



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 17, 2019 – 05:11 PM EDT

PDB ID : 6FSD  
Title : Mus musculus acetylcholinesterase in complex with 2-(4-Biphenyloxy)-N-[3-(1-piperidiny)propyl]-acetamide hydrochloride (10)  
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Deposited on : 2018-02-19  
Resolution : 2.70 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

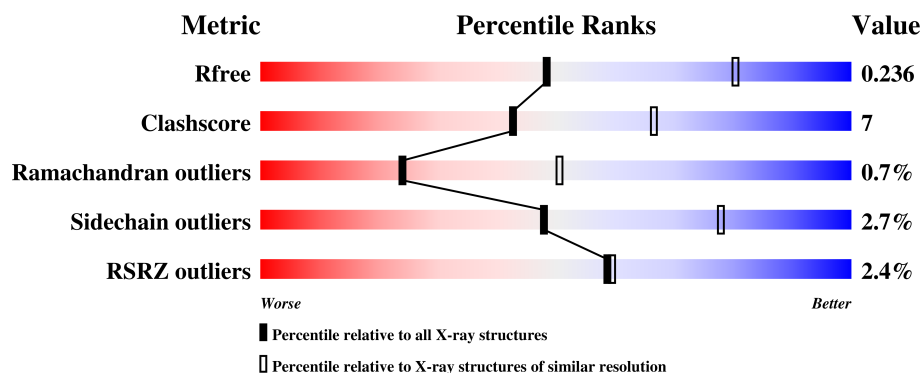
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)

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	548	<div> <div>2%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	B	548	<div> <div>3%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8586 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.

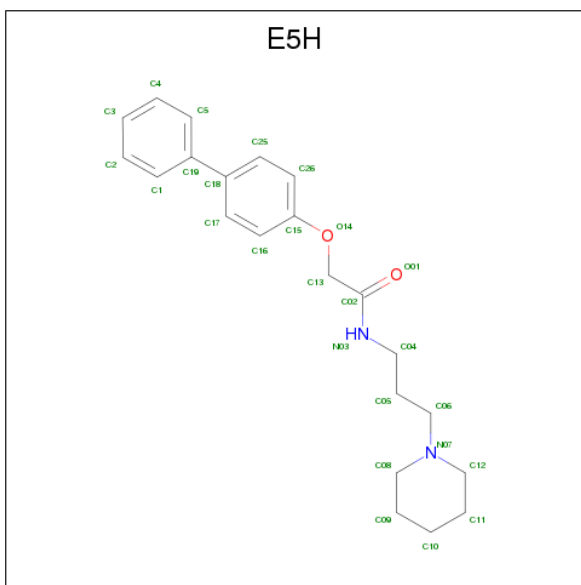
- Molecule 1 is a protein called Acetylcholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	535	Total	C	N	O	S	0	0	0
			4177	2679	725	759	14			
1	B	533	Total	C	N	O	S	0	0	0
			4158	2670	718	756	14			

There are 10 discrepancies between the modelled and reference sequences:

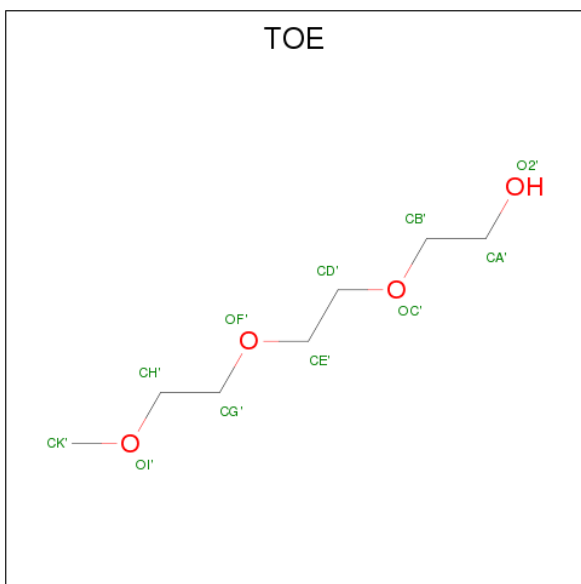
Chain	Residue	Modelled	Actual	Comment	Reference
A	544	ALA	-	expression tag	UNP P21836
A	545	THR	-	expression tag	UNP P21836
A	546	GLY	-	expression tag	UNP P21836
A	547	ALA	-	expression tag	UNP P21836
A	548	PRO	-	expression tag	UNP P21836
B	544	ALA	-	expression tag	UNP P21836
B	545	THR	-	expression tag	UNP P21836
B	546	GLY	-	expression tag	UNP P21836
B	547	ALA	-	expression tag	UNP P21836
B	548	PRO	-	expression tag	UNP P21836

