Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:14 AM GMT

PDB ID	:	2C4H
Title	:	TORPEDO CALIFORNICA ACETYLCHOLINESTERASE IN COMPLEX WITH 500MM ACETYLTHIOCHOLINE
Authors	:	Colletier, J.P.; Fournier, D.; Greenblatt, H.M.; Sussman, J.L.; Zaccai, G.; Silman, I.; Weik, M.
Deposited on	:	2005-10-19
Resolution	:	2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (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
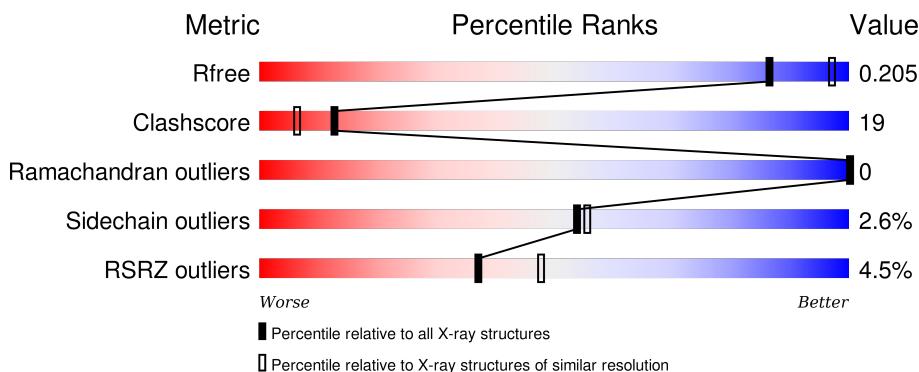
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	537	4% (red) 77% (green) 19% (yellow) •••

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	PGE	A	1539	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AT3	A	1540	-	-	X	X
5	AT3	A	1541	-	-	X	X
6	ACE	A	1543[A]	-	-	-	X
7	CL	A	1552	-	-	-	X
8	ACT	A	1555[B]	-	-	-	X

Full wwPDB X-ray Structure Validation Report

2 Entry composition (i)
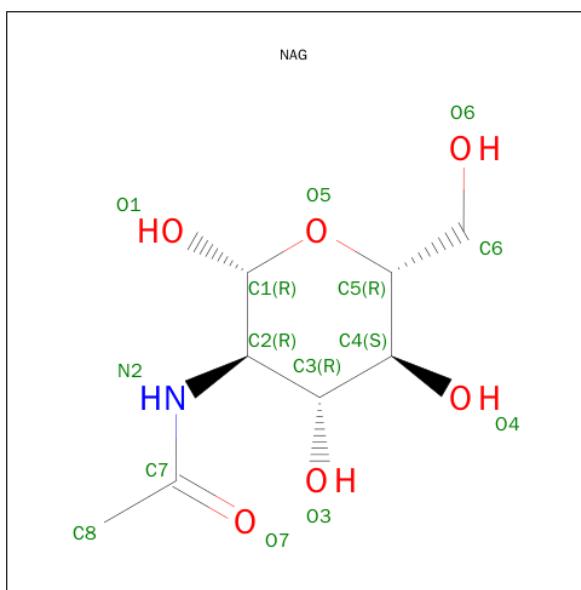
There are 9 unique types of molecules in this entry. The entry contains 5535 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.
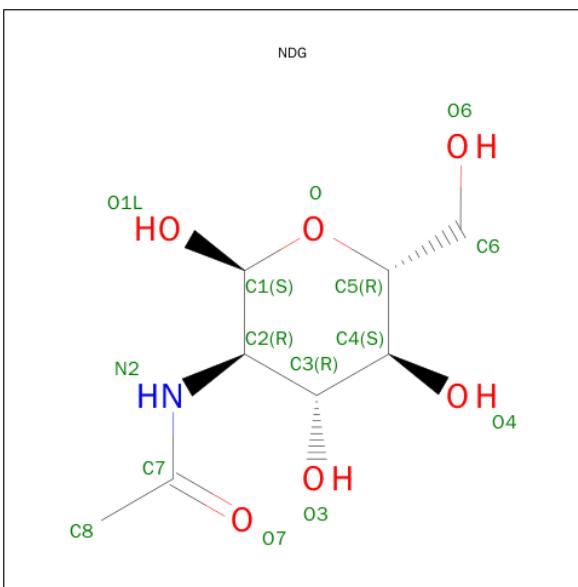
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total 4501	C 2874	N 770	O 830	S 27	0	29	1

