



Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2016 – 11:20 PM EDT

PDB ID : 5FKJ
Title : Crystal structure of mouse acetylcholinesterase in complex with C-547, an alkyl ammonium derivative of 6-methyl uracil
Authors : Nachon, F.; Villard-Wandhammer, M.; Petrov, K.; Masson, P.
Deposited on : 2015-10-16
Resolution : 3.13 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

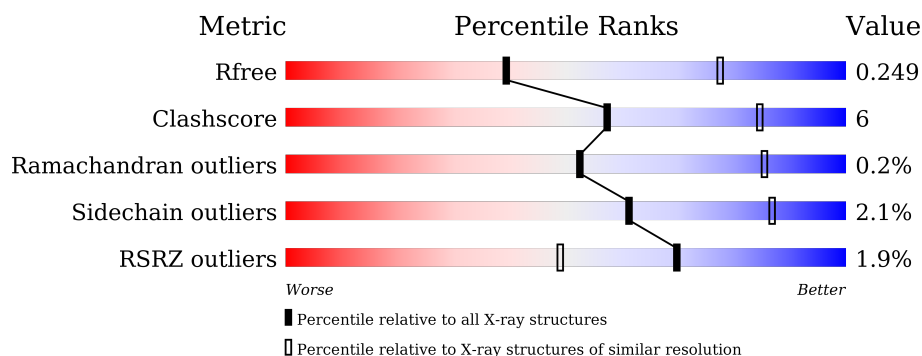
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.13 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	1095 (3.18-3.10)
Clashscore	102246	1202 (3.18-3.10)
Ramachandran outliers	100387	1162 (3.18-3.10)
Sidechain outliers	100360	1162 (3.18-3.10)
RSRZ outliers	91569	1097 (3.18-3.10)

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 $\leq 5\%$. 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	543	<div> <div></div> <div>85%14%.</div> </div>
1	B	543	<div> <div>6%</div> <div>79%19%..</div> </div>
1	C	543	<div> <div>%</div> <div>86%13%. .</div> </div>
1	D	543	<div> <div>%</div> <div>84%14%. .</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	G0W	A	550	-	-	-	X
2	G0W	B	550	-	-	-	X
2	G0W	C	550	-	-	-	X

2 Entry composition [i](#)

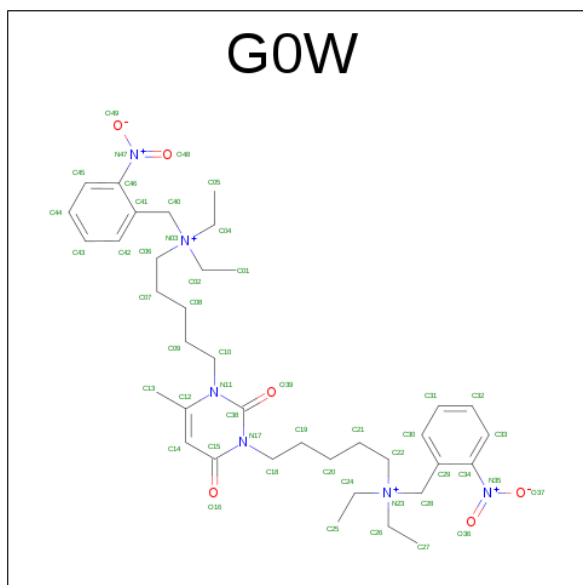
There are 6 unique types of molecules in this entry. The entry contains 17437 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	0	0
			4211	2700	732	765	14			
1	B	538	Total	C	N	O	S	0	3	0
			4207	2700	730	763	14			
1	C	536	Total	C	N	O	S	0	2	0
			4185	2686	724	761	14			
1	D	536	Total	C	N	O	S	0	0	0
			4173	2678	724	757	14			

- Molecule 2 is 1,3-BIS[5(DIETHYL-O-NITROBENZYLAMMONIUM)PENTYL]-6-METHYLURACIL (three-letter code: G0W) (formula: $C_{37}H_{56}N_6O_6$).



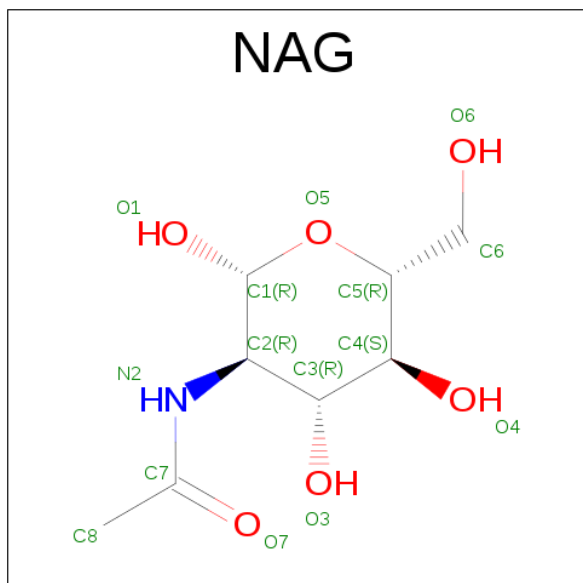
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			49	37	6	6		
2	B	1	Total	C	N	O	0	0
			31	23	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			49	37	6	6		
2	D	1	Total	C	N	O	0	0
			31	23	4	4		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

