Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:59 AM GMT

PDB ID	:	2JGK
Title	:	Crystal structure of mouse acetylcholinesterase inhibited by aged fenamiphos
Authors	:	Hornberg, A.; Tunemalm, A.-K.; Ekstrom, F.
Deposited on	:	2007-02-13
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) 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 2.90 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		7
Ramachandran outliers		0.8%
Sidechain outliers		5.3%
RSRZ outliers		1.6%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
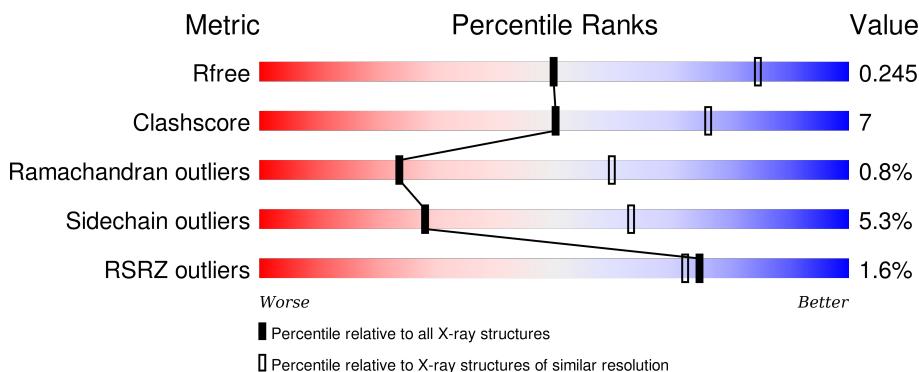
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	548	2% 82% 14% ··
1	B	548	% 78% 16% ··
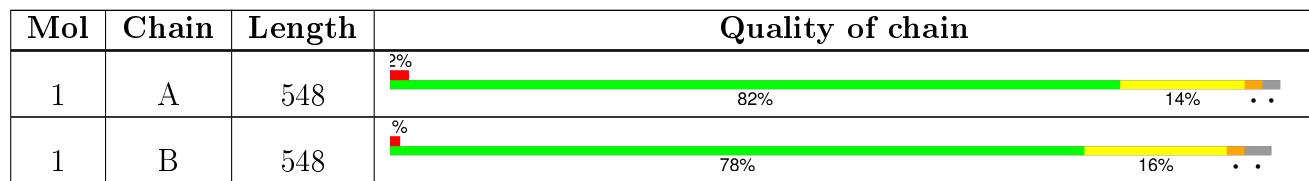
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1544	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8437 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	535	Total	C	N	O	P	S	0	0	0
			4188	2685	727	761	1	14			
1	B	530	Total	C	N	O	P	S	0	0	0
			4153	2666	719	753	1	14			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
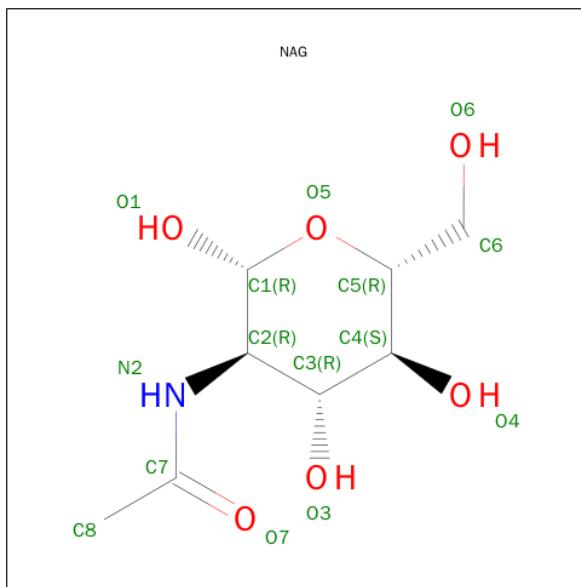
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).