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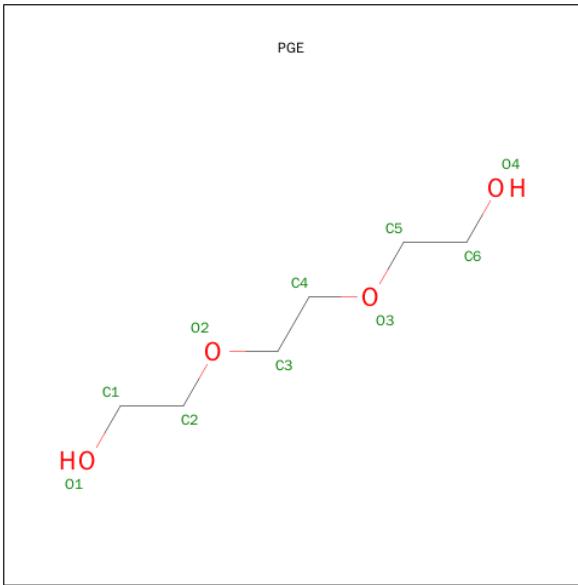
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).
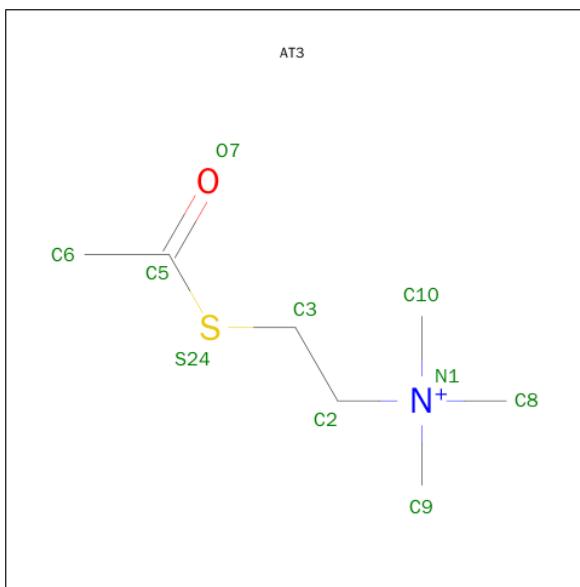
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
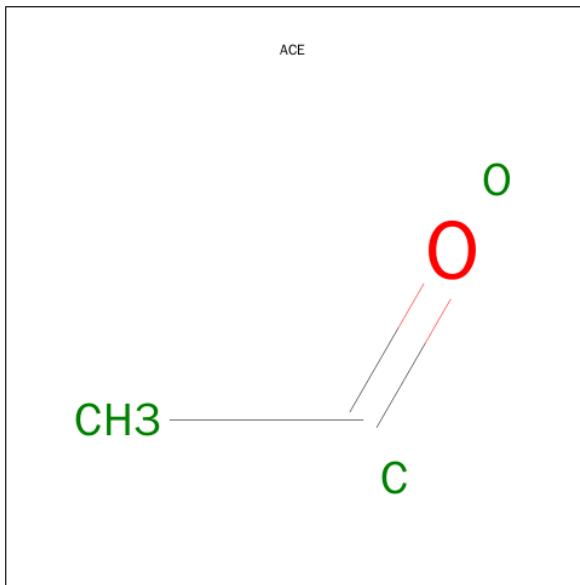
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 6	O 4	0	0
4	A	1	Total 10	C 6	O 4	0	0

- Molecule 5 is ACETYLTHIOCHOLINE (three-letter code: AT3) (formula: $C_7H_{16}NOS$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			10	7	1	1	1		
5	A	1	Total	C	N	O	S	0	0
			10	7	1	1	1		

- Molecule 6 is ACETYL GROUP (three-letter code: ACE) (formula: C_2H_4O).
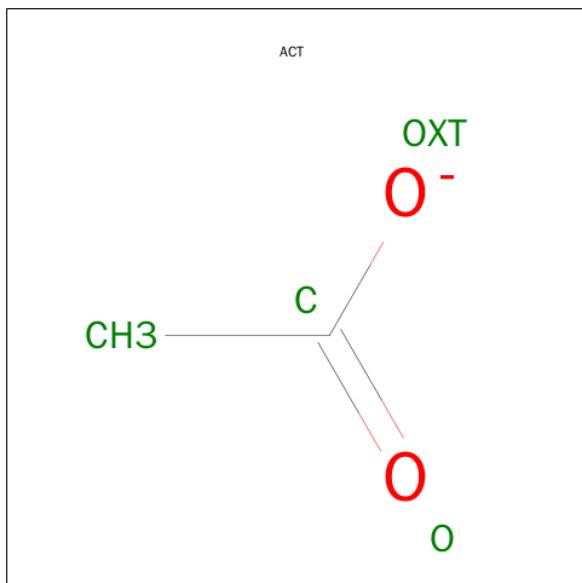
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	1
			3	2	1		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total Cl 11 11		0	0

• Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total C O 4 2 2			0	1
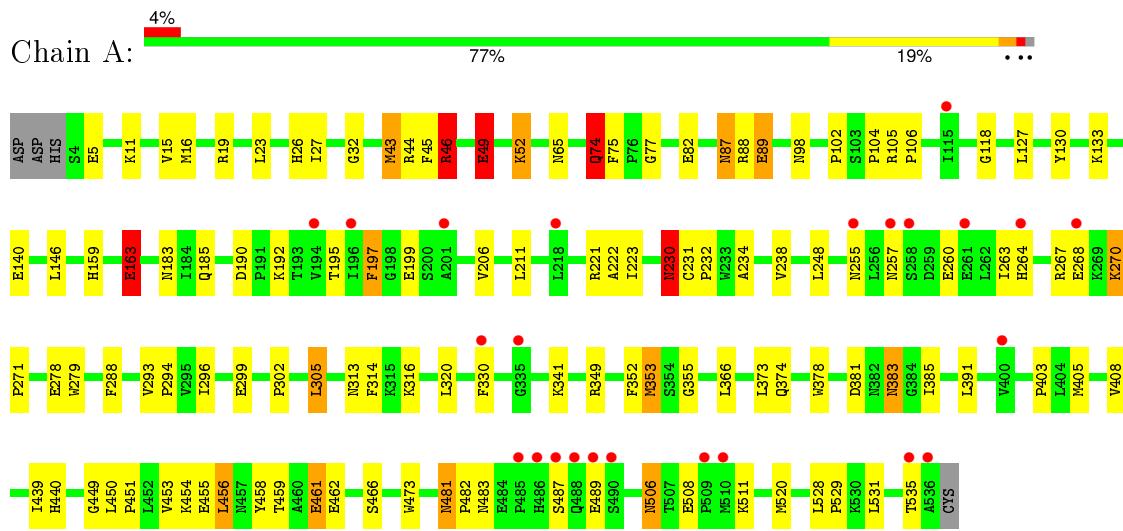
• Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	948	Total O 948 948		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

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	111.99Å 111.99Å 137.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 2.15 48.49 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.80-2.15) 99.6 (48.49-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.97 (at 2.16Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.169 , 0.209 0.165 , 0.205	Depositor DCC
R_{free} test set	2765 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.493	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 93.0	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning [2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 54312 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	5535	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PGE, NAG, ACE, CL, NDG, AT3, ACT

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	6.39	20/4627 (0.4%)	2.63	36/6277 (0.6%)

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	7

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	49[A]	GLU	CD-OE1	229.03	3.77	1.25
1	A	49[B]	GLU	CD-OE1	229.03	3.77	1.25
1	A	46[A]	ARG	CZ-NH1	170.88	3.55	1.33
1	A	46[B]	ARG	CZ-NH1	170.88	3.55	1.33
1	A	461[A]	GLU	CG-CD	66.43	2.51	1.51
1	A	461[B]	GLU	CG-CD	66.43	2.51	1.51
1	A	163[A]	GLU	CD-OE1	63.51	1.95	1.25
1	A	163[B]	GLU	CD-OE1	63.51	1.95	1.25
1	A	270[A]	LYS	CD-CE	55.23	2.89	1.51
1	A	270[B]	LYS	CD-CE	55.23	2.89	1.51
1	A	43[A]	MET	SD-CE	18.91	2.83	1.77
1	A	43[B]	MET	SD-CE	18.91	2.83	1.77
1	A	74[A]	GLN	CG-CD	18.57	1.93	1.51
1	A	74[B]	GLN	CG-CD	18.57	1.93	1.51
1	A	89[A]	GLU	CB-CG	-10.21	1.32	1.52
1	A	89[B]	GLU	CB-CG	-10.21	1.32	1.52
1	A	52[A]	LYS	CB-CG	8.89	1.76	1.52
1	A	52[B]	LYS	CB-CG	8.89	1.76	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353[A]	MET	CG-SD	-6.24	1.65	1.81
1	A	353[B]	MET	CG-SD	-6.24	1.65	1.81