- Molecule 2 is 2-(4-phenylphenoxy)- {N}-(3-piperidin-1-ylpropyl)ethanamide (three-letter code: E5H) (formula: C<sub>22</sub>H<sub>28</sub>N<sub>2</sub>O<sub>2</sub>).



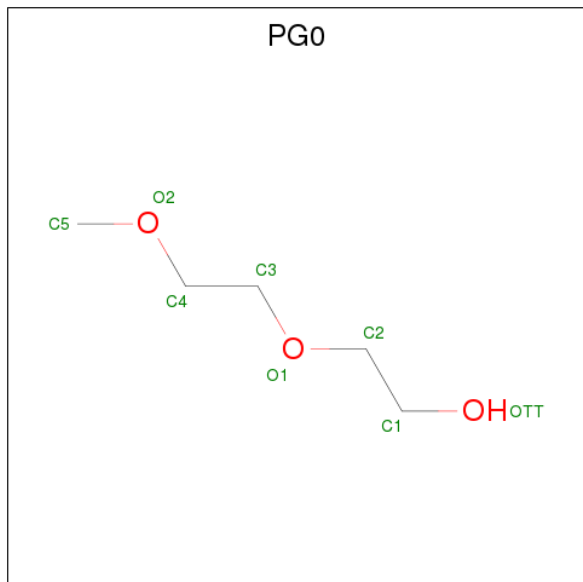
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	17	2	2		
2	B	1	Total	C	N	O	0	0
			21	17	2	2		

- Molecule 3 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>4</sub>).



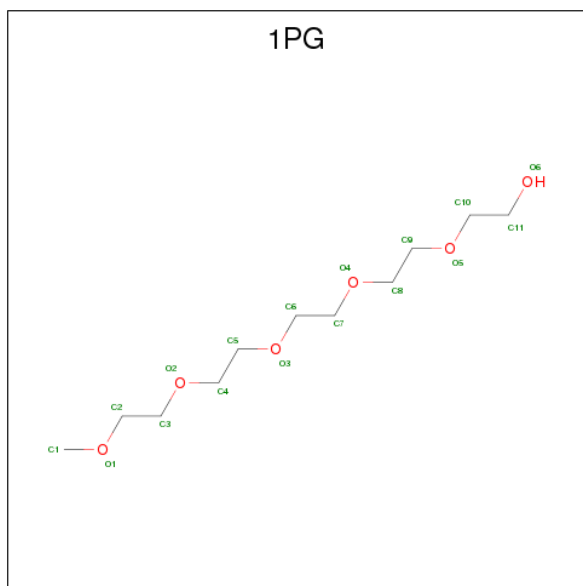
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	7	4		

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula:  $C_5H_{12}O_3$ ).



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

- Molecule 5 is 2-(2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHANOL (three-letter code: 1PG) (formula:  $C_{11}H_{24}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			17	11	6		

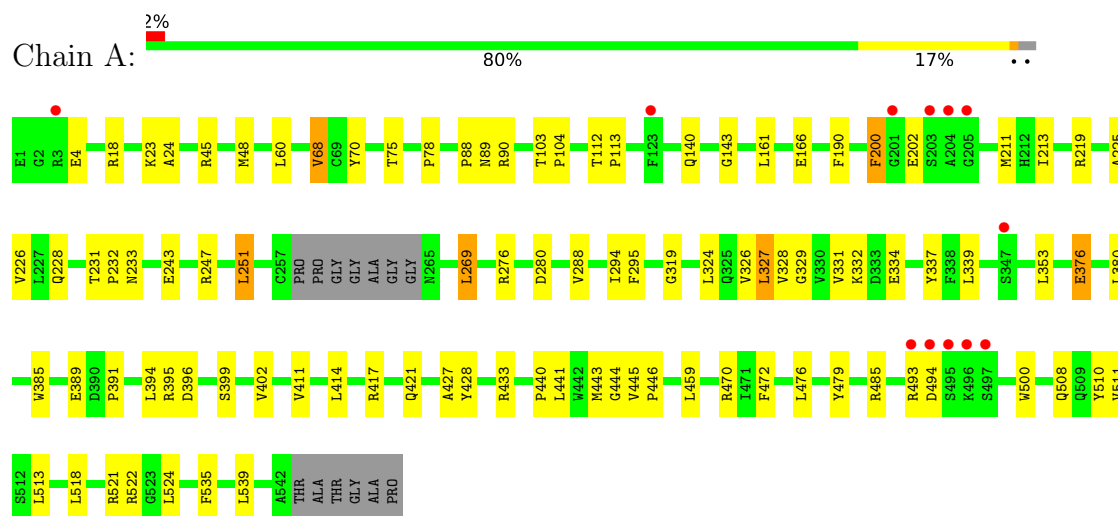
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total	O	0	0
			89	89		
6	B	76	Total	O	0	0
			76	76		

