



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:28 PM GMT

PDB ID : 3ZKM  
Title : BACE2 FAB COMPLEX  
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Deposited on : 2013-01-23  
Resolution : 1.85 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

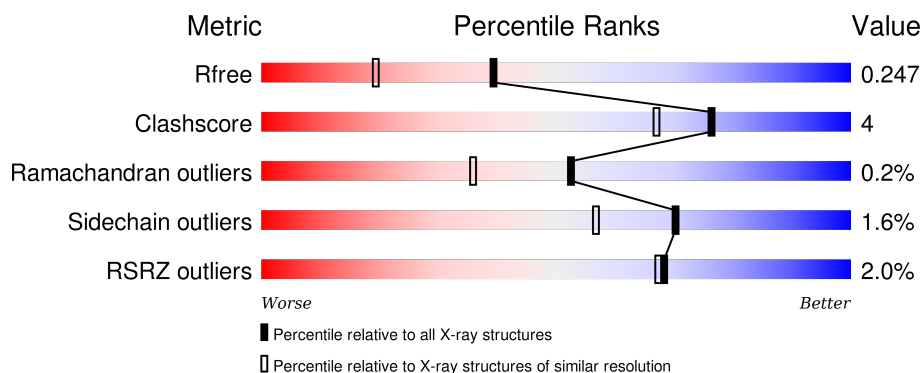
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	386	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
1	B	386	<div> <div>3%</div> <div>88%</div> <div>8%</div> <div>..</div> </div>
2	C	221	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>..</div> </div>
2	H	221	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>
3	D	218	<div> <div>2%</div> <div>90%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	218	 <div>90%9%</div>

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
4	SO4	A	1398	-	-	-	X
5	DMS	A	1399	-	-	-	X
5	DMS	B	1399	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13629 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	375	Total	C	N	O	S	0	6	0
			2959	1905	470	571	13			
1	B	375	Total	C	N	O	S	0	5	0
			2953	1902	469	569	13			

- Molecule 2 is a protein called FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	3	1
			1653	1048	273	324	8			
2	H	217	Total	C	N	O	S	0	4	1
			1658	1050	274	326	8			

- Molecule 3 is a protein called FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	217	Total	C	N	O	S	0	4	0
			1707	1057	296	347	7			
3	L	217	Total	C	N	O	S	0	5	0
			1716	1062	297	350	7			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula:  $C_2H_6OS$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

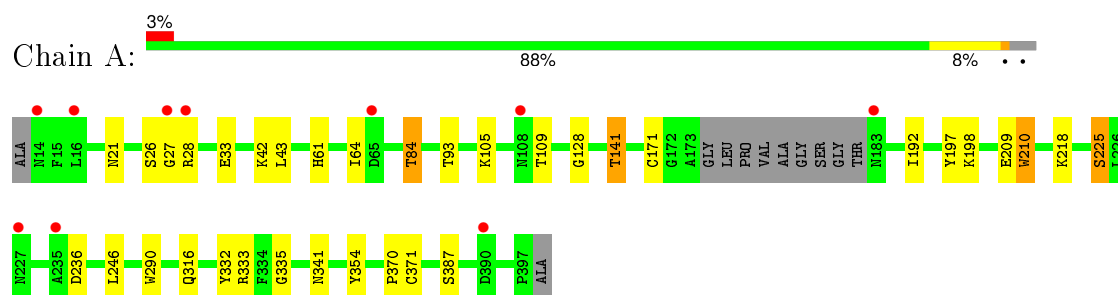
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	177	Total	O	0	0
			177	177		
7	B	174	Total	O	0	0
			174	174		
7	C	153	Total	O	0	0
			153	153		
7	D	141	Total	O	0	0
			141	141		
7	H	157	Total	O	0	0
			157	157		
7	L	151	Total	O	0	0
			151	151		

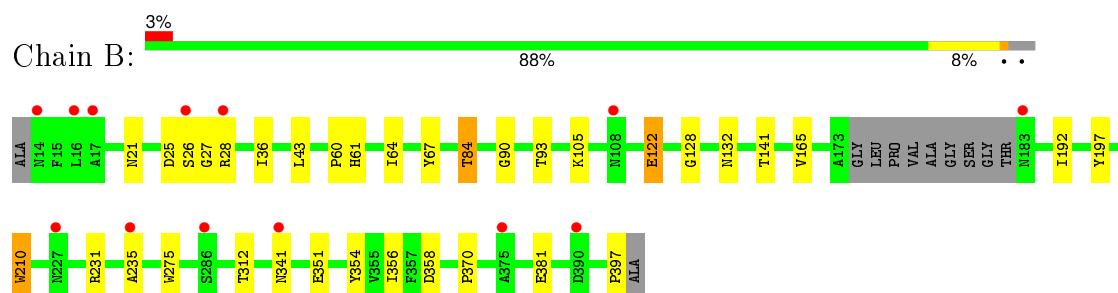
### 3 Residue-property plots [i](#)

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.

