HG3	2.01	0.43
1:A:21:GLY:HA2	1:A:83:ASP:OD1	2.19	0.43
1:A:205:ARG:HB3	1:A:286:TYR:HB2	2.01	0.43
1:B:197:TRP:CG	1:B:198:TYR:N	2.84	0.43
1:C:63:LEU:HG	1:C:81:GLY:HA2	2.01	0.43
1:B:125:GLU:OE2	1:B:195:ARG:NH2	2.37	0.42
1:A:194:ARG:HB3	1:A:200:GLU:HG2	2.01	0.42
1:A:154:LEU:O	1:A:339:GLU:HA	2.19	0.42
1:C:197:TRP:CG	1:C:198:TYR:N	2.87	0.42
1:A:267:LEU:HD12	1:A:320:TYR:O	2.19	0.42
1:B:188:LEU:HD23	1:B:355:ALA:HB2	2.01	0.42
1:A:23:PRO:HA	1:A:24:PRO:HD3	1.87	0.42
1:B:277:TRP:CZ3	1:B:306:LEU:HD12	2.55	0.42
1:B:257:PHE:HD2	1:B:268:VAL:HG21	1.85	0.42
1:A:238:LYS:O	1:A:242:GLU:HG3	2.20	0.41
1:B:134:GLU:HA	1:B:135:PRO:HD3	1.90	0.41
1:B:110:ILE:HB	1:B:113:SER:HB3	2.02	0.41
1:B:113:SER:O	1:B:114:ASN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:THR:O	1:C:336:VAL:HG13	2.20	0.41
1:C:9:LYS:HZ2	1:C:12:GLN:HG3	1.85	0.41
1:B:278:ASN:HD22	1:B:278:ASN:N	2.18	0.41
1:A:305:TYR:HB2	1:A:324:ILE:HG13	2.02	0.41
1:C:235:ARG:HB3	1:C:327:SER:HB2	2.01	0.41
1:C:255:GLU:OE1	1:C:276:PRO:HG3	2.20	0.41
1:B:224:LYS:HE2	3:B:2111:HOH:O	2.19	0.41
1:A:75:LYS:NZ	3:A:1092:HOH:O	2.54	0.41
1:A:278:ASN:HA	1:A:365:PHE:HZ	1.85	0.41
1:B:301:LEU:H	1:B:304:GLN:NE2	2.19	0.41
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.51	0.41
1:C:110:ILE:CD1	2:Z:2:LEU:HD13	2.52	0.40
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.50	0.40
1:B:63:LEU:HG	1:B:81:GLY:HA2	2.04	0.40
1:B:291:VAL:HG23	1:B:294:GLN:HB3	2.03	0.40
1:C:63:LEU:HD12	1:C:80:LEU:HB3	2.03	0.40
1:B:32:ASP:OD1	1:B:230:GLY:HA3	2.22	0.40
1:A:277:TRP:CZ3	1:A:303:GLN:HA	2.56	0.40
1:A:45:HIS:HA	1:A:46:PRO:HD3	1.96	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	372/402 (92%)	353 (95%)	18 (5%)	1 (0%)	46 36
1	B	373/402 (93%)	352 (94%)	19 (5%)	2 (0%)	34 22
1	C	372/402 (92%)	356 (96%)	16 (4%)	0	100 100
2	X	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
2	Y	2/6 (33%)	1 (50%)	1 (50%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	Z	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
All	All	1123/1224 (92%)	1064 (95%)	56 (5%)	3 (0%)	46 36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	311	ASP
1	A	315	SER
1	B	363	ASP

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/342 (94%)	318 (99%)	3 (1%)	84 84
1	B	322/342 (94%)	312 (97%)	10 (3%)	47 39
1	C	321/342 (94%)	319 (99%)	2 (1%)	90 90
2	X	3/3 (100%)	3 (100%)	0	100 100
2	Y	3/3 (100%)	3 (100%)	0	100 100
2	Z	3/3 (100%)	3 (100%)	0	100 100
All	All	973/1035 (94%)	958 (98%)	15 (2%)	72 70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	197	TRP
1	A	211	GLN
1	B	55	GLN
1	B	92	ASN
1	B	114	ASN
1	B	149	LEU
1	B	170	VAL

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Mol	Chain	Res	Type
1	B	197	TRP
1	B	266	GLN
1	B	278	ASN
1	B	279	ILE
1	B	304	GLN
1	C	79	GLU
1	C	197	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	316	GLN
1	A	326	GLN
1	B	12	GLN
1	B	55	GLN
1	B	92	ASN
1	B	114	ASN
1	B	271	GLN
1	B	278	ASN
1	B	293	ASN
1	B	304	GLN
1	B	326	GLN
1	C	53	GLN
1	C	73	GLN
1	C	114	ASN
1	C	211	GLN
1	C	271	GLN
1	C	326	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 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	$\#\|Z\| > 2$
2	24O	X	4	2	16,16,17	0.87	1 (6%)	12,22,24	2.38	3 (25%)
2	24O	Y	4	2	16,16,17	0.83	0	12,22,24	2.30	3 (25%)
2	24O	Z	4	2	16,16,17	0.78	0	12,22,24	2.26	3 (25%)