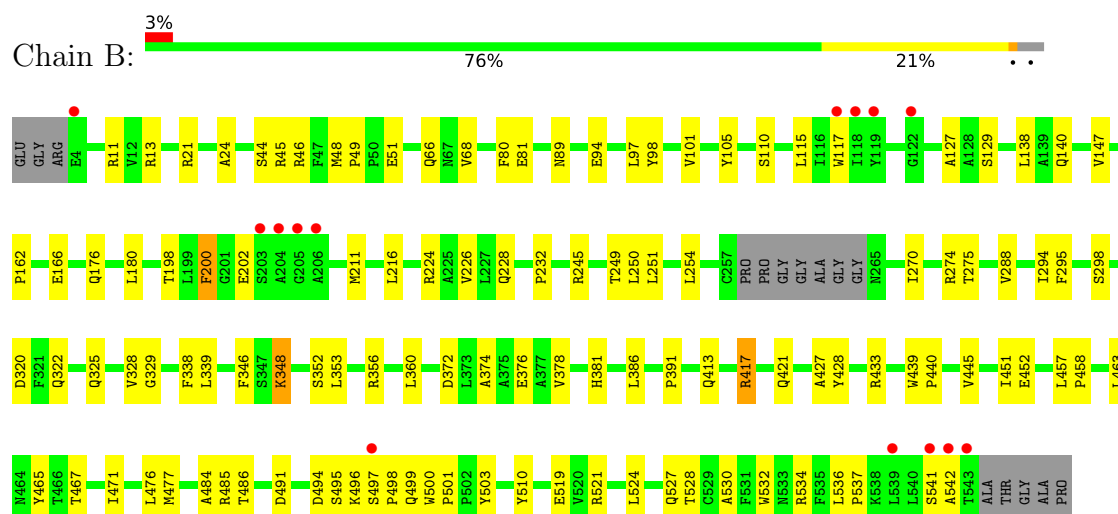
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.01Å 110.33Å 227.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.58 – 2.70 39.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (39.58-2.70) 94.9 (39.58-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.191 , 0.234 0.191 , 0.236	Depositor DCC
$R_{free}$ test set	1035 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.982	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 respectively for untwinned datasets, and 0.375, 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: TOE, E5H, PG0, 1PG

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	0.44	0/4300	0.62	0/5875
1	B	0.45	1/4281 (0.0%)	0.63	2/5851 (0.0%)
All	All	0.45	1/8581 (0.0%)	0.63	2/11726 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	81	GLU	CD-OE1	-7.27	1.17	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	THR	C-N-CA	-5.67	107.53	121.70
1	B	417	ARG	NE-CZ-NH1	5.28	122.94	120.30