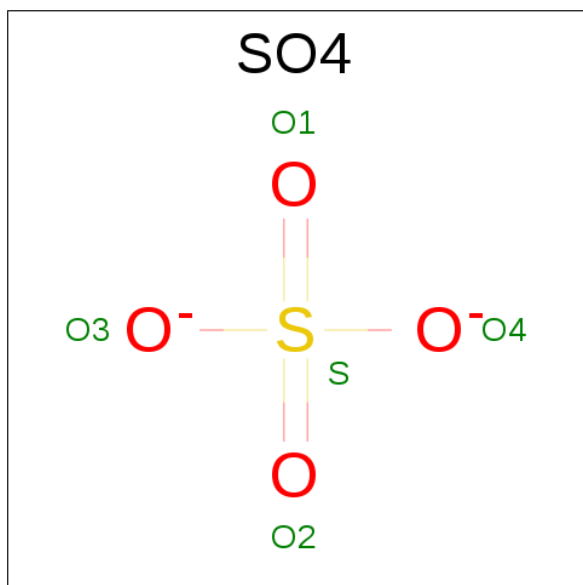
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cl	0	0
			4	4		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	9	Total	Cl	0	0
			9	9		
4	D	6	Total	Cl	0	0
			6	6		
4	C	9	Total	Cl	0	0
			9	9		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	56	Total	O	0	0
			56	56		
6	C	110	Total	O	0	0
			110	110		

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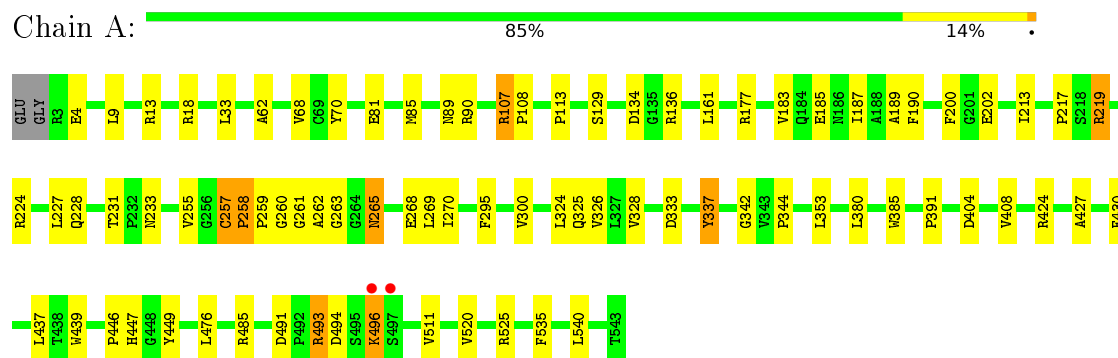
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	102	Total 102	O 102	0	0

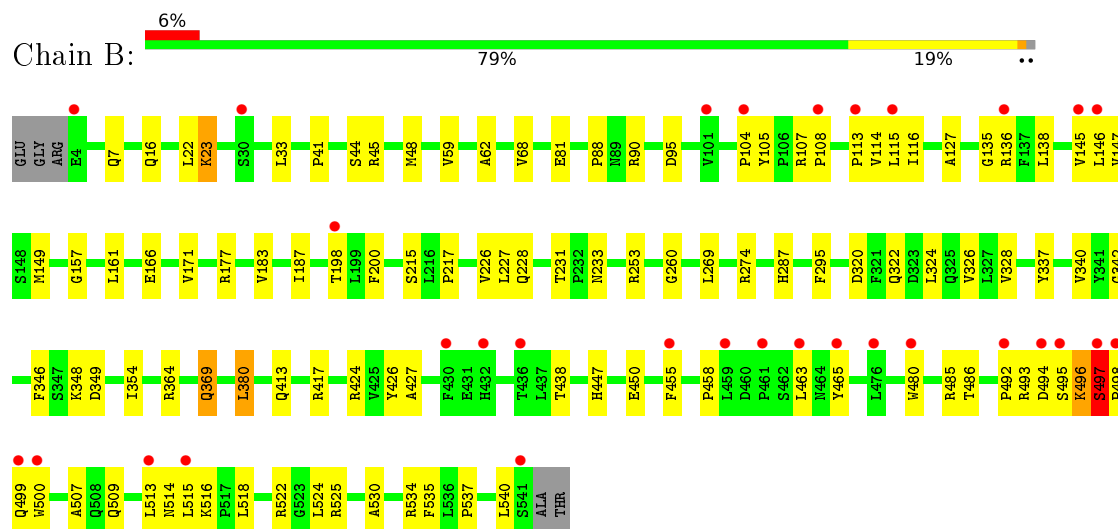
3 Residue-property plots

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.