P6G
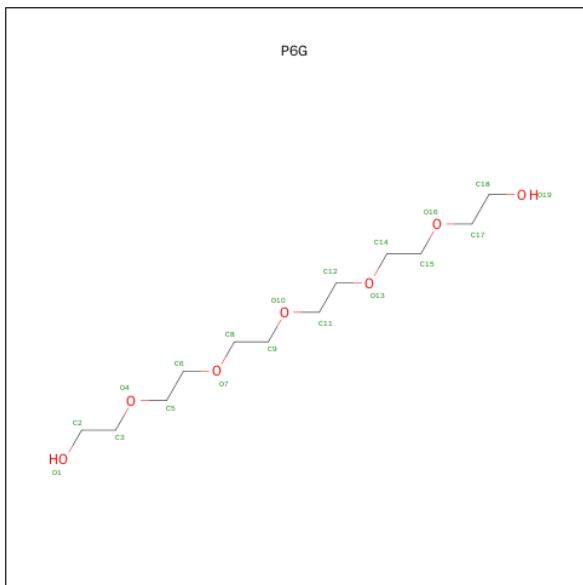
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 19	C 12	O 7	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	34	Total 34	O 34	0	0
4	B	29	Total 29	O 29	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
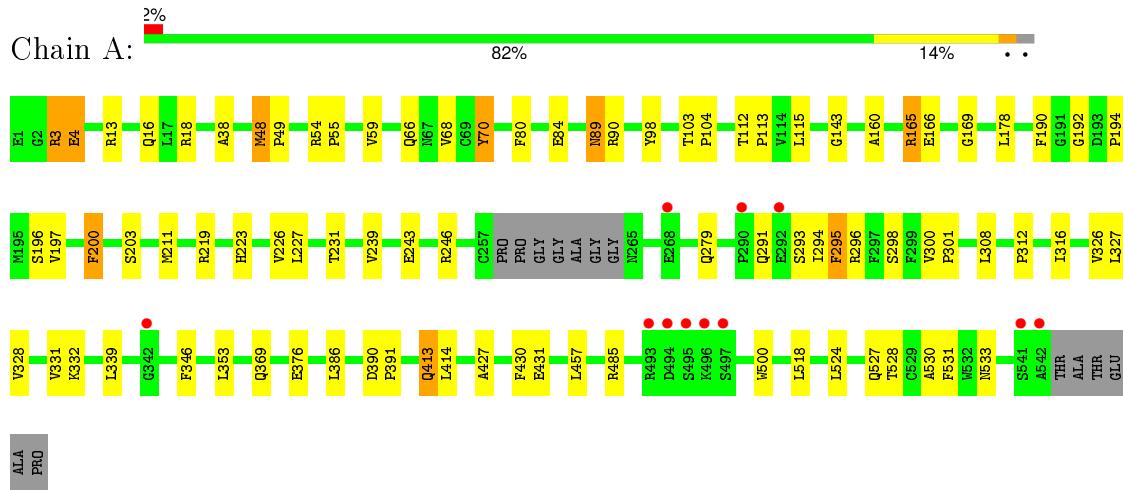
- Molecule 1: ACETYLCHOLINESTERASE
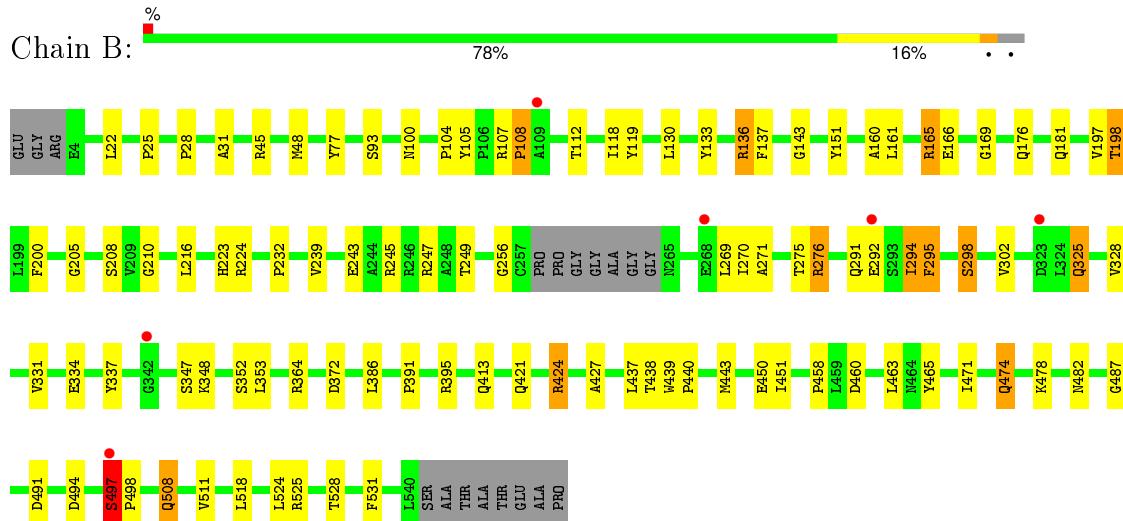
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.71Å 111.26Å 226.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.90 19.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.90) 100.0 (19.93-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.93 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.253 0.198 , 0.245	Depositor DCC
R_{free} test set	890 reflections (2.00%)	DCC
Wilson B-factor (Å^2)	59.5	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 26.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	1 of 45440 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8437	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SVZ, NAG, P6G

