Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2016 – 04:31 PM EDT

PDB ID	:	4LQG
Title	:	X-ray structure of human glutamate carboxypeptidase II (GCPII) in complex with a phosphoramidate inhibitor CTT1056
Authors	:	Barinka, C.; Skultetyova, L.
Deposited on	:	2013-07-18
Resolution	:	1.77 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 (1)) were used in the production of this report:

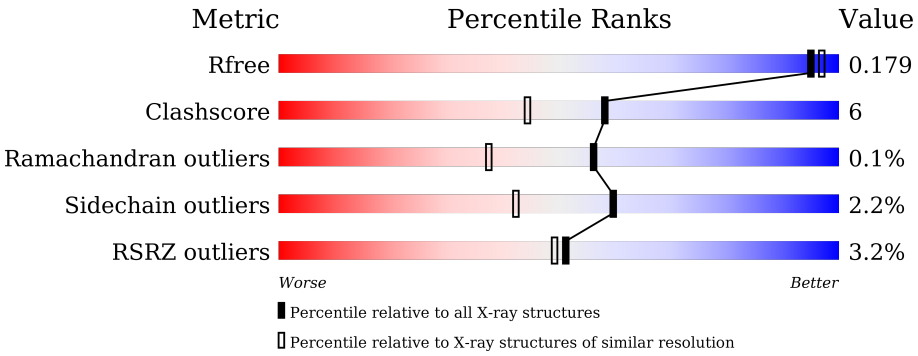
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance

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

The reported resolution of this entry is 1.77 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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	709	3% 86% 11%

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
5	NAG	A	806	-	-	-	X
6	NAG	A	807	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	NAG	A	815	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 6791 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 Glutamate carboxypeptidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	692	Total	C	N	O	S	0	75	0
			5923	3794	990	1113	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ARG	-	EXPRESSION TAG	UNP Q04609
A	43	SER	-	EXPRESSION TAG	UNP Q04609

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

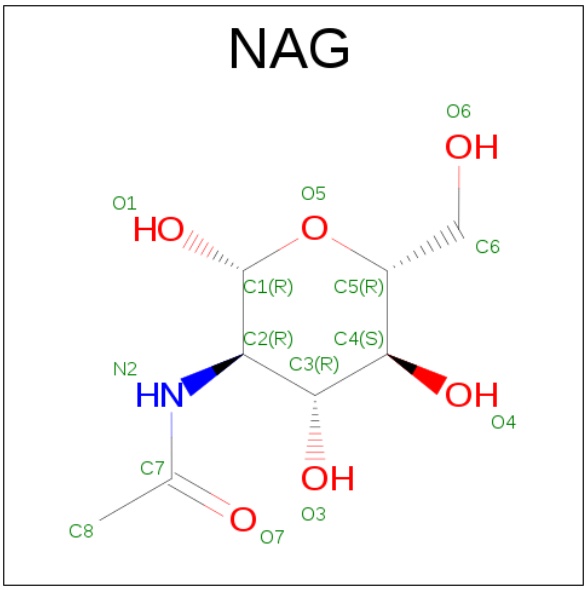
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total C N O 28 16 2 10	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total C N O 38 22 2 14	0	0
6	A	3	Total C N O 38 22 2 14	0	0

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

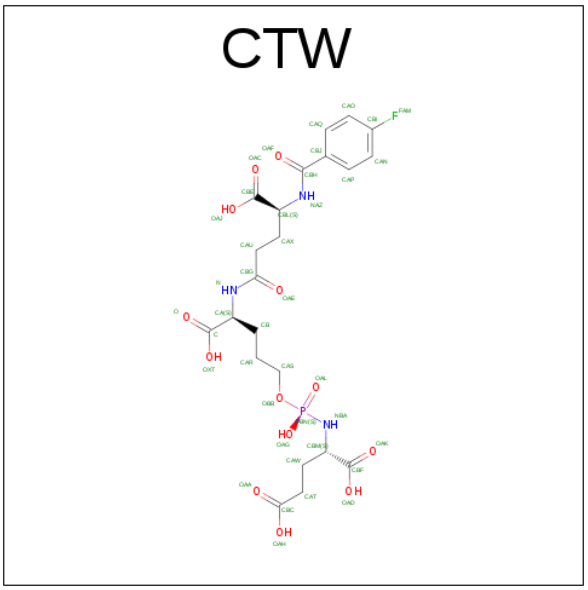
- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total C N O 39 22 2 15	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 10 is N-(4-FLUOROBENZOYL)-L-GAMMA-GLUTAMYL-5-{[(S)-{[(1S)-1,3-DICARBOXYPROPYL]AMINO}(HYDROXY)PHOSPHORYL]OXY}-L-NORVALINE (three-letter code: CTW) (formula: $C_{22}H_{29}FN_3O_{13}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	A	1	Total	C	F	N	O	P	0	0
			40	22	1	3	13	1		