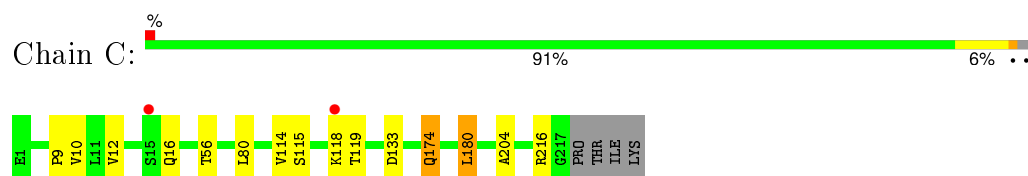
- Molecule 1: BETA-SECRETASE 2



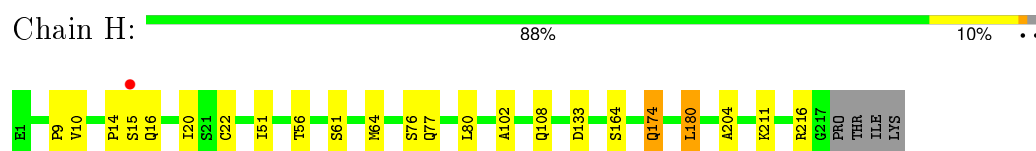
- Molecule 1: BETA-SECRETASE 2



- Molecule 2: FAB HEAVY CHAIN

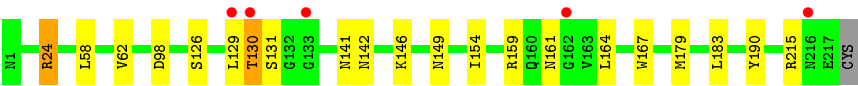


- Molecule 2: FAB HEAVY CHAIN

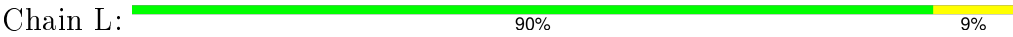


- Molecule 3: FAB LIGHT CHAIN





● Molecule 3: FAB LIGHT CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.94Å 161.10Å 163.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.86 – 1.85 43.82 – 1.85	Depositor EDS
% Data completeness (in resolution range)	84.8 (44.86-1.85) 84.8 (43.82-1.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, $R_{free}$	0.211 , 0.245 0.212 , 0.247	Depositor DCC
$R_{free}$ test set	7695 reflections (6.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.5	EDS
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	7 of 129945 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	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 49.81 % 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 7.0770e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DMS, PCA, SO4

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	0.55	0/3034	0.68	0/4129
1	B	0.54	0/3028	0.66	0/4121
2	C	0.59	1/1688 (0.1%)	0.70	1/2309 (0.0%)
2	H	0.62	1/1692 (0.1%)	0.71	1/2314 (0.0%)
3	D	0.55	0/1747	0.69	0/2377
3	L	0.57	0/1756	0.69	0/2389
All	All	0.57	2/12945 (0.0%)	0.68	2/17639 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	216	ARG	C-N	-5.10	1.23	1.33
2	C	216	ARG	C-N	-5.09	1.23	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	180	LEU	CA-CB-CG	6.27	129.73	115.30
2	C	180	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2959	0	2859	21	0
1	B	2953	0	2853	23	0
2	C	1653	0	1621	10	0
2	H	1658	0	1619	11	0
3	D	1707	0	1615	19	0
3	L	1716	0	1620	14	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	C	6	0	8	0	0
6	H	6	0	8	0	0
7	A	177	0	0	3	0
7	B	174	0	0	5	0
7	C	153	0	0	2	0
7	D	141	0	0	5	0
7	H	157	0	0	2	0
7	L	151	0	0	4	0
All	All	13629	0	12215	93	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 4.