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	0.52	0/4297	0.65	0/5868
1	B	0.52	0/4262	0.65	0/5822
All	All	0.52	0/8559	0.65	0/11690

There are no bond length outliers.

There are no bond angle outliers.

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	4188	0	4082	54	0
1	B	4153	0	4048	61	0
2	A	14	0	13	0	0
3	B	19	0	24	1	0
4	A	34	0	0	0	0
4	B	29	0	0	1	0
All	All	8437	0	8167	115	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 (115) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:HH11	1:B:424:ARG:HG3	1.01	1.07
1:A:3:ARG:HH11	1:A:3:ARG:HG3	1.13	1.06
1:A:197:VAL:H	1:A:223:HIS:HD2	1.20	0.90
1:A:4:GLU:OE2	1:A:18:ARG:HD3	1.73	0.89
1:B:497:SER:HB2	1:B:498:PRO:C	1.94	0.88
1:B:424:ARG:NH1	1:B:424:ARG:HG3	1.80	0.86
1:B:198:THR:HG23	1:B:224:ARG:HB2	1.69	0.75
1:A:112:THR:HG21	1:A:143:GLY:O	1.85	0.75
1:A:294:ILE:HB	1:A:295:PHE:CD1	2.22	0.74
1:A:295:PHE:N	1:A:295:PHE:CD1	2.55	0.74
1:B:104:PRO:HG2	1:B:108:PRO:HD3	1.72	0.70
1:B:295:PHE:HD1	1:B:295:PHE:N	1.89	0.70
1:B:508:GLN:HG2	4:B:2026:HOH:O	1.92	0.69
1:A:295:PHE:N	1:A:295:PHE:HD1	1.89	0.69
1:B:276:ARG:HH11	1:B:276:ARG:CG	2.05	0.69
1:A:3:ARG:NH1	1:A:3:ARG:HG3	1.94	0.69
1:A:294:ILE:HB	1:A:295:PHE:HD1	1.58	0.68
1:B:295:PHE:CD1	1:B:295:PHE:N	2.61	0.67
1:B:276:ARG:HG3	1:B:276:ARG:HH11	1.60	0.64
1:B:294:ILE:HB	1:B:295:PHE:CD1	2.33	0.63
1:A:3:ARG:CG	1:A:3:ARG:HH11	2.01	0.62
1:A:527:GLN:HE21	3:B:1542:P6G:H171	1.64	0.62
1:B:294:ILE:HD12	1:B:294:ILE:H	1.65	0.62
1:B:197:VAL:H	1:B:223:HIS:CD2	2.19	0.61
1:B:271:ALA:O	1:B:275:THR:HG23	2.00	0.61
1:A:211:MET:HG2	1:A:308:LEU:HD21	1.82	0.61
1:B:511:VAL:HB	1:B:518:LEU:HD22	1.83	0.61
1:B:328:VAL:O	1:B:427:ALA:HA	2.01	0.60
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.84	0.59
1:A:376:GLU:HA	1:A:376:GLU:OE1	2.03	0.59
1:A:331:VAL:HG12	1:A:430:PHE:HB3	1.85	0.59
1:B:161:LEU:HD11	1:B:269:LEU:HD23	1.87	0.57
1:A:197:VAL:H	1:A:223:HIS:CD2	2.11	0.57
1:B:497:SER:HB2	1:B:498:PRO:CA	2.35	0.57
1:A:203:SVZ:H6C1	1:A:295:PHE:HE2	1.70	0.57
1:B:424:ARG:CG	1:B:424:ARG:HH11	1.92	0.56
1:A:293:SER:O	1:A:296:ARG:HG2	2.06	0.56
1:A:89:ASN:H	1:A:89:ASN:HD22	1.54	0.56
1:B:197:VAL:H	1:B:223:HIS:HD2	1.52	0.55
1:B:460:ASP:HB3	1:B:463:LEU:HD12	1.88	0.55
1:A:48:MET:HE2	1:A:49:PRO:HD2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:LEU:HD12	1:B:31:ALA:HB2	1.90	0.52
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.92	0.52
1:A:293:SER:HB3	1:A:296:ARG:HB3	1.91	0.52
1:B:245:ARG:O	1:B:249:THR:HG23	2.10	0.51
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.45	0.51
1:A:226:VAL:HG22	1:A:327:LEU:HB3	1.92	0.51
1:A:80:PHE:O	1:A:84:GLU:HG2	2.11	0.51
1:A:243:GLU:OE2	1:A:246:ARG:NH1	2.44	0.51
1:A:312:PRO:O	1:A:316:ILE:HG23	2.11	0.51
1:A:332:LYS:HD3	1:A:431:GLU:HG2	1.93	0.50
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.46	0.50
1:B:210:GLY:HA3	1:B:232:PRO:HG3	1.93	0.50
1:A:528:THR:O	1:A:531:PHE:HB3	2.10	0.50
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.93	0.50