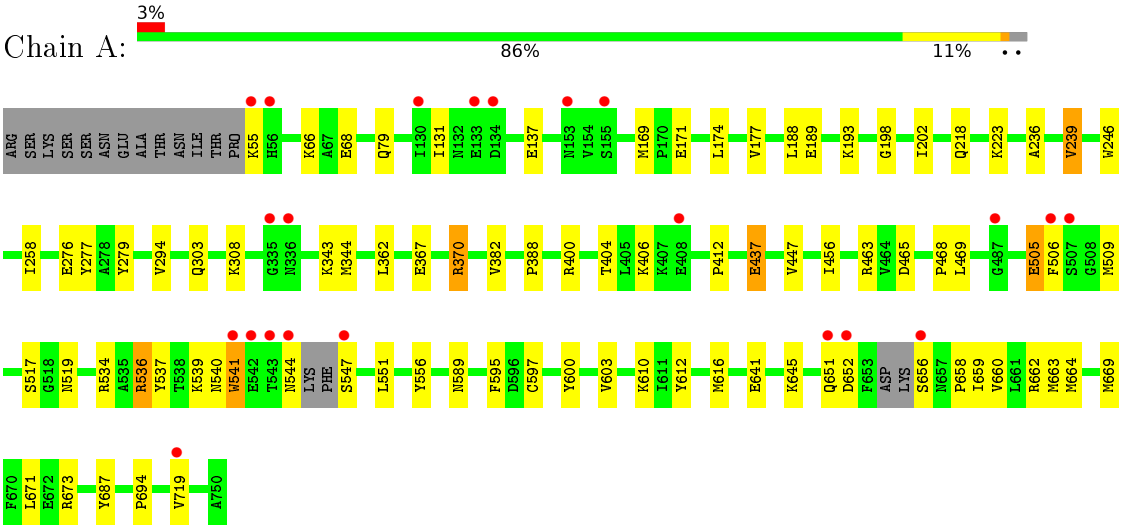
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	592	Total	O	0	0
			592	592		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate carboxypeptidase 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	101.90Å 130.23Å 158.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.51 – 1.77 19.69 – 1.77	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.51-1.77) 99.5 (19.69-1.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 1.77Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.157 , 0.182 0.156 , 0.179	Depositor DCC
R_{free} test set	5106 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	16.9	Xtriage
Anisotropy	0.641	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	6791	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, CTW, NAG, CL, CA, BMA, FUC, MAN

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	0.91	3/6239 (0.0%)	0.81	3/8442 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437[A]	GLU	CD-OE2	-5.36	1.19	1.25
1	A	437[B]	GLU	CD-OE2	-5.36	1.19	1.25
1	A	687	TYR	CD2-CE2	5.00	1.46	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	465	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	370	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	534	ARG	NE-CZ-NH1	-5.74	117.43	120.30

There are no chirality outliers.

There are no planarity outliers.

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	5923	0	5761	67	2
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	28	0	25	2	0
6	A	76	0	68	1	0
7	A	28	0	26	1	0
8	A	39	0	34	2	0
9	A	61	0	52	0	0
10	A	40	0	24	3	0
11	A	592	0	0	20	3
All	All	6791	0	5990	73	3

