



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 12:38 AM EDT

PDB ID : 1TOQ
Title : CRYSTAL STRUCTURE OF A GALACTOSE SPECIFIC LECTIN FROM ARTOCARPUS HIRSUTA IN COMPLEX WITH METHYL-a-D-GALACTOSE
Authors : Rao, K.N.; Suresh, C.G.; Katre, U.V.; Gaikwad, S.M.; Khan, M.I.
Deposited on : 2004-06-15
Resolution : 2.50 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

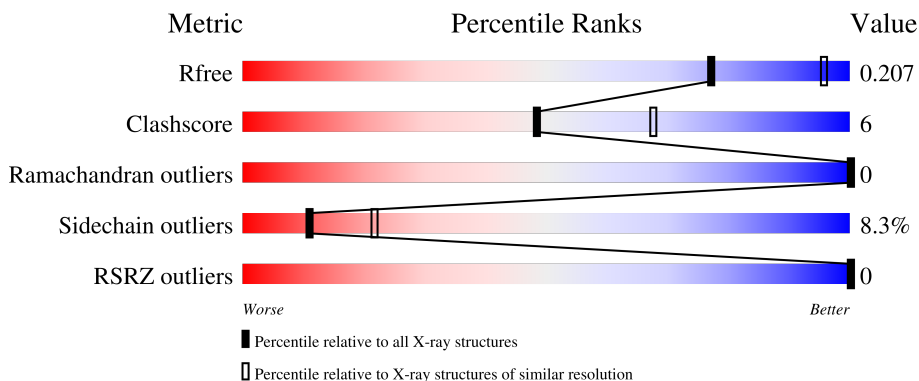
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	133	 81% 17% .
1	C	133	 76% 23% .
1	E	133	 79% 18% .
1	G	133	 77% 23% .
2	B	20	 75% 25%

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Mol	Chain	Length	Quality of chain
2	D	20	 55% 20% 25%
2	F	20	 65% 5% 5% 25%
2	H	20	 75% 25%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4726 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.

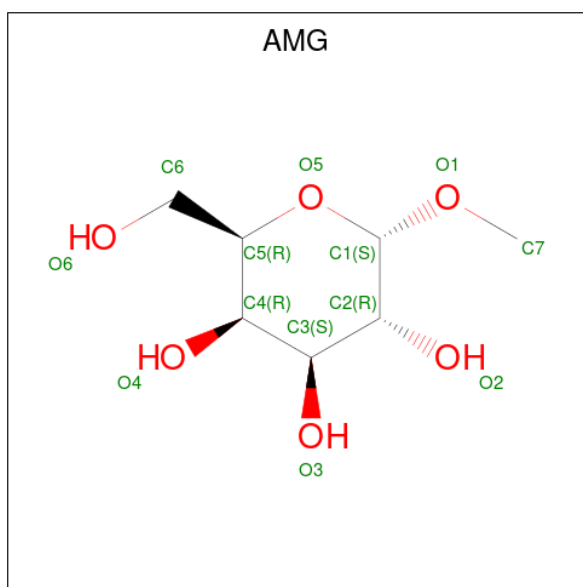
- Molecule 1 is a protein called AGGLUTININ ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	133	1035	673	159	201	2	4	0	0
1	C	133	1035	673	159	201	2	4	0	0
1	E	133	1035	673	159	201	2	4	0	0
1	G	133	1035	673	159	201	2	8	0	0

- Molecule 2 is a protein called AGGLUTININ BETA CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	15	106	68	19	19	4	0	0
2	D	15	106	68	19	19	4	0	0
2	F	15	106	68	19	19	4	0	0
2	H	15	106	68	19	19	4	0	0

- Molecule 3 is methyl alpha-D-galactopyranoside (three-letter code: AMG) (formula: C₇H₁₄O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 7 6	0	0
3	C	1	Total C O 13 7 6	0	0
3	E	1	Total C O 13 7 6	0	0
3	G	1	Total C O 13 7 6	0	0


- Molecule 4 is water.

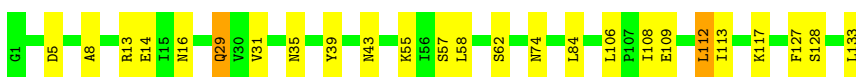
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	25	Total O 25 25	0	0
4	B	3	Total O 3 3	0	0
4	C	20	Total O 20 20	0	0
4	D	5	Total O 5 5	0	0
4	E	26	Total O 26 26	0	0
4	F	3	Total O 3 3	0	0
4	G	25	Total O 25 25	0	0
4	H	3	Total O 3 3	0	0

3 Residue-property plots


These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: AGGLUTININ ALPHA CHAIN

Chain A: 




- Molecule 1: AGGLUTININ ALPHA CHAIN

Chain C: 




- Molecule 1: AGGLUTININ ALPHA CHAIN

Chain E: 



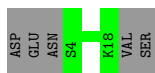
- Molecule 1: AGGLUTININ ALPHA CHAIN

Chain G: 



- Molecule 2: AGGLUTININ BETA CHAIN

Chain B: 