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46[A]	ARG	NH1-CZ-NH2	-81.70	29.52	119.40
1	A	46[B]	ARG	NH1-CZ-NH2	-81.70	29.52	119.40
1	A	15[A]	VAL	CG1-CB-CG2	-67.28	3.26	110.90
1	A	15[B]	VAL	CG1-CB-CG2	-67.28	3.26	110.90
1	A	46[A]	ARG	NE-CZ-NH1	-56.93	91.84	120.30
1	A	46[B]	ARG	NE-CZ-NH1	-56.93	91.84	120.30
1	A	49[A]	GLU	CG-CD-OE1	-42.52	33.26	118.30
1	A	49[B]	GLU	CG-CD-OE1	-42.52	33.26	118.30
1	A	163[A]	GLU	OE1-CD-OE2	-32.70	84.06	123.30
1	A	163[B]	GLU	OE1-CD-OE2	-32.70	84.06	123.30
1	A	49[A]	GLU	OE1-CD-OE2	-29.51	87.89	123.30
1	A	49[B]	GLU	OE1-CD-OE2	-29.51	87.89	123.30
1	A	163[A]	GLU	CG-CD-OE2	25.77	169.83	118.30
1	A	163[B]	GLU	CG-CD-OE2	25.77	169.83	118.30
1	A	43[A]	MET	CG-SD-CE	-19.11	69.62	100.20
1	A	43[B]	MET	CG-SD-CE	-19.11	69.62	100.20
1	A	270[A]	LYS	CG-CD-CE	-17.20	60.29	111.90
1	A	270[B]	LYS	CG-CD-CE	-17.20	60.29	111.90
1	A	461[A]	GLU	CB-CG-CD	-13.07	78.91	114.20
1	A	461[B]	GLU	CB-CG-CD	-13.07	78.91	114.20
1	A	270[A]	LYS	CD-CE-NZ	12.60	140.67	111.70
1	A	270[B]	LYS	CD-CE-NZ	12.60	140.67	111.70
1	A	74[A]	GLN	CG-CD-OE1	-11.87	97.86	121.60
1	A	74[B]	GLN	CG-CD-OE1	-11.87	97.86	121.60
1	A	74[A]	GLN	OE1-CD-NE2	10.01	144.92	121.90
1	A	74[B]	GLN	OE1-CD-NE2	10.01	144.92	121.90
1	A	163[A]	GLU	CG-CD-OE1	-7.81	102.67	118.30
1	A	163[B]	GLU	CG-CD-OE1	-7.81	102.67	118.30
1	A	230[A]	ASN	OD1-CG-ND2	-7.80	103.95	121.90
1	A	230[B]	ASN	OD1-CG-ND2	-7.80	103.95	121.90
1	A	52[A]	LYS	CA-CB-CG	-7.33	97.27	113.40
1	A	52[B]	LYS	CA-CB-CG	-7.33	97.27	113.40
1	A	74[A]	GLN	CB-CG-CD	-6.94	93.56	111.60
1	A	74[B]	GLN	CB-CG-CD	-6.94	93.56	111.60
1	A	230[A]	ASN	O-C-N	-5.89	113.27	122.70
1	A	230[B]	ASN	O-C-N	-5.89	113.27	122.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163[A]	GLU	Sidechain
1	A	230[A]	ASN	Sidechain,Mainchain
1	A	230[B]	ASN	Mainchain
1	A	46[A]	ARG	Sidechain
1	A	49[A]	GLU	Sidechain
1	A	74[A]	GLN	Sidechain

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	4501	0	4318	166	0
2	A	14	0	13	0	0
3	A	14	0	13	0	0
4	A	20	0	28	2	0
5	A	20	0	32	32	0
6	A	3	0	3	0	0
7	A	11	0	0	1	0
8	A	4	0	3	1	0
9	A	948	0	0	16	2
All	All	5535	0	4410	174	2

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 19.