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 (73) 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)
10:A:823:CTW:FAM	10:A:823:CTW:CBI	1.61	1.37
1:A:660[A]:VAL:O	1:A:664[A]:MET:HG2	1.26	1.30
1:A:536[B]:ARG:NH1	1:A:536[B]:ARG:HG2	1.59	1.11
1:A:536[B]:ARG:HH11	1:A:536[B]:ARG:HG2	1.05	1.08
1:A:658[A]:PRO:HB3	11:A:1243:HOH:O	1.52	1.07
1:A:536[B]:ARG:HH11	1:A:536[B]:ARG:CG	1.76	0.95
1:A:437[A]:GLU:OE1	11:A:1441:HOH:O	1.84	0.94
1:A:412:PRO:HA	1:A:589[B]:ASN:HD21	1.29	0.92
1:A:597[B]:CYS:SG	1:A:671:LEU:HD22	2.12	0.90
1:A:370:ARG:HD2	1:A:669[B]:MET:HE1	1.60	0.83
1:A:597[B]:CYS:SG	1:A:671:LEU:CD2	2.67	0.82
1:A:612:TYR:CZ	1:A:616[A]:MET:HG3	2.18	0.78
1:A:131[A]:ILE:HD11	1:A:171:GLU:HG3	1.66	0.78
1:A:131[A]:ILE:HG22	1:A:137:GLU:HG2	1.71	0.72
1:A:400:ARG:O	1:A:404[B]:THR:HG23	1.91	0.71
1:A:660[A]:VAL:O	1:A:664[A]:MET:CG	2.22	0.70
1:A:276[B]:GLU:HG2	1:A:277:TYR:N	2.03	0.68
1:A:189[A]:GLU:OE2	11:A:1431:HOH:O	2.11	0.66
1:A:610:LYS:HE2	11:A:1078:HOH:O	1.96	0.66
1:A:610:LYS:CE	11:A:1078:HOH:O	2.45	0.64
1:A:645[A]:LYS:HD2	11:A:1411:HOH:O	1.99	0.62
5:A:806:NAG:H81	11:A:1145:HOH:O	1.97	0.62
1:A:131[A]:ILE:HD11	1:A:171:GLU:CG	2.29	0.62
1:A:539:LYS:HD2	1:A:544:ASN:HD22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLY:O	1:A:223:LYS:HE2	2.01	0.61
1:A:412:PRO:HA	1:A:589[B]:ASN:ND2	2.10	0.61
1:A:616[B]:MET:O	1:A:616[B]:MET:HG2	2.01	0.58
1:A:370:ARG:CD	1:A:669[B]:MET:HE1	2.31	0.57
1:A:276[B]:GLU:HB3	11:A:1067:HOH:O	2.05	0.57
1:A:308:LYS:HB2	11:A:1466:HOH:O	2.05	0.56
1:A:505[A]:GLU:HG3	1:A:506:PHE:CE1	2.39	0.56
1:A:536[B]:ARG:NH1	11:A:1472:HOH:O	2.39	0.55
1:A:367:GLU:OE1	1:A:662[A]:ARG:NH1	2.37	0.55
1:A:641:GLU:HG3	11:A:1270:HOH:O	2.06	0.54