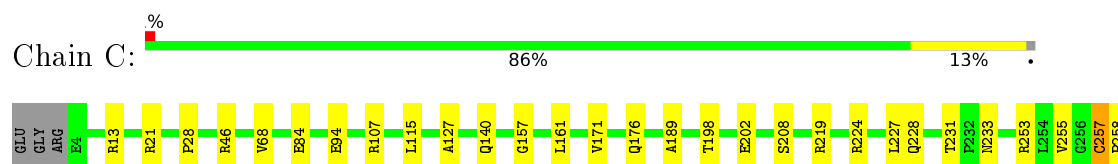
• Molecule 1: ACETYLCHOLINESTERASE

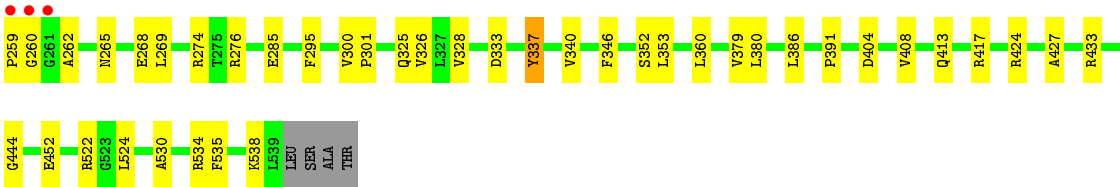


• Molecule 1: ACETYLCHOLINESTERASE

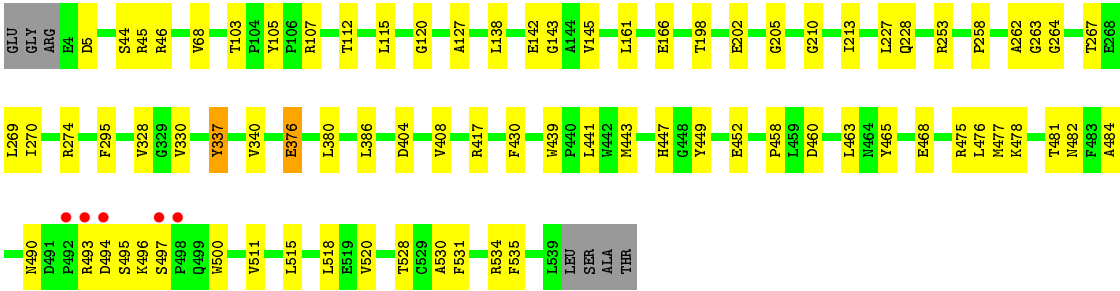
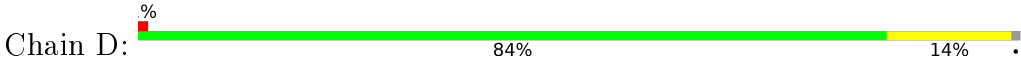


• Molecule 1: ACETYLCHOLINESTERASE





● Molecule 1: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.15Å 175.45Å 224.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	94.52 – 3.13 94.52 – 3.13	Depositor EDS
% Data completeness (in resolution range)	99.3 (94.52-3.13) 99.4 (94.52-3.13)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 3.13Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.207 , 0.249 0.205 , 0.249	Depositor DCC
R_{free} test set	1044 reflections (1.10%)	DCC
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17437	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, GOW, SO4, NAG

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	0.30	0/4337	0.53	2/5926 (0.0%)
1	B	0.29	0/4342	0.54	1/5933 (0.0%)
1	C	0.31	0/4317	0.55	2/5900 (0.0%)
1	D	0.28	0/4299	0.49	0/5876
All	All	0.29	0/17295	0.53	5/23635 (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	A	0	3
1	B	0	3
1	C	0	1
All	All	0	7

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	CYS	CA-CB-SG	6.18	125.13	114.00
1	C	524	LEU	CA-CB-CG	5.61	128.19	115.30
1	A	257	CYS	CA-CB-SG	5.31	123.56	114.00
1	A	258	PRO	C-N-CD	-5.04	109.51	120.60
1	B	524	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	260	GLY	Peptide
1	A	496	LYS	Peptide
1	A	540	LEU	Peptide
1	B	260	GLY	Peptide
1	B	342	GLY	Peptide
1	B	497	SER	Peptide
1	C	262	ALA	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4211	0	4102	52	0
1	B	4207	0	4103	71	0
1	C	4185	0	4073	38	0
1	D	4173	0	4060	51	0
2	A	49	0	0	2	0
2	B	31	0	0	0	0
2	C	49	0	0	1	0
2	D	31	0	0	0	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	0	0
3	D	28	0	26	0	0
4	A	9	0	0	0	0
4	B	4	0	0	1	0
4	C	9	0	0	0	0
4	D	6	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
6	A	106	0	0	3	0
6	B	56	0	0	2	0
6	C	110	0	0	3	0
6	D	102	0	0	2	0
All	All	17437	0	16416	201	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 6.