All (174) 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:A:52[A]:LYS:CB	1:A:52[A]:LYS:CG	1.76	1.61
1:A:461[B]:GLU:CG	1:A:461[B]:GLU:CD	1.82	1.47
1:A:74[A]:GLN:CD	1:A:74[A]:GLN:CG	1.93	1.35
1:A:74[B]:GLN:CD	1:A:74[B]:GLN:OE1	1.75	1.23
1:A:163[A]:GLU:OE1	1:A:163[A]:GLU:CD	1.95	1.04
1:A:270[A]:LYS:HG3	1:A:270[A]:LYS:CE	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461[B]:GLU:CG	1:A:461[B]:GLU:OE1	2.08	1.00
1:A:270[B]:LYS:HG2	1:A:270[B]:LYS:CE	1.91	0.99
1:A:330[B]:PHE:CG	5:A:1540:AT3:H6C2	1.99	0.98
1:A:270[B]:LYS:HG2	1:A:270[B]:LYS:HE2	1.46	0.95
1:A:46[A]:ARG:NH1	1:A:46[A]:ARG:HH21	1.71	0.88
1:A:270[A]:LYS:CG	1:A:270[A]:LYS:CE	2.51	0.87
1:A:52[A]:LYS:CA	1:A:52[A]:LYS:CG	2.53	0.87
1:A:49[A]:GLU:HG2	1:A:49[A]:GLU:OE1	1.77	0.85
1:A:330[A]:PHE:HE2	5:A:1541:AT3:C6	1.92	0.81
1:A:270[B]:LYS:CG	1:A:270[B]:LYS:CE	2.58	0.80
1:A:270[B]:LYS:CD	1:A:270[B]:LYS:CE	2.60	0.80
1:A:461[A]:GLU:CG	1:A:461[A]:GLU:CD	2.51	0.78
1:A:330[A]:PHE:CE2	5:A:1541:AT3:C6	2.67	0.78
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.82	0.78
1:A:74[A]:GLN:CD	1:A:74[A]:GLN:CB	2.52	0.78
5:A:1540:AT3:H2C1	9:A:2122:HOH:O	1.83	0.78
1:A:270[A]:LYS:HE3	1:A:270[A]:LYS:HG3	1.66	0.77
1:A:49[B]:GLU:HG3	1:A:49[B]:GLU:OE1	1.87	0.75
1:A:330[A]:PHE:HB2	5:A:1540:AT3:H6C2	1.69	0.75
1:A:330[B]:PHE:CB	5:A:1540:AT3:H6C2	2.17	0.74
1:A:330[A]:PHE:CE2	5:A:1541:AT3:H6C2	2.22	0.74
1:A:43[B]:MET:SD	1:A:43[B]:MET:CE	2.76	0.74
1:A:43[A]:MET:HG3	1:A:43[A]:MET:CE	2.18	0.73
1:A:52[A]:LYS:CB	1:A:52[A]:LYS:CD	2.65	0.72
1:A:11:LYS:H	1:A:183:ASN:ND2	1.86	0.72
1:A:199:GLU:OE1	5:A:1540:AT3:H103	1.88	0.72
1:A:238[B]:VAL:HG21	4:A:1539:PGE:H1	1.72	0.72
1:A:74[A]:GLN:CG	1:A:74[A]:GLN:OE1	2.39	0.70
1:A:279:TRP:CD2	5:A:1541:AT3:H101	2.26	0.70
1:A:74[B]:GLN:CG	1:A:74[B]:GLN:OE1	2.40	0.69
1:A:461[B]:GLU:CB	1:A:461[B]:GLU:CD	2.60	0.69
1:A:330[B]:PHE:CD1	5:A:1540:AT3:H6C2	2.27	0.68
1:A:279:TRP:CG	5:A:1541:AT3:H101	2.28	0.68
1:A:87:ASN:HD22	1:A:87:ASN:H	1.40	0.67
1:A:330[A]:PHE:CB	5:A:1540:AT3:H6C2	2.21	0.67
1:A:43[B]:MET:HG2	1:A:43[B]:MET:CE	2.25	0.67
1:A:43[A]:MET:SD	1:A:43[A]:MET:CE	2.83	0.67
5:A:1540:AT3:H101	8:A:1555[B]:ACT:O	1.95	0.66
1:A:102:PRO:HB3	1:A:140:GLU:OE1	1.95	0.66
1:A:461[A]:GLU:HB2	1:A:461[A]:GLU:CD	2.18	0.64
1:A:481:ASN:ND2	1:A:483:ASN:H	1.94	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43[A]:MET:CG	1:A:43[A]:MET:CE	2.76	0.64
5:A:1541:AT3:H9C3	9:A:2631:HOH:O	1.98	0.64
1:A:330[B]:PHE:CG	5:A:1540:AT3:C6	2.80	0.64
1:A:302:PRO:HB2	9:A:2610:HOH:O	1.97	0.63
1:A:11:LYS:HB2	1:A:183:ASN:HD21	1.63	0.63
1:A:330[A]:PHE:CG	5:A:1540:AT3:H6C2	2.34	0.62
1:A:461[A]:GLU:CD	1:A:461[A]:GLU:CB	2.67	0.62
1:A:508:GLU:HG3	9:A:2865:HOH:O	1.99	0.62
1:A:383:ASN:HD22	1:A:383:ASN:C	2.03	0.61