1:A:669[B]:MET:HE3	11:A:981:HOH:O	2.08	0.53
1:A:463:ARG:CZ	1:A:536[B]:ARG:HH21	2.22	0.53
1:A:362:LEU:CD1	1:A:406:LYS:HD2	2.39	0.53
8:A:816:NAG:H83	11:A:1110:HOH:O	2.09	0.51
1:A:177:VAL:HG12	1:A:188:LEU:HD11	1.93	0.51
1:A:506:PHE:HB2	1:A:509:MET:HG3	1.93	0.50
1:A:597[B]:CYS:SG	1:A:671:LEU:HD23	2.51	0.49
1:A:463:ARG:CZ	1:A:536[B]:ARG:NH2	2.77	0.48
1:A:169:MET:HA	1:A:344:MET:O	2.15	0.47
1:A:174[A]:LEU:HG	1:A:202:ILE:HG22	1.97	0.47
1:A:659[B]:ILE:O	1:A:663[B]:MET:HG3	2.15	0.46
1:A:469:LEU:O	1:A:595:PHE:HA	2.16	0.46
1:A:669[B]:MET:HE2	1:A:669[B]:MET:HB2	1.61	0.45
1:A:131[A]:ILE:HD13	1:A:343:LYS:HB2	1.98	0.45
1:A:544:ASN:OD1	11:A:1490:HOH:O	2.20	0.45
1:A:517:SER:HB2	1:A:694:PRO:HG3	1.98	0.45
10:A:823:CTW:CBH	10:A:823:CTW:H19	2.47	0.44
1:A:79[B]:GLN:CD	5:A:805:NAG:H81	2.38	0.44
1:A:551:LEU:HD22	1:A:556:TYR:HB2	1.99	0.43
1:A:597[B]:CYS:HG	1:A:671:LEU:HD22	1.77	0.43
8:A:816:NAG:C8	11:A:1110:HOH:O	2.64	0.43
1:A:218[A]:GLN:NE2	11:A:1306:HOH:O	2.50	0.43
1:A:236:ALA:O	1:A:239[A]:VAL:HG13	2.19	0.43
1:A:719[B]:VAL:HG22	11:A:1424:HOH:O	2.19	0.42
1:A:539:LYS:HZ1	1:A:547:SER:N	2.17	0.42
1:A:447:VAL:HG22	1:A:669[B]:MET:HE2	2.02	0.42
1:A:246:TRP:CD1	7:A:814:NAG:H83	2.55	0.41
1:A:303:GLN:HE21	1:A:303:GLN:HB2	1.69	0.41
1:A:719[A]:VAL:O	1:A:719[A]:VAL:HG12	2.20	0.41
1:A:66[B]:LYS:HB3	1:A:68[B]:GLU:HG2	2.03	0.41
1:A:468:PRO:HG3	1:A:603:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:807:NAG:H83	11:A:1109:HOH:O	2.18	0.41
1:A:651[B]:GLN:NE2	1:A:652:ASP:OD2	2.54	0.41
1:A:258:ILE:HD13	1:A:294:VAL:HB	2.02	0.41
1:A:541:TRP:NE1	10:A:823:CTW:H26	2.36	0.40
1:A:610:LYS:HD3	11:A:1078:HOH:O	2.22	0.40
1:A:79[B]:GLN:NE2	11:A:1357:HOH:O	2.29	0.40
1:A:131[A]:ILE:HG21	1:A:131[A]:ILE:HD13	1.82	0.40