All (201) 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:HB2	1:C:260:GLY:H	1.42	0.84
1:A:265:ASN:HB2	1:A:268:GLU:H	1.51	0.76
1:A:535:PHE:HB2	1:B:380:LEU:HD13	1.69	0.74
1:D:530:ALA:O	1:D:534:ARG:HB2	1.87	0.72
1:B:513:LEU:HD23	1:B:518:LEU:HD21	1.70	0.72
1:A:342:GLY:HA2	1:D:263:GLY:HA2	1.73	0.70
1:C:538:LYS:HE3	1:D:376:GLU:HG2	1.77	0.67
1:C:353:LEU:HB3	1:C:391:PRO:HB2	1.77	0.66
1:D:161:LEU:HD11	1:D:269:LEU:HD22	1.78	0.66
1:B:424:ARG:NH1	1:B:426:TYR:OH	2.28	0.66
1:B:161:LEU:HD11	1:B:269:LEU:HD22	1.77	0.65
1:A:404:ASP:HA	1:A:408:VAL:HB	1.79	0.65
1:C:258:PRO:HB2	1:C:260:GLY:N	2.11	0.65
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.77	0.65
1:B:498:PRO:CG	1:B:518:LEU:HB2	2.28	0.64
1:A:344:PRO:HG3	1:D:264:GLY:HA3	1.80	0.64
1:C:258:PRO:CB	1:C:260:GLY:H	2.12	0.63
1:D:258:PRO:HG2	1:D:262:ALA:HA	1.80	0.63
1:A:380:LEU:HD12	1:B:535:PHE:HB2	1.80	0.63
1:B:369[A]:GLN:NE2	6:B:2048:HOH:O	2.32	0.62
1:D:439:TRP:HE1	1:D:449:TYR:HH	1.48	0.62
1:D:103:THR:HG22	1:D:145:VAL:HG22	1.80	0.61
1:B:113:PRO:HG3	1:B:485:ARG:HB3	1.83	0.61
1:C:274:ARG:NH2	6:C:2043:HOH:O	2.33	0.61
1:C:360:LEU:HD13	1:C:379:VAL:HG21	1.83	0.60
1:B:499:GLN:HG3	1:B:500:TRP:H	1.67	0.60
1:C:380:LEU:HD22	1:D:535:PHE:HB2	1.83	0.60
1:C:107:ARG:NH1	1:C:189:ALA:O	2.35	0.59
1:B:183:VAL:O	1:B:187:ILE:HB	2.02	0.59
1:A:265:ASN:HB2	1:A:268:GLU:HB2	1.86	0.58
2:A:550:GOW:O48	1:D:262:ALA:HB2	2.02	0.58
1:B:494:ASP:OD1	1:B:495:SER:N	2.28	0.57
1:A:224:ARG:HG2	1:A:325:GLN:HB2	1.87	0.57
1:A:408:VAL:HG11	1:A:525:ARG:HD2	1.86	0.57
1:B:115:LEU:HD23	1:B:198:THR:HB	1.87	0.57
1:C:161:LEU:HD11	1:C:269:LEU:HD23	1.86	0.56
1:D:161:LEU:HD12	1:D:270:ILE:HD11	1.87	0.56
1:A:446:PRO:HG2	1:A:449:TYR:CD2	2.41	0.56
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.87	0.56
1:A:300:VAL:O	6:A:2047:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ARG:HH11	1:C:28:PRO:HB3	1.71	0.55
1:D:495:SER:C	1:D:497:SER:H	2.09	0.55
1:B:7:GLN:HG3	1:B:105:TYR:HE1	1.72	0.55
1:C:452:GLU:HG3	6:C:2099:HOH:O	2.07	0.55
1:D:166:GLU:HG2	1:D:274:ARG:HH22	1.72	0.55
1:A:491:ASP:HB3	1:A:494:ASP:HB3	1.89	0.54
1:B:498:PRO:HG2	1:B:518:LEU:HB2	1.89	0.54
1:B:348:LYS:NZ	1:B:349:ASP:OD1	2.39	0.54
1:B:104:PRO:HG2	1:B:108:PRO:HG3	1.87	0.54
1:C:68:VAL:HG13	1:C:127:ALA:HB2	1.90	0.53
1:B:45:ARG:HD3	1:B:48:MET:HB2	1.89	0.53
1:D:478:LYS:O	1:D:482:ASN:ND2	2.42	0.53
1:D:115:LEU:HD23	1:D:198:THR:HB	1.89	0.53
1:A:107:ARG:NH1	1:A:189:ALA:O	2.42	0.53
1:D:452:GLU:HG3	6:D:2091:HOH:O	2.09	0.52
1:B:138:LEU:HD21	1:B:455:PHE:HA	1.91	0.52
1:C:46:ARG:NH2	1:C:94:GLU:OE2	2.26	0.52
1:B:68:VAL:HG23	1:B:90:ARG:HB2	1.91	0.52
1:D:112:THR:HG21	1:D:143:GLY:O	2.09	0.52
1:B:200:PHE:HB2	1:B:226:VAL:HB	1.91	0.52
1:B:320:ASP:OD1	1:B:322:GLN:HG3	2.11	0.51
1:B:413:GLN:NE2	4:B:607:CL:CL	2.72	0.51
1:A:13:ARG:NE	1:A:185:GLU:HB3	2.25	0.51
1:B:157:GLY:O	1:B:171:VAL:HG22	2.10	0.51
1:A:107:ARG:HG3	1:A:108:PRO:HD2	1.91	0.51
1:B:227:LEU:HB2	1:B:328:VAL:HG12	1.92	0.51
1:C:224:ARG:HG2	1:C:325:GLN:HB2	1.93	0.51
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.47	0.50