1:A:16:GLN:HB3	1:A:59:VAL:HG22	1.93	0.50
1:B:294:ILE:HB	1:B:295:PHE:HD1	1.76	0.50
1:B:165:ARG:HB3	1:B:165:ARG:HH11	1.77	0.49
1:A:294:ILE:HB	1:A:295:PHE:CE1	2.48	0.49
1:A:38:ALA:HB2	1:A:178:LEU:HD23	1.95	0.48
1:A:295:PHE:H	1:A:295:PHE:HD1	1.61	0.48
1:B:337:TYR:HA	1:B:443:MET:HE1	1.95	0.48
1:B:352:SER:O	1:B:395:ARG:HG3	2.13	0.48
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.96	0.48
1:A:68:VAL:HG23	1:A:90:ARG:HB2	1.95	0.48
1:A:339:LEU:HD13	1:A:346:PHE:CE2	2.49	0.48
1:B:247:ARG:HH11	1:B:298:SER:HA	1.79	0.47
1:A:413:GLN:HB2	1:A:533:ASN:ND2	2.28	0.47
1:A:328:VAL:O	1:A:427:ALA:HA	2.14	0.47
1:B:337:TYR:HA	1:B:443:MET:CE	2.45	0.47
1:A:231:THR:HG22	1:A:414:LEU:HD22	1.97	0.47
1:B:331:VAL:HG22	1:B:334:GLU:OE2	2.15	0.47
1:B:471:ILE:HA	1:B:474:GLN:HG3	1.96	0.47
1:A:200:PHE:CB	1:A:226:VAL:HB	2.45	0.46
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.48	0.46
1:B:104:PRO:O	1:B:107:ARG:HA	2.15	0.46
1:B:197:VAL:N	1:B:223:HIS:HD2	2.13	0.46
1:B:325:GLN:HE21	1:B:487:GLY:HA3	1.81	0.46
1:B:136:ARG:HG2	1:B:137:PHE:N	2.31	0.46
1:A:66:GLN:HG3	1:A:98:TYR:CD1	2.51	0.46
1:A:227:LEU:HB2	1:A:328:VAL:HG12	1.97	0.45
1:A:70:TYR:HE2	1:A:279:GLN:OE1	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ASP:HB3	1:B:494:ASP:HB3	1.98	0.45
1:A:300:VAL:HB	1:A:301:PRO:HD2	1.99	0.44
1:B:112:THR:HG21	1:B:143:GLY:O	2.17	0.44
1:B:364:ARG:HH12	1:B:372:ASP:HA	1.82	0.44
1:B:166:GLU:HG2	1:B:270:ILE:HD13	2.00	0.44
1:B:478:LYS:O	1:B:482:ASN:HB2	2.17	0.44
1:B:439:TRP:HB3	1:B:440:PRO:HD2	1.99	0.44
1:B:424:ARG:CG	1:B:424:ARG:NH1	2.60	0.43
1:B:528:THR:O	1:B:531:PHE:HB3	2.18	0.43
1:B:118:ILE:HG22	1:B:205:GLY:HA2	2.00	0.43
1:A:192:GLY:O	1:A:194:PRO:HD3	2.19	0.43
1:B:243:GLU:HG3	1:B:247:ARG:HE	1.84	0.42
1:A:165:ARG:NH1	1:A:166:GLU:HG3	2.34	0.42
1:B:160:ALA:HB2	1:B:169:GLY:HA3	2.01	0.42
1:A:89:ASN:N	1:A:89:ASN:HD22	2.17	0.42
1:B:276:ARG:NH1	1:B:276:ARG:CG	2.71	0.41
1:B:474:GLN:HE21	1:B:474:GLN:HB3	1.69	0.41
1:B:176:GLN:OE1	1:B:208:SER:HB3	2.19	0.41
1:B:28:PRO:O	1:B:105:TYR:HB3	2.20	0.41
1:B:119:TYR:CE1	1:B:151:TYR:CE1	3.08	0.41
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.03	0.41
1:A:527:GLN:O	1:A:530:ALA:HB3	2.20	0.41
1:B:239:VAL:HG23	1:B:302:VAL:HG23	2.03	0.41
1:A:219:ARG:HA	1:A:219:ARG:HD2	1.83	0.41
1:A:160:ALA:HB2	1:A:169:GLY:HA2	2.01	0.41
1:B:450:GLU:HG2	1:B:451:ILE:N	2.35	0.41
1:B:130:LEU:HD12	1:B:133:TYR:CE2	2.56	0.41
1:A:203:SVZ:H6C1	1:A:295:PHE:CE2	2.52	0.40
1:A:390:ASP:HA	1:A:391:PRO:HD3	1.86	0.40
1:B:48:MET:HE1	1:B:165:ARG:O	2.22	0.40
1:B:77:TYR:CZ	1:B:348:LYS:HG2	2.56	0.40
1:A:54:ARG:HA	1:A:55:PRO:HD3	1.99	0.40
1:B:294:ILE:HB	1:B:295:PHE:CE1	2.56	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	530/548 (97%)	495 (93%)	33 (6%)	2 (0%)	39	74
1	B	525/548 (96%)	494 (94%)	25 (5%)	6 (1%)	17	51
All	All	1055/1096 (96%)	989 (94%)	58 (6%)	8 (1%)	24	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	292	GLU
1	B	291	GLN
1	A	291	GLN
1	B	108	PRO
1	A	104	PRO
1	B	25	PRO
1	B	497	SER
1	B	256	GLY