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	4177	0	4065	55	0
1	B	4158	0	4047	69	0
2	A	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	21	0	0	0	0
3	A	11	0	16	2	0
4	A	8	0	12	1	0
4	B	8	0	12	1	0
5	B	17	0	24	2	0
6	A	89	0	0	1	0
6	B	76	0	0	0	0
All	All	8586	0	8176	122	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 (122) 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:381:HIS:HE1	1:B:528:THR:HG22	1.39	0.87
1:B:176:GLN:O	1:B:180:LEU:HD13	1.75	0.85
1:A:113:PRO:HG2	1:A:485:ARG:HG2	1.70	0.74
1:A:353:LEU:HB3	1:A:391:PRO:HB2	1.75	0.69
1:A:522:ARG:HH21	1:B:386:LEU:HD11	1.58	0.69
1:A:219:ARG:NH2	6:A:701:HOH:O	2.26	0.69
1:B:250:LEU:O	1:B:254:LEU:HD12	1.97	0.64
1:A:417:ARG:HD2	4:A:603:PG0:H32	1.79	0.64
1:B:89:ASN:ND2	1:B:129:SER:O	2.32	0.63
1:B:381:HIS:CE1	1:B:528:THR:HG22	2.30	0.61
1:B:202:GLU:OE1	1:B:451:ILE:HD11	2.01	0.60
1:A:535:PHE:CE2	1:A:539:LEU:HD12	2.36	0.60
1:B:294:ILE:HD11	1:B:338:PHE:O	2.02	0.60
1:A:213:ILE:HD13	1:A:324:LEU:HD21	1.84	0.60
1:A:276:ARG:NH2	1:A:280:ASP:OD2	2.34	0.60
1:B:166:GLU:HG2	1:B:270:ILE:HD13	1.83	0.59
1:A:440:PRO:HG2	1:A:443:MET:HG3	1.85	0.59
1:B:101:VAL:HG22	1:B:147:VAL:HG22	1.85	0.58
1:A:376:GLU:O	1:A:380:LEU:HD22	2.05	0.57
1:B:46:ARG:HB3	1:B:274:ARG:HG2	1.87	0.56
1:B:328:VAL:O	1:B:427:ALA:HA	2.06	0.56
1:A:89:ASN:O	1:A:90:ARG:NH1	2.39	0.55
1:A:327:LEU:HD11	1:A:500:TRP:CH2	2.42	0.55
1:A:104:PRO:HG3	1:A:143:GLY:HA2	1.88	0.54
1:B:48:MET:HE3	1:B:49:PRO:HD2	1.90	0.54
1:B:46:ARG:NH2	1:B:94:GLU:OE1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:PHE:CB	1:B:226:VAL:HB	2.38	0.53
1:B:497:SER:O	1:B:499:GLN:N	2.42	0.53
1:B:329:GLY:HA3	1:B:428:TYR:CZ	2.43	0.53
1:A:24:ALA:HB3	1:A:140:GLN:HG3	1.90	0.53
1:B:417:ARG:O	1:B:421:GLN:HG3	2.09	0.52
1:B:353:LEU:HB3	1:B:391:PRO:HB2	1.92	0.52
1:B:499:GLN:O	1:B:501:PRO:HD3	2.09	0.51
1:A:524:LEU:HD22	3:A:602:TOE:H15	1.92	0.51
1:B:138:LEU:HD23	1:B:477:MET:HE3	1.91	0.51
1:A:166:GLU:N	1:A:166:GLU:OE1	2.43	0.51
1:B:458:PRO:HA	1:B:465:TYR:CD2	2.46	0.51
1:A:511:VAL:HB	1:A:518:LEU:HD22	1.92	0.51
1:B:356:ARG:O	1:B:360:LEU:HD12	2.11	0.51
1:A:510:TYR:CZ	1:A:521:ARG:HB2	2.46	0.50
1:B:202:GLU:HA	1:B:228:GLN:O	2.11	0.50
1:B:372:ASP:O	1:B:376:GLU:HG3	2.10	0.50
1:B:115:LEU:HD23	1:B:198:THR:HB	1.93	0.50
1:A:68:VAL:HG21	1:A:88:PRO:HB3	1.95	0.49
1:B:21:ARG:HD3	1:B:105:TYR:CZ	2.47	0.49
1:B:329:GLY:HA3	1:B:428:TYR:CE2	2.48	0.49
1:A:231:THR:HG23	1:A:411:VAL:HG22	1.95	0.49
1:B:24:ALA:HB3	1:B:140:GLN:HG3	1.95	0.49
1:B:68:VAL:HG13	1:B:127:ALA:HB2	1.94	0.49
1:A:441:LEU:H	1:A:441:LEU:HD12	1.79	0.48
1:A:524:LEU:HD22	3:A:602:TOE:H13	1.94	0.48
1:B:457:LEU:O	1:B:463:LEU:HD12	2.12	0.48
1:A:75:THR:O	1:A:78:PRO:HD3	2.14	0.48
1:A:4:GLU:OE1	1:A:18:ARG:HD3	2.14	0.47
1:A:329:GLY:HA3	1:A:428:TYR:CE2	2.49	0.47
1:A:459:LEU:HD12	1:A:470:ARG:HG2	1.97	0.47
1:B:413:GLN:O	1:B:417:ARG:HG2	2.13	0.47
1:A:444:GLY:O	1:A:446:PRO:HD3	2.15	0.47
1:B:45:ARG:HD3	1:B:51:GLU:OE2	2.14	0.47
1:B:381:HIS:NE2	5:B:602:1PG:H112	2.30	0.47