1:B:68:VAL:HG13	1:B:127:ALA:HB2	1.93	0.50
1:A:437:LEU:HD11	1:A:446:PRO:HD2	1.94	0.50
1:B:44:SER:HA	1:B:274:ARG:HD2	1.94	0.50
1:B:337:TYR:O	1:B:340:VAL:HG22	2.12	0.49
1:D:337:TYR:CZ	1:D:447:HIS:HB3	2.47	0.49
1:B:16:GLN:HB2	1:B:59:VAL:HA	1.95	0.48
1:D:337:TYR:O	1:D:340:VAL:HG22	2.12	0.48
1:B:492:PRO:HG2	1:B:493[A]:ARG:HD2	1.95	0.48
1:D:142:GLU:HB3	1:D:481:THR:HG21	1.95	0.48
1:D:468:GLU:HB3	1:D:515:LEU:HD11	1.95	0.48
1:A:257:CYS:N	1:A:258:PRO:HD3	2.28	0.48
1:C:346:PHE:HA	1:C:352:SER:OG	2.13	0.48
1:A:213:ILE:HA	1:A:219:ARG:HD3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:VAL:O	1:C:427:ALA:HA	2.14	0.48
1:D:44:SER:HA	1:D:274:ARG:HD2	1.95	0.48
1:D:202:GLU:HA	1:D:228:GLN:O	2.14	0.48
1:A:107:ARG:HD2	1:A:190:PHE:HA	1.96	0.48
2:A:550:GOW:C44	1:D:253:ARG:HG3	2.44	0.47
1:B:497:SER:HB3	1:B:498:PRO:CD	2.43	0.47
1:C:231:THR:HB	1:C:233:ASN:OD1	2.14	0.47
1:B:287:HIS:CD2	1:C:253:ARG:HH12	2.32	0.47
1:D:490:ASN:HD21	1:D:500:TRP:H	1.63	0.47
1:B:515:LEU:HD23	1:B:515:LEU:HA	1.69	0.47
1:B:200:PHE:CB	1:B:226:VAL:HB	2.45	0.47
1:B:287:HIS:CD2	1:C:253:ARG:HH22	2.32	0.47
1:A:177:ARG:CZ	1:A:217:PRO:HB2	2.45	0.47
1:C:522:ARG:HE	1:D:386:LEU:HD21	1.78	0.47
1:A:161:LEU:HD12	1:A:270:ILE:HD11	1.96	0.47
1:B:114:VAL:HG12	1:B:145:VAL:HB	1.97	0.47
1:B:166:GLU:N	1:B:166:GLU:OE1	2.48	0.46
1:A:161:LEU:HD11	1:A:269:LEU:HD23	1.97	0.46
1:A:81:GLU:O	1:A:85:MET:HB3	2.15	0.46
1:B:135:GLY:HA3	1:B:146:LEU:HD22	1.98	0.46
1:B:116:ILE:HA	1:B:147:VAL:O	2.16	0.46
1:C:404:ASP:HA	1:C:408:VAL:HB	1.97	0.46
1:B:516:LYS:HG3	1:B:516:LYS:H	1.50	0.46
1:B:537:PRO:O	1:B:540:LEU:HD23	2.16	0.46
1:B:177:ARG:NH2	1:B:215:SER:OG	2.49	0.46
1:C:115:LEU:HD23	1:C:198:THR:HB	1.97	0.46
1:B:507:ALA:HB1	1:B:509:GLN:HG3	1.98	0.46
1:C:326:VAL:HG12	1:C:328:VAL:HG13	1.99	0.45
1:D:5:ASP:OD2	1:D:105:TYR:OH	2.29	0.45
1:A:328:VAL:O	1:A:427:ALA:HA	2.16	0.45
1:B:463:LEU:HD23	1:B:463:LEU:O	2.16	0.45
1:A:33:LEU:N	1:A:62:ALA:O	2.33	0.45
1:D:166:GLU:OE1	1:D:267:THR:HG22	2.17	0.45
1:D:528:THR:O	1:D:531:PHE:HB3	2.16	0.45
1:A:261:GLY:O	1:A:263:GLY:N	2.47	0.45
1:B:177:ARG:CZ	1:B:217:PRO:HB2	2.47	0.45
1:B:537:PRO:HA	1:B:540:LEU:HD22	1.99	0.45
1:B:324:LEU:HG	1:B:326:VAL:HG23	1.99	0.45
1:D:458:PRO:HA	1:D:465:TYR:CD2	2.52	0.45
1:D:430:PHE:HE1	1:D:476:LEU:HD11	1.82	0.45
1:A:424:ARG:NH1	6:A:2092:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASP:OD1	6:B:2012:HOH:O	2.21	0.44
1:A:337:TYR:CZ	1:A:447:HIS:HB3	2.52	0.44
1:D:210:GLY:O	1:D:213:ILE:HB	2.18	0.44
1:D:46:ARG:HB3	1:D:274:ARG:HG2	1.99	0.44
1:B:514:ASN:O	1:B:515:LEU:C	2.53	0.44
1:C:424:ARG:NH1	6:C:2091:HOH:O	2.51	0.44
1:B:33:LEU:H	1:B:62:ALA:HB1	1.83	0.44
1:A:113:PRO:HG2	1:A:485:ARG:HG3	2.00	0.44
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.80	0.43
1:B:413:GLN:O	1:B:417:ARG:HG2	2.18	0.43
1:B:530:ALA:O	1:B:534:ARG:HB2	2.18	0.43
1:B:81:GLU:HB3	1:B:438:THR:HG21	2.00	0.43
1:A:255:VAL:HG23	1:A:257:CYS:HB2	2.00	0.43
1:B:33:LEU:N	1:B:62:ALA:HB1	2.32	0.43
1:B:68:VAL:HG11	1:B:88:PRO:HB3	1.99	0.43