All (3) 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)
11:A:1115:HOH:O	11:A:1426:HOH:O[2_565]	1.77	0.43
1:A:656[B]:SER:O	11:A:1243:HOH:O[4_566]	1.88	0.32
1:A:656[B]:SER:OG	11:A:1243:HOH:O[4_566]	2.18	0.02

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	758/709 (107%)	739 (98%)	18 (2%)	1 (0%)	56 37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	382	VAL

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	662/605 (109%)	646 (98%)	16 (2%)	57 38

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LYS
1	A	193	LYS
1	A	239[A]	VAL
1	A	239[B]	VAL
1	A	388	PRO
1	A	456	ILE
1	A	505[A]	GLU
1	A	505[B]	GLU
1	A	519	ASN
1	A	536[A]	ARG
1	A	536[B]	ARG
1	A	537	TYR
1	A	540	ASN
1	A	541	TRP
1	A	600	TYR
1	A	673	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	136	ASN
1	A	303	GLN
1	A	347	HIS
1	A	540	ASN
1	A	544	ASN

5.3.3 RNA

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)

16 carbohydrates 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	$\#\|Z\|>2$
5	NAG	A	805	1,5	14,14,15	0.52	0	15,19,21	1.04	1 (6%)
5	NAG	A	806	5	14,14,15	0.63	0	15,19,21	1.14	1 (6%)
6	NAG	A	807	1,6	14,14,15	0.73	0	15,19,21	0.97	0
6	NAG	A	808	6	14,14,15	0.39	0	15,19,21	1.24	2 (13%)
6	FUC	A	809	6	10,10,11	0.72	0	13,14,16	1.14	0
6	NAG	A	810	1,6	14,14,15	0.51	0	15,19,21	0.98	0
6	NAG	A	811	6	14,14,15	0.52	0	15,19,21	1.08	2 (13%)
6	FUC	A	812	6	10,10,11	0.79	0	13,14,16	1.04	1 (7%)
8	NAG	A	815	1,8	14,14,15	0.89	1 (7%)	15,19,21	0.88	0
8	NAG	A	816	8	14,14,15	0.61	0	15,19,21	1.16	2 (13%)
8	BMA	A	817	8	11,11,12	0.86	0	15,15,17	1.39	3 (20%)
9	NAG	A	818	9,1	14,14,15	0.77	0	15,19,21	1.26	2 (13%)
9	NAG	A	819	9	14,14,15	0.73	1 (7%)	15,19,21	1.67	5 (33%)
9	BMA	A	820	9	11,11,12	0.60	0	15,15,17	1.00	0
9	MAN	A	821	9	11,11,12	0.70	0	15,15,17	1.21	2 (13%)
9	MAN	A	822	9	11,11,12	0.58	0	15,15,17	1.05	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
5	NAG	A	805	1,5	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	806	5	-	0/6/23/26	0/1/1/1
6	NAG	A	807	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	808	6	-	0/6/23/26	0/1/1/1
6	FUC	A	809	6	-	0/0/17/20	0/1/1/1
6	NAG	A	810	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	811	6	-	0/6/23/26	0/1/1/1
6	FUC	A	812	6	-	0/0/17/20	0/1/1/1
8	NAG	A	815	1,8	-	0/6/23/26	0/1/1/1
8	NAG	A	816	8	-	0/6/23/26	0/1/1/1
8	BMA	A	817	8	-	0/2/19/22	0/1/1/1
9	NAG	A	818	9,1	-	0/6/23/26	0/1/1/1
9	NAG	A	819	9	-	0/6/23/26	0/1/1/1
9	BMA	A	820	9	-	0/2/19/22	0/1/1/1
9	MAN	A	821	9	-	0/2/19/22	0/1/1/1
9	MAN	A	822	9	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	819	NAG	O5-C1	-2.03	1.40	1.43
8	A	815	NAG	O7-C7	2.11	1.28	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	819	NAG	C3-C4-C5	-2.83	105.18	110.23
9	A	819	NAG	C2-N2-C7	-2.32	120.09	123.11
5	A	805	NAG	O4-C4-C3	-2.26	105.26	110.36
6	A	811	NAG	C3-C4-C5	-2.26	106.20	110.23
9	A	818	NAG	O4-C4-C5	-2.16	103.53	109.23
6	A	812	FUC	O5-C1-C2	-2.15	107.46	110.89
8	A	816	NAG	O7-C7-C8	-2.14	118.13	122.07
9	A	819	NAG	O4-C4-C5	-2.09	103.72	109.23
9	A	819	NAG	C4-C3-C2	-2.03	108.19	111.34
6	A	808	NAG	C3-C4-C5	-2.01	106.64	110.23
8	A	817	BMA	C1-O5-C5	2.08	115.19	112.14
6	A	811	NAG	O4-C4-C5	2.28	115.23	109.23
8	A	817	BMA	O5-C5-C4	2.37	114.06	110.13
5	A	806	NAG	C2-N2-C7	2.37	126.19	123.11
9	A	821	MAN	O3-C3-C2	2.54	114.65	110.01
9	A	819	NAG	C8-C7-N2	2.78	121.42	116.10
9	A	821	MAN	O5-C5-C6	2.84	113.42	107.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	816	NAG	C8-C7-N2	3.06	121.96	116.10
8	A	817	BMA	C3-C4-C5	3.21	115.95	110.23
6	A	808	NAG	C1-O5-C5	3.26	116.93	112.14
9	A	818	NAG	C1-O5-C5	3.57	117.39	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	NAG	1	0
5	A	806	NAG	1	0
6	A	807	NAG	1	0
8	A	816	NAG	2	0

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
7	NAG	A	813	1	14,14,15	0.61	0	15,19,21	2.50	2 (13%)
7	NAG	A	814	1	14,14,15	0.83	0	15,19,21	1.26	2 (13%)
10	CTW	A	823	2	27,40,40	3.96	9 (33%)	33,54,54	1.60	7 (21%)