All (93) 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)
3:D:131:SER:HB2	7:D:2096:HOH:O	1.64	0.98
3:D:149:ASN:HB3	7:D:2107:HOH:O	1.76	0.84
2:H:51:ILE:CB	2:H:51:ILE:CD1	2.56	0.83
1:A:341:ASN:OD1	7:A:2110:HOH:O	1.96	0.83
1:A:171:CYS:HG	1:A:371:CYS:HG	1.06	0.82
1:B:165:VAL:HG13	1:B:358:ASP:HA	1.62	0.81
2:H:108:GLN:NE2	7:H:2079:HOH:O	2.14	0.79
2:H:174:GLN:HE21	3:L:164:LEU:HD21	1.51	0.76
3:L:149:ASN:HB3	7:L:2112:HOH:O	1.88	0.73
3:D:129:LEU:O	3:D:131:SER:N	2.21	0.72
2:C:174:GLN:HE21	3:D:164:LEU:HD21	1.56	0.71
3:D:129:LEU:C	3:D:131:SER:H	1.94	0.70
1:B:28:ARG:HB2	7:B:2003:HOH:O	1.94	0.68
1:B:341:ASN:OD1	7:B:2108:HOH:O	2.12	0.67
1:A:218:LYS:HD3	1:A:225:SER:HB2	1.79	0.62
3:L:127[B]:GLU:HG3	7:L:2095:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:HIS:HB3	1:A:64:ILE:HG12	1.84	0.60
1:A:84[B]:THR:HG23	7:A:2042:HOH:O	2.02	0.59
3:L:140:LEU:HD13	3:L:179:MET:HE2	1.84	0.59
1:A:236:ASP:OD2	1:A:341:ASN:HB2	2.03	0.59
1:A:33:GLU:CD	1:A:42:LYS:HD2	2.22	0.59
3:D:190:TYR:CE2	3:D:215:ARG:HD3	2.39	0.58
3:L:24[B]:ARG:HD2	7:L:2022:HOH:O	2.05	0.56
7:B:2136:HOH:O	2:C:56[A]:THR:HG21	2.06	0.56
3:L:190:TYR:CE2	3:L:215:ARG:HD3	2.41	0.56
1:B:84[B]:THR:HG23	7:B:2042:HOH:O	2.06	0.55
1:B:26:SER:OG	1:B:27:GLY:N	2.40	0.55
1:A:141:THR:HG21	1:A:209:GLU:O	2.07	0.54
2:C:118:LYS:HG2	2:C:119:THR:N	2.22	0.54
1:B:36:ILE:HD12	1:B:43[B]:LEU:HD13	1.90	0.54
2:C:118:LYS:HG2	2:C:119:THR:H	1.74	0.53
3:L:41:GLN:HB2	3:L:51:LEU:HD11	1.92	0.52
2:H:61:SER:O	2:H:64:MET:HG2	2.09	0.52
1:B:90:GLY:HA2	1:B:122:GLU:O	2.10	0.52
3:D:129:LEU:C	3:D:131:SER:N	2.62	0.51
3:D:146:LYS:HE3	7:D:2100:HOH:O	2.09	0.51
1:B:192:ILE:HG23	1:B:354:TYR:HE2	1.75	0.51
1:A:26:SER:OG	1:A:27:GLY:N	2.45	0.50
3:D:24[B]:ARG:HD2	7:D:2024:HOH:O	2.11	0.49
3:D:126:SER:O	3:D:130:THR:N	2.37	0.49
7:A:2139:HOH:O	2:H:56[A]:THR:HG21	2.14	0.48
1:B:84[B]:THR:HG22	1:B:93:THR:OG1	2.13	0.48
2:C:115:SER:O	7:C:2085:HOH:O	2.19	0.48
3:D:154:ILE:HD11	3:D:183:LEU:HD21	1.94	0.48
3:L:140:LEU:HD13	3:L:179:MET:CE	2.43	0.48
1:A:141:THR:HG23	1:A:210:TRP:HA	1.96	0.47
1:B:21:ASN:HA	1:B:105:LYS:HD3	1.95	0.47
1:B:141:THR:CG2	1:B:210:TRP:HA	2.44	0.47
3:D:159:ARG:HD2	3:D:161:ASN:O	2.14	0.47
2:H:9:PRO:HG3	7:H:2016:HOH:O	2.14	0.47
1:A:141:THR:CG2	1:A:210:TRP:HA	2.45	0.47