1:A:511:VAL:HG12	1:A:520:VAL:HG22	2.01	0.43
1:B:22:LEU:HD23	1:B:23:LYS:N	2.34	0.43
1:A:231:THR:HB	1:A:233:ASN:OD1	2.18	0.43
1:B:253:ARG:HG3	2:C:550:GOW:C44	2.49	0.43
1:B:41:PRO:HA	1:B:45:ARG:HB3	1.99	0.43
1:C:535:PHE:HB2	1:D:380:LEU:HD22	2.00	0.43
1:D:494:ASP:HB3	1:D:495:SER:H	1.59	0.43
1:B:514:ASN:OD1	1:B:514:ASN:N	2.51	0.43
1:D:404:ASP:HA	1:D:408:VAL:HB	2.00	0.43
1:A:437:LEU:CD2	1:A:439:TRP:H	2.31	0.43
1:D:518:LEU:HA	1:D:518:LEU:HD23	1.88	0.43
1:A:342:GLY:HA2	1:D:263:GLY:CA	2.47	0.43
1:A:380:LEU:HD22	1:A:385:TRP:CZ2	2.54	0.43
1:A:491:ASP:OD1	1:A:493:ARG:HD3	2.19	0.43
1:C:157:GLY:O	1:C:171:VAL:HG22	2.18	0.43
1:C:300:VAL:HB	1:C:301:PRO:HD2	2.01	0.43
1:D:120:GLY:HA2	1:D:205:GLY:H	1.84	0.43
1:D:495:SER:C	1:D:497:SER:N	2.71	0.43
1:A:353:LEU:HB3	1:A:391:PRO:HB2	2.01	0.42
1:B:228:GLN:HB3	1:B:450:GLU:OE2	2.18	0.42
1:B:231:THR:HB	1:B:233:ASN:OD1	2.19	0.42
1:D:138:LEU:HD23	1:D:477:MET:HE3	2.00	0.42
1:D:460:ASP:HB3	1:D:463:LEU:HD12	2.02	0.42
1:A:326:VAL:HG12	1:A:328:VAL:HG13	2.01	0.42
1:C:202:GLU:HA	1:C:228:GLN:O	2.20	0.42
1:D:330:VAL:HG11	1:D:408:VAL:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:PHE:CE1	1:B:354:ILE:HG21	2.55	0.42
1:B:7:GLN:O	1:B:107:ARG:NH2	2.34	0.42
1:A:89:ASN:ND2	1:A:129:SER:O	2.40	0.42
1:D:511:VAL:HG12	1:D:520:VAL:HG22	2.01	0.42
1:B:7:GLN:OE1	1:B:107:ARG:HG2	2.20	0.42
1:D:115:LEU:HD21	1:D:484:ALA:HB2	2.02	0.42
1:B:485:ARG:HG3	1:B:486:THR:HG23	2.02	0.42
1:C:176:GLN:OE1	1:C:208:SER:HB3	2.19	0.42
1:C:257:CYS:N	1:C:258:PRO:HD3	2.35	0.41
1:C:227:LEU:HB2	1:C:328:VAL:HG12	2.01	0.41
1:C:433:ARG:HD2	1:C:444:GLY:O	2.19	0.41
1:D:490:ASN:ND2	1:D:500:TRP:H	2.18	0.41
1:A:183:VAL:O	1:A:187:ILE:HB	2.19	0.41
1:A:430:PHE:HE2	1:A:476:LEU:HD11	1.84	0.41
1:B:497:SER:HB3	1:B:498:PRO:HD3	2.02	0.41
1:C:530:ALA:O	1:C:534:ARG:HB2	2.21	0.41
1:D:227:LEU:HB2	1:D:328:VAL:HG12	2.01	0.41
1:B:48:MET:HE2	1:B:48:MET:HB3	1.88	0.41
1:C:413:GLN:O	1:C:417:ARG:HG2	2.20	0.41
1:A:134:ASP:OD2	1:A:136:ARG:HD2	2.21	0.41
1:A:380:LEU:HD22	1:A:385:TRP:HZ2	1.85	0.41
1:D:68:VAL:HG13	1:D:127:ALA:HB2	2.03	0.41
1:A:4:GLU:OE1	1:A:18:ARG:NH1	2.54	0.41
1:A:4:GLU:OE2	1:A:18:ARG:HD3	2.21	0.41
1:A:496:LYS:HD2	1:A:496:LYS:HA	1.81	0.41
1:B:22:LEU:HD13	1:B:136:ARG:HH12	1.86	0.41
1:A:202:GLU:HA	1:A:228:GLN:O	2.21	0.41
1:D:475:ARG:NH2	6:D:2093:HOH:O	2.51	0.41
1:C:255:VAL:HG23	1:C:257:CYS:HB2	2.04	0.40
1:C:337:TYR:O	1:C:340:VAL:HG22	2.21	0.40
1:D:493:ARG:HD2	1:D:493:ARG:HA	1.89	0.40
1:B:337:TYR:CZ	1:B:447:HIS:HB3	2.57	0.40
1:D:337:TYR:HB3	1:D:443:MET:CE	2.51	0.40
1:A:107:ARG:HG2	6:A:2032:HOH:O	2.22	0.40
1:B:328:VAL:O	1:B:427:ALA:HA	2.22	0.40
1:C:265:ASN:HB3	1:C:268:GLU:HB2	2.03	0.40
1:A:324:LEU:HG	1:A:326:VAL:HG23	2.03	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	539/543 (99%)	523 (97%)	14 (3%)	2 (0%)	39	77
1	B	539/543 (99%)	521 (97%)	17 (3%)	1 (0%)	52	85
1	C	536/543 (99%)	521 (97%)	14 (3%)	1 (0%)	52	85
1	D	534/543 (98%)	518 (97%)	15 (3%)	1 (0%)	52	85
All	All	2148/2172 (99%)	2083 (97%)	60 (3%)	5 (0%)	52	85