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	24O	X	4	2	-	0/13/26/28	0/1/1/1
2	24O	Y	4	2	-	0/13/26/28	0/1/1/1
2	24O	Z	4	2	-	0/13/26/28	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	4	24O	C49-C59	2.03	1.53	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	4	24O	C95-C92-C41	-2.97	109.21	115.77
2	Z	4	24O	C95-C92-C41	-2.89	109.39	115.77
2	Y	4	24O	C95-C92-C41	-2.77	109.66	115.77
2	X	4	24O	O60-C59-C49	-2.58	118.62	125.56
2	Y	4	24O	O60-C59-C49	-2.43	119.04	125.56
2	Z	4	24O	O60-C59-C49	-2.14	119.82	125.56
2	Z	4	24O	C55-C54-C51	6.12	114.30	108.88
2	Y	4	24O	C55-C54-C51	6.27	114.43	108.88
2	X	4	24O	C55-C54-C51	6.46	114.60	108.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	4	24O	1	0
2	Y	4	24O	1	0
2	Z	4	24O	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	376/402 (93%)	0.63	31 (8%) 14 16	30, 44, 74, 107	0
1	B	377/402 (93%)	0.69	47 (12%) 5 5	28, 46, 90, 113	0
1	C	376/402 (93%)	0.47	25 (6%) 22 24	30, 44, 69, 79	0
2	X	3/6 (50%)	0.87	0 100 100	37, 37, 40, 45	0
2	Y	3/6 (50%)	0.80	0 100 100	36, 36, 41, 43	0
2	Z	3/6 (50%)	1.13	0 100 100	38, 38, 40, 44	0
All	All	1138/1224 (92%)	0.60	103 (9%) 11 12	28, 45, 77, 113	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	312	VAL	14.2
1	A	313	ALA	10.9
1	A	315	SER	9.0
1	B	313	ALA	8.7
1	A	312	VAL	8.7
1	B	314	THR	7.9
1	A	314	THR	6.8
1	B	270	TRP	5.9
1	B	254	THR	5.8
1	B	253	SER	5.8
1	B	256	LYS	5.3
1	A	311	ASP	5.2
1	A	259	ASP	5.0
1	B	316	GLN	4.9
1	A	316	GLN	4.8
1	A	170	VAL	4.8
1	C	314	THR	4.5
1	C	313	ALA	4.4
1	C	259	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	257	PHE	4.3
1	B	311	ASP	4.3
1	C	266	GLN	3.9
1	A	309	VAL	3.9
1	C	256	LYS	3.8
1	B	365	PHE	3.8
1	C	55	GLN	3.6
1	A	257	PHE	3.6
1	A	256	LYS	3.6
1	C	312	VAL	3.6
1	A	157	ALA	3.6
1	B	317	ASP	3.5
1	A	21	GLY	3.5
1	B	274	THR	3.5
1	C	316	GLN	3.4
1	B	364	GLU	3.4
1	A	365	PHE	3.3
1	A	266	GLN	3.2
1	C	64	ARG	3.2
1	B	315	SER	3.2
1	B	262	TRP	3.2
1	A	64	ARG	3.1
1	A	23	PRO	3.0
1	A	253	SER	3.0
1	C	-2	SER	3.0
1	C	59	THR	3.0
1	B	267	LEU	3.0
1	B	266	GLN	3.0
1	C	315	SER	3.0
1	A	271	GLN	3.0
1	B	157	ALA	3.0
1	B	260	GLY	2.9
1	C	365	PHE	2.9
1	B	271	GLN	2.9
1	A	258	PRO	2.7
1	B	280	PHE	2.7
1	C	271	GLN	2.7
1	A	56	LEU	2.7
1	B	23	PRO	2.7
1	B	258	PRO	2.7
1	B	268	VAL	2.7
1	B	309	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	59	THR	2.7
1	C	56	LEU	2.6
1	A	364	GLU	2.6
1	B	250	ALA	2.6
1	B	51	TYR	2.6
1	A	55	GLN	2.6
1	B	154	LEU	2.6
1	C	257	PHE	2.5
1	B	64	ARG	2.5
1	A	269	CYS	2.5
1	B	319	CYS	2.5
1	B	170	VAL	2.5
1	C	145	HIS	2.4
1	C	258	PRO	2.4
1	B	56	LEU	2.4
1	C	279	ILE	2.4
1	A	49	HIS	2.4
1	A	361	VAL	2.3
1	B	279	ILE	2.3
1	B	156	GLY	2.3
1	C	260	GLY	2.3
1	A	227	VAL	2.3
1	B	367	THR	2.3
1	B	60	TYR	2.3
1	B	275	THR	2.2
1	A	310	GLU	2.2
1	C	310	GLU	2.2
1	A	317	ASP	2.2
1	B	362	HIS	2.1
1	B	6	LEU	2.1
1	B	59	THR	2.1
1	B	55	GLN	2.1
1	B	261	PHE	2.1
1	B	363	ASP	2.1
1	C	268	VAL	2.1
1	B	145	HIS	2.0
1	C	63	LEU	2.0
1	B	22	SER	2.0
1	C	254	THR	2.0
1	B	9	LYS	2.0
1	C	359	CYS	2.0
1	A	154	LEU	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
2	24O	Y	4	16/17	0.97	0.14	-	34,36,38,39	0
2	24O	X	4	16/17	0.96	0.18	-	35,37,37,37	0
2	24O	Z	4	16/17	0.98	0.17	-	35,37,38,39	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.