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	439/445 (99%)	419 (95%)	20 (5%)	33	69
1	B	436/445 (98%)	410 (94%)	26 (6%)	24	57
All	All	875/890 (98%)	829 (95%)	46 (5%)	28	63

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	GLU
1	A	13	ARG
1	A	48	MET
1	A	70	TYR
1	A	89	ASN
1	A	115	LEU
1	A	165	ARG
1	A	196	SER
1	A	200	PHE
1	A	239	VAL
1	A	295	PHE
1	A	298	SER
1	A	326	VAL
1	A	369	GLN
1	A	386	LEU
1	A	413	GLN
1	A	457	LEU
1	A	518	LEU
1	A	524	LEU
1	B	45	ARG
1	B	93	SER
1	B	100	ASN
1	B	136	ARG
1	B	165	ARG
1	B	181	GLN
1	B	198	THR
1	B	200	PHE
1	B	216	LEU
1	B	276	ARG
1	B	294	ILE
1	B	295	PHE
1	B	298	SER
1	B	325	GLN
1	B	347	SER
1	B	386	LEU
1	B	413	GLN
1	B	421	GLN
1	B	424	ARG
1	B	437	LEU
1	B	438	THR
1	B	474	GLN
1	B	497	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	508	GLN
1	B	524	LEU
1	B	525	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	ASN
1	A	223	HIS
1	A	509	GLN
1	B	223	HIS
1	B	284	HIS
1	B	325	GLN
1	B	369	GLN
1	B	464	ASN
1	B	474	GLN
1	B	499	GLN

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	$\#|Z| > 2$
1	SVZ	A	203	1	11,12,13	4.30	2 (18%)	11,16,18	4.12	8 (72%)
1	SVZ	B	203	1	11,12,13	4.44	2 (18%)	11,16,18	4.84	6 (54%)