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	ALA
1	D	496	LYS
1	C	259	PRO
1	B	497	SER
1	A	259	PRO

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	442/443 (100%)	432 (98%)	10 (2%)	58	85
1	B	443/443 (100%)	432 (98%)	11 (2%)	55	84
1	C	440/443 (99%)	430 (98%)	10 (2%)	58	85
1	D	438/443 (99%)	431 (98%)	7 (2%)	70	90
All	All	1763/1772 (100%)	1725 (98%)	38 (2%)	61	86

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	70	TYR
1	A	107	ARG
1	A	200	PHE
1	A	219	ARG
1	A	265	ASN
1	A	295	PHE
1	A	333	ASP
1	A	337	TYR
1	A	493	ARG
1	B	23	LYS
1	B	149	MET
1	B	295	PHE
1	B	364	ARG
1	B	369[A]	GLN
1	B	369[B]	GLN
1	B	380	LEU
1	B	480	TRP
1	B	496	LYS
1	B	522	ARG
1	B	525	ARG
1	C	13	ARG
1	C	84	GLU
1	C	140	GLN
1	C	219	ARG
1	C	276	ARG
1	C	285	GLU
1	C	295	PHE
1	C	333	ASP
1	C	337	TYR
1	C	386	LEU
1	D	45	ARG
1	D	107	ARG
1	D	295	PHE
1	D	337	TYR
1	D	376	GLU
1	D	417	ARG
1	D	441	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	287	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 ⓘ