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
7	NAG	A	813	1	-	0/6/23/26	0/1/1/1
7	NAG	A	814	1	-	0/6/23/26	0/1/1/1
10	CTW	A	823	2	-	0/32/47/47	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	823	CTW	PBN-OAG	-3.40	1.47	1.56
10	A	823	CTW	CBJ-CBH	-3.40	1.43	1.50
10	A	823	CTW	CB-CA	-2.53	1.49	1.53
10	A	823	CTW	CBL-NAZ	2.05	1.49	1.46
10	A	823	CTW	CAO-CBI	2.40	1.41	1.37
10	A	823	CTW	CAW-CBM	2.99	1.57	1.53
10	A	823	CTW	PBN-NBA	7.04	1.68	1.61
10	A	823	CTW	FAM-CBI	10.58	1.61	1.36
10	A	823	CTW	PBN-OAL	13.78	1.61	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	A	823	CTW	OAL-PBN-NBA	-4.14	105.95	112.84
10	A	823	CTW	C-CA-N	-3.65	105.65	112.93
10	A	823	CTW	CAR-CB-CA	-3.23	104.04	113.90
7	A	813	NAG	C4-C3-C2	-2.94	106.78	111.34
10	A	823	CTW	CAO-CBI-CAN	-2.64	119.03	122.87
7	A	814	NAG	O7-C7-C8	-2.55	117.37	122.07
10	A	823	CTW	CB-CAR-CAS	-2.01	107.28	113.39
10	A	823	CTW	FAM-CBI-CAO	2.01	121.73	118.53
10	A	823	CTW	CAQ-CAO-CBI	2.14	120.62	118.34
7	A	814	NAG	C1-O5-C5	2.32	115.56	112.14
7	A	813	NAG	C1-O5-C5	8.36	124.44	112.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	814	NAG	1	0
10	A	823	CTW	3	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^{th} 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	692/709 (97%)	-0.27	22 (3%) 51 49	9, 19, 37, 64	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	TRP	8.4
1	A	543	THR	4.4
1	A	542	GLU	4.3
1	A	544	ASN	4.2
1	A	719[A]	VAL	3.9
1	A	55	LYS	3.8
1	A	507	SER	3.3
1	A	134	ASP	3.2
1	A	56	HIS	2.9
1	A	487	GLY	2.8
1	A	656[A]	SER	2.7
1	A	133	GLU	2.6
1	A	336	ASN	2.5
1	A	506	PHE	2.5
1	A	130	ILE	2.4
1	A	153	ASN	2.4
1	A	335	GLY	2.3
1	A	155[A]	SER	2.3
1	A	651[A]	GLN	2.2
1	A	547	SER	2.2
1	A	652	ASP	2.1
1	A	408	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
5	NAG	A	806	14/15	0.75	0.31	9.88	35,42,49,50	0
8	NAG	A	815	14/15	0.94	0.11	5.49	23,26,31,32	0
6	NAG	A	807	14/15	0.77	0.23	2.69	38,45,56,58	0
5	NAG	A	805	14/15	0.95	0.10	1.96	27,33,38,40	0
9	NAG	A	818	14/15	0.93	0.10	0.80	16,22,28,36	0
9	MAN	A	821	11/12	0.95	0.14	0.58	36,38,40,41	0
6	NAG	A	810	14/15	0.94	0.13	-	36,39,44,45	0
6	FUC	A	809	10/11	0.83	0.34	-	62,63,64,64	0
8	NAG	A	816	14/15	0.89	0.20	-	38,43,49,56	0
9	BMA	A	820	11/12	0.92	0.11	-	33,35,43,47	0
6	FUC	A	812	10/11	0.83	0.28	-	51,54,56,56	0
9	MAN	A	822	11/12	0.79	0.30	-	54,59,61,67	0
6	NAG	A	811	14/15	0.67	0.32	-	47,56,63,63	0
6	NAG	A	808	14/15	0.78	0.39	-	60,64,66,66	0
9	NAG	A	819	14/15	0.89	0.22	-	31,34,45,45	0
8	BMA	A	817	11/12	0.64	0.36	-	63,69,71,72	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
10	CTW	A	823	40/40	0.95	0.12	0.91	11,32,52,53	0
3	CA	A	803	1/1	1.00	0.06	-0.31	11,11,11,11	0
4	CL	A	804	1/1	1.00	0.04	-1.10	18,18,18,18	0
2	ZN	A	802	1/1	1.00	0.03	-2.40	13,13,13,13	0
2	ZN	A	801	1/1	1.00	0.03	-5.53	12,12,12,12	0
7	NAG	A	813	14/15	0.71	0.24	-	61,68,70,71	0
7	NAG	A	814	14/15	0.90	0.11	-	24,38,42,43	0

6.5 Other polymers (i)

There are no such residues in this entry.