1:B:510:TYR:OH	1:B:521:ARG:HD2	2.14	0.47
1:B:162:PRO:HD2	1:B:245:ARG:HB2	1.96	0.47
1:A:202:GLU:HA	1:A:228:GLN:O	2.15	0.46
1:A:385:TRP:HD1	1:B:527:GLN:OE1	1.98	0.46
1:A:45:ARG:HD3	1:A:48:MET:HB2	1.97	0.46
1:A:479:TYR:OH	1:A:518:LEU:HG	2.16	0.46
5:B:602:1PG:H82	5:B:602:1PG:H111	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:SER:HA	1:B:274:ARG:HD2	1.97	0.46
1:A:103:THR:HG21	1:A:190:PHE:HB3	1.98	0.45
1:B:510:TYR:CZ	1:B:521:ARG:HB2	2.50	0.45
1:B:433:ARG:HB2	1:B:445:VAL:HG22	1.98	0.45
1:B:162:PRO:O	1:B:245:ARG:NH1	2.50	0.45
1:A:231:THR:HB	1:A:233:ASN:OD1	2.17	0.44
1:A:243:GLU:O	1:A:247:ARG:HG3	2.17	0.44
1:B:519:GLU:CD	1:B:521:ARG:HH22	2.20	0.44
1:A:45:ARG:HH21	1:A:48:MET:HG3	1.82	0.44
1:B:491:ASP:HB3	1:B:494:ASP:HB3	2.00	0.44
1:B:485:ARG:HB2	1:B:486:THR:HG23	1.98	0.44
1:B:320:ASP:OD1	1:B:322:GLN:HG2	2.19	0.43
1:A:319:GLY:O	1:A:421:GLN:NE2	2.49	0.43
1:B:339:LEU:HD13	1:B:346:PHE:CE2	2.54	0.43
1:B:503:TYR:CE2	1:B:524:LEU:HD23	2.54	0.43
1:A:225:ALA:O	1:A:326:VAL:HA	2.19	0.43
1:A:472:PHE:CZ	1:A:476:LEU:HD11	2.54	0.43
1:B:245:ARG:O	1:B:249:THR:HG23	2.19	0.43
1:A:339:LEU:HD11	1:A:399:SER:HA	2.00	0.43
1:A:200:PHE:CB	1:A:226:VAL:HB	2.49	0.43
1:B:117:TRP:HA	1:B:200:PHE:O	2.18	0.42
1:B:417:ARG:HE	1:B:417:ARG:HB3	1.62	0.42
1:B:13:ARG:HB3	1:B:13:ARG:NH1	2.34	0.42
1:B:439:TRP:HB3	1:B:440:PRO:HD2	2.00	0.42
1:A:112:THR:HG21	1:A:143:GLY:O	2.19	0.42
1:A:328:VAL:O	1:A:427:ALA:HA	2.18	0.42
1:A:251:LEU:HB2	1:A:288:VAL:HG11	2.01	0.42
1:A:395:ARG:HD2	1:A:396:ASP:OD1	2.20	0.42
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.78	0.42
1:B:467:THR:O	1:B:471:ILE:HG12	2.20	0.42
1:A:211:MET:HG3	1:A:232:PRO:HB3	2.01	0.42
1:A:433:ARG:HB2	1:A:445:VAL:HG22	2.01	0.42
1:B:216:LEU:HD13	4:B:603:PG0:H53	2.01	0.42
1:B:428:TYR:HB3	1:B:500:TRP:CZ2	2.55	0.41
1:B:200:PHE:HB2	1:B:226:VAL:HB	2.02	0.41
1:B:13:ARG:HB3	1:B:13:ARG:HH11	1.86	0.41
1:B:224:ARG:HG2	1:B:325:GLN:HB2	2.02	0.41
1:B:80:PHE:CE2	1:B:348:LYS:HD2	2.56	0.41
1:B:491:ASP:HB3	1:B:494:ASP:CB	2.51	0.41
1:A:226:VAL:HG22	1:A:327:LEU:HB3	2.03	0.41
1:A:508:GLN:HE22	1:B:386:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:THR:HG21	1:A:411:VAL:HA	2.02	0.41
1:A:389:GLU:HA	1:A:394:LEU:HD11	2.03	0.41
1:B:374:ALA:O	1:B:378:VAL:HG23	2.20	0.41
1:B:530:ALA:HA	1:B:534:ARG:HD2	2.03	0.41
1:B:48:MET:SD	1:B:166:GLU:HA	2.61	0.41
1:B:211:MET:HG3	1:B:232:PRO:HB3	2.02	0.41
1:B:532:TRP:O	1:B:537:PRO:HD3	2.21	0.41
1:A:161:LEU:HD11	1:A:269:LEU:HD22	2.03	0.40
1:B:288:VAL:CG2	1:B:298:SER:HB3	2.52	0.40
1:B:115:LEU:HD21	1:B:484:ALA:HB2	2.03	0.40
1:A:331:VAL:HG22	1:A:334:GLU:OE1	2.20	0.40
1:A:476:LEU:HD22	1:A:513:LEU:HD13	2.02	0.40
1:B:66:GLN:HG3	1:B:98:TYR:CD1	2.57	0.40
1:A:294:ILE:HD11	1:A:402:VAL:HG21	2.02	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	531/548 (97%)	504 (95%)	26 (5%)	1 (0%)	49 77
1	B	529/548 (96%)	496 (94%)	27 (5%)	6 (1%)	16 38
All	All	1060/1096 (97%)	1000 (94%)	53 (5%)	7 (1%)	24 50