1:A:43[B]:MET:CG	1:A:43[B]:MET:CE	2.78	0.61
1:A:330[A]:PHE:CD1	5:A:1540:AT3:H6C2	2.34	0.61
1:A:230[B]:ASN:CG	1:A:230[B]:ASN:O	2.39	0.60
1:A:238[A]:VAL:HG21	4:A:1539:PGE:H1	1.83	0.60
1:A:487:SER:OG	1:A:489:GLU:HG2	2.02	0.60
1:A:313:ASN:ND2	9:A:2610:HOH:O	2.34	0.60
5:A:1541:AT3:H3C1	9:A:2631:HOH:O	2.00	0.59
1:A:453:VAL:HB	1:A:456:LEU:HD22	1.83	0.59
1:A:163[A]:GLU:OE1	1:A:163[A]:GLU:OE2	2.19	0.59
1:A:46[A]:ARG:NH1	1:A:46[A]:ARG:NH2	2.48	0.58
1:A:163[A]:GLU:HG3	9:A:2154:HOH:O	2.05	0.57
1:A:440:HIS:HB3	5:A:1540:AT3:H6C3	1.86	0.57
1:A:481:ASN:HD22	1:A:482:PRO:N	2.02	0.57
1:A:481:ASN:HD22	1:A:482:PRO:CD	2.18	0.57
1:A:159:HIS:HB3	1:A:238[B]:VAL:HG13	1.87	0.56
1:A:330[B]:PHE:HB2	5:A:1540:AT3:H6C2	1.85	0.56
1:A:279:TRP:CE2	5:A:1541:AT3:H101	2.40	0.56
1:A:264[B]:HIS:O	1:A:268[B]:GLU:HG3	2.06	0.56
1:A:279:TRP:CD1	5:A:1541:AT3:H101	2.41	0.55
1:A:506:ASN:HD22	1:A:506:ASN:C	2.10	0.55
1:A:231[B]:CYS:HB2	1:A:232:PRO:HD2	1.89	0.55
1:A:373:LEU:HD12	1:A:378:TRP:HE1	1.72	0.54
1:A:87:ASN:ND2	1:A:87:ASN:H	2.05	0.54
1:A:531:LEU:HD23	1:A:531:LEU:C	2.28	0.54
1:A:87:ASN:HD22	1:A:87:ASN:N	2.01	0.54
1:A:366:LEU:HD23	1:A:535:THR:HG21	1.89	0.54
1:A:481:ASN:HD22	1:A:482:PRO:HD2	1.73	0.54
1:A:255:ASN:HD21	1:A:257:ASN:HD22	1.54	0.54
1:A:481:ASN:C	1:A:481:ASN:HD22	2.11	0.54
1:A:5:GLU:OE2	1:A:104:PRO:HA	2.07	0.54
1:A:159:HIS:CB	1:A:238[B]:VAL:HG13	2.38	0.54
1:A:330[A]:PHE:C	1:A:330[A]:PHE:CD2	2.81	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330[A]:PHE:CZ	5:A:1541:AT3:H6C2	2.43	0.53
1:A:77:GLY:N	1:A:82[A]:GLU:OE1	2.36	0.52
1:A:27:ILE:HD11	1:A:133:LYS:HB2	1.91	0.52
5:A:1541:AT3:O7	9:A:2947:HOH:O	2.18	0.51
1:A:278:GLU:HB2	9:A:2558:HOH:O	2.11	0.51
1:A:197:PHE:CB	1:A:223:ILE:HB	2.40	0.51
1:A:481:ASN:HD21	1:A:483:ASN:HD22	1.57	0.51
1:A:506:ASN:ND2	1:A:508:GLU:H	2.08	0.51
1:A:211:LEU:HD23	1:A:314:PHE:HB3	1.92	0.51
1:A:127:LEU:HD12	1:A:130:TYR:CE2	2.46	0.51
1:A:195:THR:OG1	1:A:221:ARG:HG3	2.11	0.50
1:A:260:GLU:HG3	1:A:264[A]:HIS:CE1	2.46	0.50
1:A:270[A]:LYS:CD	1:A:270[A]:LYS:CE	2.89	0.50
1:A:255:ASN:HD21	1:A:257:ASN:ND2	2.07	0.50
1:A:506:ASN:HD22	1:A:508:GLU:H	1.58	0.50
1:A:461[B]:GLU:HG3	1:A:461[B]:GLU:OE1	2.07	0.50
1:A:330[A]:PHE:CD1	5:A:1540:AT3:C6	2.95	0.50
1:A:185:GLN:NE2	9:A:2464:HOH:O	2.44	0.49
1:A:264[B]:HIS:HE1	1:A:268[B]:GLU:OE2	1.96	0.49
1:A:449:GLY:HA2	1:A:466:SER:OG	2.12	0.49
1:A:459:THR:OG1	1:A:462:GLU:HG3	2.12	0.49
1:A:163[A]:GLU:HB2	1:A:263:ILE:HD13	1.94	0.49
1:A:223:ILE:HA	1:A:320:LEU:O	2.13	0.48
1:A:163[B]:GLU:HB3	1:A:267:ARG:NH2	2.27	0.48
1:A:374:GLN:HE21	1:A:520:MET:CE	2.26	0.48
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.48	0.48
1:A:296:ILE:HD12	1:A:305:LEU:HD13	1.96	0.47
1:A:11:LYS:H	1:A:183:ASN:HD21	1.62	0.47