Of 41 ligands modelled in this entry, 28 are monoatomic - leaving 13 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	G0W	A	550	-	43,51,51	1.70	5 (11%)	45,70,70	1.47	5 (11%)
3	NAG	A	560	1	14,14,15	0.34	0	15,19,21	0.34	0
5	SO4	B	1542	-	4,4,4	0.18	0	6,6,6	0.13	0
2	G0W	B	550	-	27,29,51	1.16	4 (14%)	28,38,70	0.96	1 (3%)
3	NAG	B	560	1	14,14,15	0.49	0	15,19,21	0.51	0
3	NAG	B	561	1	14,14,15	0.38	0	15,19,21	0.48	0
5	SO4	C	1541	-	4,4,4	0.17	0	6,6,6	0.09	0
2	G0W	C	550	-	43,51,51	1.65	7 (16%)	45,70,70	1.43	5 (11%)
3	NAG	C	560	1	14,14,15	0.54	0	15,19,21	0.76	1 (6%)
5	SO4	D	1540	-	4,4,4	0.15	0	6,6,6	0.11	0
2	G0W	D	550	-	27,29,51	1.31	5 (18%)	28,38,70	1.09	2 (7%)
3	NAG	D	560	1	14,14,15	0.52	0	15,19,21	0.58	1 (6%)
3	NAG	D	561	1	14,14,15	0.43	0	15,19,21	0.34	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	G0W	A	550	-	-	0/46/48/48	0/3/3/3
3	NAG	A	560	1	-	0/6/23/26	0/1/1/1
5	SO4	B	1542	-	-	0/0/0/0	0/0/0/0
2	G0W	B	550	-	-	0/34/25/48	0/1/1/3
3	NAG	B	560	1	-	0/6/23/26	0/1/1/1
3	NAG	B	561	1	-	0/6/23/26	0/1/1/1
5	SO4	C	1541	-	-	0/0/0/0	0/0/0/0
2	G0W	C	550	-	-	0/46/48/48	0/3/3/3
3	NAG	C	560	1	-	0/6/23/26	0/1/1/1
5	SO4	D	1540	-	-	0/0/0/0	0/0/0/0
2	G0W	D	550	-	-	0/34/25/48	0/1/1/3
3	NAG	D	560	1	-	0/6/23/26	0/1/1/1
3	NAG	D	561	1	-	0/6/23/26	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	550	G0W	C34-C29	2.03	1.43	1.40
2	D	550	G0W	C38-N11	2.05	1.44	1.33
2	D	550	G0W	C34-C29	2.15	1.43	1.40
2	B	550	G0W	C38-N11	2.15	1.45	1.33
2	B	550	G0W	C15-N17	2.17	1.44	1.39
2	B	550	G0W	C10-N11	2.20	1.54	1.46
2	D	550	G0W	C28-N23	2.26	1.57	1.53
2	A	550	G0W	C46-C41	2.30	1.43	1.40
2	B	550	G0W	C22-N23	2.42	1.61	1.52
2	A	550	G0W	C22-N23	2.44	1.61	1.52
2	D	550	G0W	C22-N23	2.53	1.61	1.52
2	D	550	G0W	C15-N17	2.55	1.45	1.39
2	C	550	G0W	C22-N23	2.62	1.61	1.52
2	C	550	G0W	C40-C41	2.68	1.56	1.51
2	C	550	G0W	C46-C41	3.29	1.45	1.40
2	C	550	G0W	C40-N03	3.67	1.60	1.53
2	A	550	G0W	C15-N17	4.16	1.44	1.38
2	C	550	G0W	C15-N17	4.57	1.45	1.38
2	C	550	G0W	C12-N11	4.97	1.41	1.36
2	A	550	G0W	C40-N03	5.22	1.63	1.53
2	A	550	G0W	C12-N11	5.65	1.42	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	550	G0W	C42-C41-C46	-3.38	114.21	118.01
2	A	550	G0W	C42-C41-C46	-2.89	114.77	118.01
2	D	550	G0W	C30-C29-C34	-2.57	115.12	118.01
2	C	550	G0W	C30-C29-C34	-2.16	115.58	118.01
2	A	550	G0W	C30-C29-C34	-2.14	115.61	118.01
2	D	550	G0W	O39-C38-N11	-2.10	117.77	123.42
2	B	550	G0W	C30-C29-C34	-2.09	115.66	118.01
3	D	560	NAG	C1-O5-C5	2.00	115.08	112.14
2	A	550	G0W	C18-N17-C15	2.21	121.21	119.06
2	A	550	G0W	C15-C14-C12	2.24	123.91	117.25
2	C	550	G0W	C15-C14-C12	2.26	123.96	117.25
2	C	550	G0W	C18-N17-C15	2.44	121.42	119.06
3	C	560	NAG	C1-O5-C5	2.66	116.05	112.14
2	C	550	G0W	C10-N11-C12	5.54	123.16	119.47
2	A	550	G0W	C10-N11-C12	6.57	123.85	119.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	550	G0W	2	0
2	C	550	G0W	1	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, 95th 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	541/543 (99%)	-0.02	2 (0%) 93 86	44, 58, 87, 117	1 (0%)
1	B	538/543 (99%)	0.39	31 (5%) 26 10	50, 89, 156, 196	0
1	C	536/543 (98%)	-0.08	3 (0%) 90 81	44, 58, 78, 119	0
1	D	536/543 (98%)	0.17	5 (0%) 85 73	45, 66, 97, 132	1 (0%)
All	All	2151/2172 (99%)	0.12	41 (1%) 70 49	44, 64, 127, 196	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	494	ASP	4.6
1	B	463	LEU	4.0
1	B	30	SER	3.8
1	C	260	GLY	3.5
1	B	198	THR	3.5
1	B	108	PRO	3.4
1	B	146	LEU	3.3
1	B	115	LEU	3.2
1	B	101	VAL	3.1
1	B	480	TRP	2.9
1	B	136	ARG	2.8
1	A	497	SER	2.7
1	B	541	SER	2.7
1	B	492	PRO	2.7
1	B	500	TRP	2.7
1	B	498	PRO	2.7
1	B	459	LEU	2.7
1	B	495	SER	2.6
1	B	465	TYR	2.6
1	B	515	LEU	2.6
1	D	494	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	261	GLY	2.4
1	B	497	SER	2.4
1	B	513	LEU	2.4
1	D	493	ARG	2.4
1	B	113	PRO	2.4
1	C	259	PRO	2.4
1	B	104	PRO	2.4
1	B	499	GLN	2.3
1	B	430	PHE	2.3
1	B	432	HIS	2.2
1	B	455	PHE	2.2
1	D	492	PRO	2.2
1	B	436	THR	2.2
1	B	461	PRO	2.1
1	A	496	LYS	2.1
1	B	4	GLU	2.1
1	D	497	SER	2.1
1	B	476	LEU	2.1
1	D	498	PRO	2.1
1	B	145	VAL	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, 95th 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	G0W	A	550	49/49	0.95	0.40	3.73	49,59,103,106	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	G0W	C	550	49/49	0.94	0.34	2.84	50,65,98,101	0
2	G0W	B	550	31/49	0.92	0.38	2.33	63,69,86,89	0
3	NAG	D	561	14/15	0.73	0.31	1.91	85,91,95,97	0
3	NAG	B	561	14/15	0.71	0.35	1.70	91,98,103,106	0
2	G0W	D	550	31/49	0.95	0.29	1.07	49,55,59,63	0
4	CL	C	610	1/1	0.86	0.22	-0.09	78,78,78,78	0
4	CL	C	606	1/1	0.95	0.20	-0.12	73,73,73,73	0
5	SO4	D	1540	5/5	0.96	0.16	-0.93	73,73,74,74	5
4	CL	A	604	1/1	0.96	0.14	-3.47	77,77,77,77	0
4	CL	A	609	1/1	0.92	0.16	-4.66	77,77,77,77	0
3	NAG	C	560	14/15	0.86	0.25	-	92,97,101,101	14
4	CL	B	607	1/1	0.88	0.14	-	77,77,77,77	0
4	CL	A	607	1/1	0.83	0.29	-	103,103,103,103	0
4	CL	C	603	1/1	0.62	0.27	-	114,114,114,114	0
3	NAG	A	560	14/15	0.84	0.20	-	101,108,114,115	0
4	CL	C	605	1/1	0.90	0.18	-	74,74,74,74	0
4	CL	B	605	1/1	0.77	0.23	-	94,94,94,94	0
4	CL	A	610	1/1	0.91	0.21	-	115,115,115,115	0
4	CL	D	608	1/1	0.90	0.23	-	55,55,55,55	0
4	CL	A	605	1/1	0.73	0.30	-	88,88,88,88	0
4	CL	A	611	1/1	0.82	0.14	-	90,90,90,90	0
4	CL	A	608	1/1	0.75	0.17	-	75,75,75,75	0
4	CL	C	608	1/1	0.90	0.31	-	120,120,120,120	0
3	NAG	B	560	14/15	0.71	0.24	-	96,101,106,109	0
4	CL	A	601	1/1	0.87	0.18	-	107,107,107,107	0
4	CL	D	605	1/1	0.98	0.21	-	69,69,69,69	0
4	CL	D	606	1/1	0.90	0.26	-	95,95,95,95	0
4	CL	D	609	1/1	0.97	0.11	-	63,63,63,63	0
4	CL	C	607	1/1	0.94	0.07	-	61,61,61,61	0
4	CL	B	606	1/1	0.89	0.08	-	82,82,82,82	0
4	CL	D	610	1/1	0.93	0.12	-	97,97,97,97	0
5	SO4	C	1541	5/5	0.96	0.15	-	86,86,87,88	0
5	SO4	B	1542	5/5	0.94	0.15	-	81,82,82,83	5
4	CL	B	608	1/1	0.72	0.33	-	85,85,85,85	0
4	CL	C	612	1/1	0.73	0.35	-	80,80,80,80	0
4	CL	D	607	1/1	0.65	0.17	-	89,89,89,89	0
4	CL	C	609	1/1	0.87	0.20	-	89,89,89,89	0
3	NAG	D	560	14/15	0.82	0.18	-	84,92,98,103	0
4	CL	C	611	1/1	0.96	0.19	-	46,46,46,46	0
4	CL	A	606	1/1	0.95	0.20	-	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.