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
1	SVZ	A	203	1	-	0/10/13/15	0/0/0/0
1	SVZ	B	203	1	-	0/10/13/15	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	203	SVZ	P1-O4	5.16	1.52	1.46
1	B	203	SVZ	P1-O4	5.34	1.52	1.46
1	A	203	SVZ	P1-N3	13.07	1.75	1.61
1	B	203	SVZ	P1-N3	13.47	1.75	1.61

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	203	SVZ	OG-P1-O4	-6.72	85.51	113.31
1	B	203	SVZ	O4-P1-N3	-5.64	102.98	113.08
1	A	203	SVZ	P1-OG-CB	-3.93	108.82	120.79
1	A	203	SVZ	P1-N3-C5	-3.90	117.31	124.73
1	A	203	SVZ	O4-P1-N3	-2.99	107.72	113.08
1	A	203	SVZ	OG-P1-O4	-2.61	102.50	113.31
1	A	203	SVZ	O-C-CA	-2.38	119.28	125.49
1	B	203	SVZ	O-C-CA	-2.04	120.16	125.49
1	A	203	SVZ	OG-CB-CA	3.79	111.51	108.27
1	A	203	SVZ	O2-P1-O4	4.41	119.20	110.00
1	B	203	SVZ	OG-CB-CA	4.53	112.14	108.27
1	B	203	SVZ	O2-P1-O4	5.35	121.17	110.00
1	A	203	SVZ	O2-P1-OG	10.00	135.82	106.60
1	B	203	SVZ	O2-P1-OG	10.95	138.58	106.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	203	SVZ	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	NAG	A	1544	1	14,14,15	0.70	0	15,19,21	1.55	2 (13%)
3	P6G	B	1542	-	18,18,18	1.74	5 (27%)	17,17,17	2.15	8 (47%)

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	NAG	A	1544	1	-	0/6/23/26	0/1/1/1
3	P6G	B	1542	-	-	0/16/16/16	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1542	P6G	C9-C8	-2.93	1.33	1.48
3	B	1542	P6G	C15-C14	-2.82	1.34	1.48
3	B	1542	P6G	C6-C5	-2.81	1.34	1.48
3	B	1542	P6G	C3-C2	-2.76	1.34	1.49
3	B	1542	P6G	C17-C18	-2.68	1.34	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1542	P6G	O4-C3-C2	2.16	120.38	110.43
3	B	1542	P6G	O16-C17-C18	2.29	120.98	110.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1544	NAG	O5-C5-C6	2.35	112.43	107.35
3	B	1542	P6G	O4-C5-C6	2.62	122.02	110.36
3	B	1542	P6G	O10-C9-C8	2.77	122.66	110.36
3	B	1542	P6G	O16-C15-C14	2.86	123.06	110.36
3	B	1542	P6G	O13-C14-C15	2.95	123.46	110.36
3	B	1542	P6G	O7-C8-C9	3.12	124.25	110.36
3	B	1542	P6G	O7-C6-C5	3.17	124.45	110.36
2	A	1544	NAG	C1-O5-C5	4.09	117.44	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1542	P6G	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 (i)

6.1 Protein, DNA and RNA chains (i)

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(Å²)	Q<0.9
1	A	534/548 (97%)	-0.46	11 (2%)	67	62	32, 50, 73, 93	0
1	B	529/548 (96%)	-0.42	6 (1%)	82	80	34, 54, 77, 102	0
All	All	1063/1096 (96%)	-0.44	17 (1%)	74	72	32, 52, 76, 102	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	292	GLU	4.5
1	A	495	SER	3.8
1	A	292	GLU	3.7
1	A	496	LYS	3.6
1	B	497	SER	3.3
1	A	541	SER	3.1
1	A	494	ASP	2.7
1	A	497	SER	2.6
1	A	493	ARG	2.6
1	B	342	GLY	2.5
1	A	342	GLY	2.3
1	B	268	GLU	2.3
1	A	542	ALA	2.2
1	B	109	ALA	2.2
1	A	290	PRO	2.1
1	A	268	GLU	2.1
1	B	323	ASP	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, 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
1	SVZ	A	203	13/14	0.98	0.10	-	40,43,54,54	0
1	SVZ	B	203	13/14	0.98	0.10	-	43,46,57,57	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, 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	NAG	A	1544	14/15	0.86	0.45	4.78	82,85,90,91	0
3	P6G	B	1542	19/19	0.86	0.26	1.82	76,79,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.