1:A:314:PHE:O	1:A:316:LYS:HD2	2.14	0.47
1:A:32:GLY:H	1:A:98:ASN:HD22	1.61	0.47
1:A:511:LYS:HE2	9:A:2867:HOH:O	2.14	0.47
1:A:481:ASN:ND2	1:A:482:PRO:HD2	2.30	0.47
1:A:352:PHE:HD2	1:A:353[A]:MET:HE2	1.80	0.46
1:A:16[B]:MET:HE3	9:A:2065:HOH:O	2.15	0.46
1:A:163[B]:GLU:HB3	1:A:267:ARG:HH22	1.80	0.46
1:A:271:PRO:HD2	7:A:1550:CL:CL	2.52	0.46
1:A:270[A]:LYS:CG	1:A:270[A]:LYS:HE3	2.36	0.46
1:A:450:LEU:N	1:A:451:PRO:CD	2.78	0.46
1:A:231[B]:CYS:SG	1:A:234:ALA:HB2	2.56	0.46
5:A:1541:AT3:H3C1	5:A:1541:AT3:H8C2	1.72	0.46
1:A:19[A]:ARG:NH1	1:A:26:HIS:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:HE3	9:A:2645:HOH:O	2.16	0.45
1:A:383:ASN:HD21	1:A:385:ILE:HB	1.81	0.45
1:A:278:GLU:HB3	9:A:2566:HOH:O	2.16	0.45
1:A:405:MET:O	1:A:408:VAL:HG12	2.17	0.45
1:A:330[A]:PHE:CG	5:A:1540:AT3:C6	3.00	0.44
1:A:32:GLY:H	1:A:98:ASN:ND2	2.14	0.44
1:A:197:PHE:HB3	1:A:223:ILE:HB	1.98	0.44
1:A:43[A]:MET:HG3	1:A:43[A]:MET:HE3	2.00	0.44
1:A:268[A]:GLU:HA	1:A:268[A]:GLU:OE2	2.18	0.44
1:A:453:VAL:HG12	1:A:455:GLU:HG2	1.99	0.43
1:A:206:VAL:CG1	1:A:222:ALA:HB1	2.48	0.43
1:A:230[B]:ASN:O	1:A:230[B]:ASN:ND2	2.51	0.43
1:A:231[B]:CYS:SG	1:A:234:ALA:CB	3.07	0.43
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.99	0.43
1:A:349:ARG:HD3	1:A:381:ASP:O	2.19	0.43
1:A:461[B]:GLU:HB3	1:A:461[B]:GLU:CD	2.37	0.43
1:A:163[A]:GLU:OE1	1:A:163[A]:GLU:HA	2.19	0.43
1:A:44:ARG:O	1:A:45:PHE:HB2	2.18	0.43
1:A:439:ILE:HG22	1:A:440:HIS:N	2.34	0.43
1:A:279:TRP:CD1	5:A:1541:AT3:C10	3.03	0.42
1:A:260:GLU:O	1:A:264[A]:HIS:ND1	2.52	0.42
1:A:355:GLY:HA3	1:A:391:LEU:HD11	2.01	0.42
1:A:481:ASN:HD22	1:A:483:ASN:H	1.65	0.42
1:A:19[A]:ARG:NH1	1:A:26:HIS:CB	2.82	0.42
1:A:293:VAL:HB	1:A:294:PRO:HD2	2.01	0.42
1:A:146:LEU:HD12	1:A:146:LEU:C	2.39	0.42
1:A:43[B]:MET:HG2	1:A:43[B]:MET:HE2	1.99	0.42
1:A:118:GLY:N	5:A:1540:AT3:C9	2.83	0.42
1:A:299:GLU:HG3	9:A:2586:HOH:O	2.20	0.42
1:A:230[B]:ASN:O	1:A:403:PRO:HB3	2.20	0.42
5:A:1540:AT3:H3C2	5:A:1540:AT3:H102	1.77	0.41
5:A:1540:AT3:H8C1	9:A:2373:HOH:O	2.20	0.41
1:A:65:ASN:OD1	1:A:89[B]:GLU:HG2	2.21	0.41
1:A:330[A]:PHE:CZ	5:A:1541:AT3:C6	3.01	0.41
1:A:87:ASN:ND2	1:A:87:ASN:N	2.66	0.41
1:A:461[A]:GLU:OE1	1:A:461[A]:GLU:N	2.46	0.41
1:A:197:PHE:HB2	1:A:223:ILE:HB	2.03	0.41
1:A:349:ARG:O	1:A:353[B]:MET:HG3	2.21	0.41
1:A:105:ARG:HA	1:A:106:PRO:HD3	1.97	0.41
1:A:74[A]:GLN:OE1	1:A:74[A]:GLN:CB	2.68	0.40
1:A:43[A]:MET:HE1	1:A:49[A]:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ARG:HA	1:A:349:ARG:HD2	1.79	0.40
1:A:74[A]:GLN:HG3	1:A:75:PHE:CE2	2.56	0.40
1:A:87:ASN:ND2	1:A:88[A]:ARG:HG2	2.36	0.40
1:A:456:LEU:HA	1:A:456:LEU:HD12	1.84	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:2342:HOH:O	9:A:2342:HOH:O[4_556]	1.71	0.49
9:A:2919:HOH:O	9:A:2919:HOH:O[4_556]	2.05	0.15