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	494	ASP
1	B	542	ALA
1	B	495	SER
1	B	496	LYS

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Mol	Chain	Res	Type
1	B	97	LEU
1	B	498	PRO
1	B	541	SER

### 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	439/445 (99%)	425 (97%)	14 (3%)	42	73
1	B	438/445 (98%)	428 (98%)	10 (2%)	53	82
All	All	877/890 (98%)	853 (97%)	24 (3%)	48	78

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	60	LEU
1	A	68	VAL
1	A	70	TYR
1	A	200	PHE
1	A	251	LEU
1	A	269	LEU
1	A	295	PHE
1	A	327	LEU
1	A	332	LYS
1	A	337	TYR
1	A	376	GLU
1	A	414	LEU
1	A	493	ARG
1	B	11	ARG
1	B	110	SER
1	B	200	PHE
1	B	251	LEU
1	B	295	PHE
1	B	348	LYS

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Mol	Chain	Res	Type
1	B	352	SER
1	B	452	GLU
1	B	476	LEU
1	B	536	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	181	GLN
1	A	508	GLN
1	B	279	GLN
1	B	381	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 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	$\# Z  > 2$
2	E5H	A	601	-	22,22,28	2.62	11 (50%)	27,27,35	1.98	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	TOE	A	602	-	10,10,10	0.67	0	9,9,9	0.70	0
4	PG0	A	603	-	7,7,7	0.52	0	6,6,6	0.93	0
2	E5H	B	601	-	22,22,28	2.27	8 (36%)	27,27,35	2.05	7 (25%)
5	1PG	B	602	-	16,16,16	0.66	0	15,15,15	1.22	2 (13%)
4	PG0	B	603	-	7,7,7	0.48	0	6,6,6	0.92	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	E5H	A	601	-	-	0/12/20/24	0/2/2/3
3	TOE	A	602	-	-	0/8/8/8	0/0/0/0
4	PG0	A	603	-	-	0/5/5/5	0/0/0/0
2	E5H	B	601	-	-	0/12/20/24	0/2/2/3
5	1PG	B	602	-	-	0/14/14/14	0/0/0/0
4	PG0	B	603	-	-	0/5/5/5	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	E5H	C16-C15	2.03	1.42	1.38
2	A	601	E5H	C26-C25	2.08	1.42	1.38
2	A	601	E5H	C16-C17	2.15	1.42	1.38
2	B	601	E5H	C12-N07	2.16	1.52	1.47
2	A	601	E5H	C26-C15	2.23	1.43	1.38
2	A	601	E5H	C12-N07	2.24	1.52	1.47
2	B	601	E5H	C26-C15	2.36	1.43	1.38
2	A	601	E5H	C04-N03	2.62	1.52	1.46
2	B	601	E5H	C16-C17	2.69	1.43	1.38
2	B	601	E5H	O14-C15	2.75	1.44	1.37
2	A	601	E5H	O14-C15	2.75	1.44	1.37
2	B	601	E5H	C26-C25	2.86	1.44	1.38
2	A	601	E5H	C08-N07	2.97	1.54	1.47
2	B	601	E5H	C06-N07	2.97	1.54	1.47
2	A	601	E5H	C06-N07	3.12	1.54	1.47
2	A	601	E5H	C13-C02	4.55	1.60	1.51
2	B	601	E5H	C13-C02	4.61	1.60	1.51
2	B	601	E5H	C02-N03	5.70	1.46	1.33
2	A	601	E5H	C02-N03	7.67	1.50	1.33