1:B:235:ALA:HA	1:B:397:PRO:HG2	1.95	0.47
3:D:141:ASN:HB3	3:D:142:ASN:HD22	1.79	0.47
2:H:10:VAL:HG11	2:H:204:ALA:HA	1.98	0.46
3:L:167:TRP:CD2	3:L:179:MET:HG3	2.51	0.45
2:H:22:CYS:O	2:H:77:GLN:HA	2.17	0.45
1:B:61:HIS:HB3	1:B:64:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ARG:HD2	1:B:128:GLY:O	2.17	0.45
1:B:275[A]:TRP:CH2	3:D:98[A]:ASP:CB	3.00	0.45
1:B:192:ILE:HG12	1:B:356:ILE:HG12	1.99	0.44
2:C:174:GLN:HB2	3:D:164:LEU:HD21	1.99	0.44
1:A:84[B]:THR:HG22	1:A:93:THR:HG23	2.00	0.44
2:H:211:LYS:HA	2:H:211:LYS:HD3	1.85	0.44
3:D:58:LEU:HD11	3:D:62:VAL:HG12	2.00	0.44
1:B:26:SER:HB3	1:B:351:GLU:OE2	2.17	0.43
3:D:159:ARG:HG2	3:D:183:LEU:HD11	2.01	0.43
1:A:42:LYS:O	1:A:43[A]:LEU:HD23	2.17	0.43
2:H:20:ILE:HD12	2:H:80:LEU:HD22	1.99	0.43
1:A:197:TYR:HA	1:A:370:PRO:HD3	2.00	0.43
3:L:12:ALA:HA	3:L:109:GLU:O	2.19	0.43
1:B:231:ARG:HB3	1:B:397:PRO:HG3	2.01	0.43
2:C:9:PRO:HG3	7:C:2016:HOH:O	2.18	0.42
2:C:10:VAL:HG11	2:C:204:ALA:HB2	2.01	0.42
2:H:14:PRO:C	2:H:16:GLN:H	2.23	0.42
3:D:130:THR:HA	7:D:2129:HOH:O	2.18	0.42
2:C:12:VAL:O	2:C:114:VAL:HA	2.20	0.42
1:B:25:ASP:HB2	7:B:2004:HOH:O	2.18	0.42
1:B:60:PRO:HG3	1:B:67:TYR:CE1	2.54	0.42
3:L:30:ASP:HA	3:L:34:HIS:O	2.20	0.42
1:A:28:ARG:HD2	1:A:128:GLY:O	2.18	0.42
1:A:246:LEU:HD22	1:A:335:GLY:HA2	2.01	0.42
1:B:312:THR:HB	1:B:381:GLU:HB2	2.02	0.41
3:L:141:ASN:HB3	3:L:142:ASN:HD22	1.84	0.41
1:A:21:ASN:HA	1:A:105:LYS:HD3	2.03	0.41
1:B:197:TYR:HA	1:B:370:PRO:HD3	2.01	0.41
3:L:10:SER:HB3	7:L:2011:HOH:O	2.21	0.41
1:A:192:ILE:HG23	1:A:354:TYR:HE2	1.86	0.41
1:A:290:TRP:CD2	1:A:316:GLN:HG3	2.55	0.41
1:A:43[A]:LEU:HA	1:A:43[A]:LEU:HD23	1.89	0.41
1:A:332:TYR:HB2	3:L:32:TYR:OH	2.21	0.41
3:D:167:TRP:CD2	3:D:179:MET:HG3	2.56	0.40
1:B:21:ASN:HB3	1:B:105:LYS:HB3	2.03	0.40
2:C:80:LEU:C	2:C:80:LEU:HD23	2.41	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	377/386 (98%)	366 (97%)	11 (3%)	0	100	100
1	B	376/386 (97%)	366 (97%)	10 (3%)	0	100	100
2	C	218/221 (99%)	208 (95%)	9 (4%)	1 (0%)	34	17
2	H	219/221 (99%)	211 (96%)	6 (3%)	2 (1%)	21	7
3	D	219/218 (100%)	209 (95%)	9 (4%)	1 (0%)	34	17
3	L	220/218 (101%)	213 (97%)	7 (3%)	0	100	100
All	All	1629/1650 (99%)	1573 (97%)	52 (3%)	4 (0%)	52	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	130	THR
2	H	15	SER
2	C	16	GLN
2	H	102	ALA