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	560/537 (104%)	538 (96%)	22 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	494/469 (105%)	482 (98%)	12 (2%)	57 60

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	87	ASN
1	A	197	PHE
1	A	248	LEU
1	A	288	PHE
1	A	305	LEU
1	A	383	ASN
1	A	454	LYS
1	A	456	LEU
1	A	473	TRP
1	A	481	ASN
1	A	506	ASN

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	68	GLN
1	A	87	ASN
1	A	98	ASN
1	A	183	ASN
1	A	257	ASN
1	A	324	ASN
1	A	362	HIS
1	A	374	GLN
1	A	383	ASN
1	A	387	ASN
1	A	481	ASN
1	A	506	ASN
1	A	519	GLN
1	A	525	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 11 are monoatomic - leaving 8 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	NAG	A	1536	1	14,14,15	0.51	0	15,19,21	0.78	1 (6%)
3	NDG	A	1537	1	14,14,15	0.89	1 (7%)	15,19,21	0.83	0
4	PGE	A	1538	-	9,9,9	0.96	0	8,8,8	1.00	1 (12%)
4	PGE	A	1539	-	9,9,9	0.90	1 (11%)	8,8,8	1.20	2 (25%)
5	AT3	A	1540	-	9,9,9	1.57	1 (11%)	11,12,12	0.41	0
5	AT3	A	1541	-	9,9,9	1.54	1 (11%)	11,12,12	0.35	0
6	ACE	A	1543[A]	1	2,2,2	0.83	0	0,1,1	0.00	-
8	ACT	A	1555[B]	-	1,3,3	1.70	0	0,3,3	0.00	-

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	1536	1	-	0/6/23/26	0/1/1/1
3	NDG	A	1537	1	-	2/6/23/26	0/1/1/1
4	PGE	A	1538	-	-	0/7/7/7	0/0/0/0
4	PGE	A	1539	-	-	0/7/7/7	0/0/0/0
5	AT3	A	1540	-	-	0/7/7/7	0/0/0/0
5	AT3	A	1541	-	-	0/7/7/7	0/0/0/0
6	ACE	A	1543[A]	1	-	0/0/0/0	0/0/0/0
8	ACT	A	1555[B]	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1539	PGE	O3-C5	2.05	1.50	1.42
3	A	1537	NDG	C1-C2	2.90	1.56	1.52
5	A	1541	AT3	O7-C5	4.17	1.43	1.21
5	A	1540	AT3	O7-C5	4.23	1.43	1.21

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1536	NAG	C2-N2-C7	-2.39	119.97	123.04
4	A	1539	PGE	O2-C3-C4	-2.06	101.23	110.36
4	A	1539	PGE	O3-C5-C6	2.05	119.87	110.43
4	A	1538	PGE	O2-C2-C1	2.13	120.23	110.43

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1537	NDG	O7-C7-N2-C2
3	A	1537	NDG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1539	PGE	2	0
5	A	1540	AT3	18	0
5	A	1541	AT3	14	0
8	A	1555[B]	ACT	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(Å^2)	Q<0.9
1	A	533/537 (99%)	-0.02	24 (4%)	37	48	23, 34, 53, 84	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	HIS	6.8
1	A	488	GLN	5.2
1	A	485	PRO	4.5
1	A	509	PRO	3.5
1	A	487	SER	3.4
1	A	257	ASN	3.3
1	A	489	GLU	3.0
1	A	510[A]	MET	2.9
1	A	264[A]	HIS	2.8
1	A	536	ALA	2.7
1	A	330[A]	PHE	2.6
1	A	535	THR	2.5
1	A	218	LEU	2.4
1	A	201	ALA	2.3
1	A	490	SER	2.3
1	A	261	GLU	2.2
1	A	255	ASN	2.2
1	A	268[A]	GLU	2.2
1	A	400	VAL	2.1
1	A	335	GLY	2.0
1	A	258	SER	2.0
1	A	194	VAL	2.0
1	A	115	ILE	2.0
1	A	196	ILE	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
8	ACT	A	1555[B]	4/4	0.98	0.35	6.62	19,20,21,23	4
7	CL	A	1552	1/1	0.97	0.26	6.07	82,82,82,82	0
6	ACE	A	1543[A]	3/3	0.98	0.32	5.29	32,32,38,39	3
5	AT3	A	1541	10/10	0.87	0.39	4.90	81,82,83,84	0
4	PGE	A	1539	10/10	0.82	0.27	4.16	67,69,77,79	0
5	AT3	A	1540	10/10	0.91	0.28	2.67	76,77,78,79	0
7	CL	A	1551	1/1	0.97	0.12	1.97	79,79,79,79	0
4	PGE	A	1538	10/10	0.90	0.19	1.51	48,57,60,60	0
7	CL	A	1547	1/1	0.88	0.11	0.15	82,82,82,82	0
7	CL	A	1550	1/1	0.86	0.17	0.01	80,80,80,80	0
7	CL	A	1548	1/1	0.98	0.09	-0.26	69,69,69,69	0
7	CL	A	1546	1/1	0.93	0.09	-0.35	58,58,58,58	0
7	CL	A	1549	1/1	0.89	0.13	-1.00	88,88,88,88	0
7	CL	A	1545	1/1	1.00	0.08	-1.39	35,35,35,35	0
7	CL	A	1544	1/1	0.98	0.06	-	49,49,49,49	0
7	CL	A	1553	1/1	0.92	0.07	-	69,69,69,69	0
7	CL	A	1554	1/1	0.81	0.19	-	75,75,75,75	0
3	NDG	A	1537	14/15	0.76	0.28	-	67,71,72,73	0
2	NAG	A	1536	14/15	0.91	0.18	-	53,56,59,62	0

6.5 Other polymers (i)

There are no such residues in this entry.