All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	E5H	C26-C15-C16	-4.49	113.19	120.18
2	A	601	E5H	C26-C15-C16	-4.13	113.76	120.18
2	A	601	E5H	C06-N07-C08	-3.43	102.44	111.23
2	B	601	E5H	C25-C18-C17	-3.35	110.69	118.12
2	B	601	E5H	C06-N07-C12	-3.05	103.40	111.23
2	A	601	E5H	C25-C18-C17	-3.02	111.42	118.12
2	B	601	E5H	C06-N07-C08	-2.78	104.09	111.23
2	A	601	E5H	C06-N07-C12	-2.32	105.27	111.23
5	B	602	1PG	C10-O5-C9	2.15	122.62	113.30
2	A	601	E5H	C13-C02-N03	2.20	120.25	116.57
5	B	602	1PG	C8-O4-C7	2.24	123.00	113.30
2	A	601	E5H	C12-N07-C08	2.28	113.89	108.86
2	B	601	E5H	O14-C13-C02	2.45	117.65	110.83
2	A	601	E5H	C05-C04-N03	2.51	119.45	112.21
2	A	601	E5H	O14-C13-C02	2.57	117.98	110.83
2	A	601	E5H	C25-C26-C15	3.23	123.73	119.73
2	B	601	E5H	C25-C26-C15	3.32	123.84	119.73
2	A	601	E5H	C16-C17-C18	3.71	126.42	121.38
2	B	601	E5H	C16-C17-C18	3.90	126.69	121.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	TOE	2	0
4	A	603	PG0	1	0
5	B	602	1PG	2	0
4	B	603	PG0	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, 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	535/548 (97%)	-0.11	12 (2%) 62 62	34, 48, 67, 107	0
1	B	533/548 (97%)	-0.03	14 (2%) 56 56	36, 52, 71, 89	0
All	All	1068/1096 (97%)	-0.07	26 (2%) 59 59	34, 50, 69, 107	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	542	ALA	4.0
1	A	497	SER	3.9
1	B	497	SER	3.5
1	B	543	THR	3.4
1	B	205	GLY	3.4
1	A	496	LYS	3.3
1	B	4	GLU	3.1
1	A	347	SER	3.1
1	B	118	ILE	3.0
1	A	495	SER	3.0
1	A	203	SER	2.9
1	B	204	ALA	2.7
1	B	541	SER	2.7
1	A	493	ARG	2.6
1	B	203	SER	2.6
1	A	204	ALA	2.5
1	A	3	ARG	2.5
1	A	201	GLY	2.4
1	B	119	TYR	2.4
1	A	494	ASP	2.4
1	B	122	GLY	2.4
1	A	205	GLY	2.3
1	B	206	ALA	2.2
1	B	117	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	123	PHE	2.1
1	B	539	LEU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	E5H	B	601	21/26	0.73	0.35	60,71,82,83	0
2	E5H	A	601	21/26	0.82	0.25	50,67,74,78	0
4	PG0	B	603	8/8	0.85	0.29	66,71,76,77	0
4	PG0	A	603	8/8	0.85	0.19	61,67,69,72	0
3	TOE	A	602	11/11	0.87	0.20	44,53,63,74	0
5	1PG	B	602	17/17	0.89	0.18	50,59,67,68	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.