### 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	321/320 (100%)	312 (97%)	9 (3%)	51	33
1	B	320/320 (100%)	315 (98%)	5 (2%)	70	57
2	C	190/191 (100%)	187 (98%)	3 (2%)	70	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	190/191 (100%)	185 (97%)	5 (3%)	54	36
3	D	193/190 (102%)	191 (99%)	2 (1%)	82	76
3	L	194/190 (102%)	193 (100%)	1 (0%)	92	90
All	All	1408/1402 (100%)	1383 (98%)	25 (2%)	70	52

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84[A]	THR
1	A	84[B]	THR
1	A	109	THR
1	A	141	THR
1	A	198	LYS
1	A	210	TRP
1	A	225	SER
1	A	333	ARG
1	A	387	SER
1	B	84[A]	THR
1	B	84[B]	THR
1	B	122	GLU
1	B	132	ASN
1	B	210	TRP
2	C	133	ASP
2	C	174	GLN
2	C	180	LEU
3	D	24[A]	ARG
3	D	24[B]	ARG
2	H	76	SER
2	H	133	ASP
2	H	164	SER
2	H	174	GLN
2	H	180	LEU
3	L	217	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	108	ASN
1	A	285	ASN

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Mol	Chain	Res	Type
1	B	285	ASN
2	C	16	GLN
2	C	101	ASN
2	C	174	GLN
3	D	141	ASN
3	D	142	ASN
3	D	160	GLN
2	H	101	ASN
2	H	174	GLN
3	L	141	ASN
3	L	142	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	$\# Z  > 2$
2	PCA	C	1	2	7,8,9	0.42	0	9,10,12	0.87	0
2	PCA	H	1	2	7,8,9	0.47	0	9,10,12	0.88	0

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	PCA	C	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1



There are no bond length outliers.

There are no bond angle outliers.

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](#)

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	$\# Z  > 2$
4	SO4	A	1398	-	4,4,4	0.37	0	6,6,6	0.19	0
5	DMS	A	1399	-	3,3,3	0.42	0	3,3,3	0.59	0
4	SO4	B	1398	-	4,4,4	0.41	0	6,6,6	0.21	0
5	DMS	B	1399	-	3,3,3	0.45	0	3,3,3	0.56	0
6	GOL	C	1217	-	5,5,5	0.38	0	5,5,5	0.67	0
6	GOL	H	1217	-	5,5,5	0.17	0	5,5,5	0.50	0

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
4	SO4	A	1398	-	-	0/0/0/0	0/0/0/0
5	DMS	A	1399	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1398	-	-	0/0/0/0	0/0/0/0
5	DMS	B	1399	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	C	1217	-	-	0/4/4/4	0/0/0/0
6	GOL	H	1217	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	375/386 (97%)	0.13	10 (2%) 58 55	10, 21, 40, 57	5 (1%)
1	B	375/386 (97%)	0.19	13 (3%) 48 45	11, 22, 42, 53	6 (1%)
2	C	216/221 (97%)	0.06	2 (0%) 85 85	8, 21, 39, 50	3 (1%)
2	H	216/221 (97%)	-0.12	1 (0%) 91 91	9, 17, 30, 52	4 (1%)
3	D	217/218 (99%)	-0.02	5 (2%) 64 62	9, 19, 43, 66	2 (0%)
3	L	217/218 (99%)	-0.14	1 (0%) 91 91	9, 18, 38, 62	2 (0%)
All	All	1616/1650 (97%)	0.04	32 (1%) 68 67	8, 20, 40, 66	22 (1%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	235	ALA	6.9
2	H	15	SER	6.1
1	B	108	ASN	4.8
1	B	183	ASN	4.3
2	C	15	SER	4.1
1	B	28	ARG	3.7
1	B	235	ALA	3.7
1	A	108	ASN	3.6
1	A	390	ASP	3.3
3	D	129	LEU	3.3
1	B	14	ASN	3.1
1	A	183	ASN	3.1
1	B	390	ASP	3.0
1	B	17	ALA	3.0
1	B	16	LEU	2.9
3	D	216	ASN	2.9
3	D	133	GLY	2.8
1	B	375	ALA	2.7
1	A	227	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	14	ASN	2.7
1	B	26	SER	2.6
3	L	216	ASN	2.6
1	A	27	GLY	2.5
1	A	16	LEU	2.5
1	B	227	ASN	2.4
1	A	28	ARG	2.4
2	C	118	LYS	2.2
3	D	162	GLY	2.2
1	B	286	SER	2.1
3	D	130	THR	2.1
1	B	341	ASN	2.1
1	A	65	ASP	2.1

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PCA	C	1	8/9	0.96	0.09	-	16,18,20,21	0
2	PCA	H	1	8/9	0.95	0.10	-	16,20,23,23	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	DMS	B	1399	4/4	0.98	0.17	3.06	35,37,39,39	0
4	SO4	A	1398	5/5	0.93	0.14	2.12	58,62,65,65	0
5	DMS	A	1399	4/4	0.96	0.14	2.10	36,37,39,41	0
4	SO4	B	1398	5/5	0.94	0.12	1.55	58,58,63,64	0
6	GOL	C	1217	6/6	0.95	0.08	-1.19	22,23,24,24	0
6	GOL	H	1217	6/6	0.96	0.08	-1.37	26,26,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.