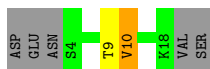


- Molecule 2: AGGLUTININ BETA CHAIN

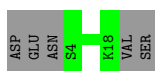
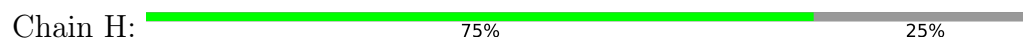
Chain D: 



- Molecule 2: AGGLUTININ BETA CHAIN



- Molecule 2: AGGLUTININ BETA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.37Å 98.66Å 164.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.50 41.22 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.50) 88.8 (41.22-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.51Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.235 0.174 , 0.207	Depositor DCC
R_{free} test set	2358 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.7	Xtrriage
Anisotropy	0.437	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: AMG

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	0.56	0/1064	1.34	7/1443 (0.5%)
1	C	0.73	1/1064 (0.1%)	1.40	7/1443 (0.5%)
1	E	0.61	1/1064 (0.1%)	1.28	6/1443 (0.4%)
1	G	0.56	0/1064	1.25	2/1443 (0.1%)
2	B	0.58	0/108	1.30	0/145
2	D	0.72	0/108	1.28	0/145
2	F	0.65	0/108	1.31	0/145
2	H	0.71	0/108	1.17	0/145
All	All	0.62	2/4688 (0.0%)	1.32	22/6352 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	LYS	CB-CG	-15.54	1.10	1.52
1	E	21	LYS	CB-CG	-9.79	1.26	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	LYS	CA-CB-CG	13.45	142.98	113.40
1	C	13	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	A	112	LEU	CA-CB-CG	8.54	134.94	115.30
1	A	5	ASP	CB-CG-OD1	8.14	125.63	118.30
1	E	112	LEU	CA-CB-CG	8.01	133.71	115.30
1	A	109	GLU	OE1-CD-OE2	7.88	132.75	123.30
1	E	17	LEU	CA-CB-CG	7.12	131.68	115.30
1	E	21	LYS	CA-CB-CG	7.05	128.90	113.40
1	G	5	ASP	CB-CG-OD1	6.83	124.44	118.30
1	A	39	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	C	126	TYR	CB-CG-CD1	6.28	124.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	5	ASP	CB-CG-OD1	6.14	123.83	118.30
1	C	21	LYS	CB-CG-CD	6.13	127.53	111.60
1	A	5	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	C	13	ARG	CD-NE-CZ	5.87	131.82	123.60
1	E	18	SER	CB-CA-C	-5.62	99.41	110.10
1	A	13	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	112	LEU	CA-CB-CG	5.43	127.78	115.30
1	A	13	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	109	GLU	OE1-CD-OE2	5.14	129.47	123.30
1	C	59	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	E	5	ASP	CB-CG-OD1	5.09	122.88	118.30

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	1035	0	995	11	0
1	C	1035	0	995	19	0
1	E	1035	0	995	13	0
1	G	1035	0	995	15	0
2	B	106	0	110	0	0
2	D	106	0	110	1	0
2	F	106	0	110	1	0
2	H	106	0	110	0	0
3	A	13	0	14	0	0
3	C	13	0	14	0	0
3	E	13	0	14	0	0
3	G	13	0	14	0	0
4	A	25	0	0	1	0
4	B	3	0	0	0	0
4	C	20	0	0	1	0
4	D	5	0	0	0	0
4	E	26	0	0	0	0
4	F	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	25	0	0	0	0
4	H	3	0	0	0	0
All	All	4726	0	4476	54	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (54) 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:29:GLN:HG3	1:A:43:ASN:HA	1.49	0.92
1:C:68:VAL:HG21	1:C:129:MET:CE	2.12	0.80
1:C:108:ILE:HD11	1:C:113:ILE:HD11	1.66	0.78
1:C:29:GLN:HG3	1:C:43:ASN:HA	1.73	0.70
1:C:68:VAL:HG21	1:C:129:MET:HE1	1.74	0.68
1:E:18:SER:HB2	1:E:27:ASP:H	1.58	0.68
1:C:18:SER:HB3	1:C:51:PHE:HB3	1.79	0.65
1:G:80:VAL:HG11	1:G:123:TRP:HB2	1.81	0.62
1:G:18:SER:HB3	1:G:51:PHE:HB3	1.81	0.61
1:G:29:GLN:HG3	1:G:43:ASN:HA	1.84	0.60
1:G:18:SER:HB2	1:G:27:ASP:H	1.68	0.59
1:A:35:ASN:ND2	4:A:509:HOH:O	2.35	0.58
1:A:16:ASN:HD21	1:A:55:LYS:HG3	1.69	0.57
1:C:68:VAL:HG21	1:C:129:MET:HE3	1.87	0.57
1:C:8:ALA:H	1:G:35:ASN:HD21	1.51	0.56
1:G:83:SER:HB2	1:G:96:TYR:O	2.05	0.56
1:A:35:ASN:HD21	1:E:8:ALA:H	1.55	0.55
1:C:20:ASN:HB3	1:C:23:THR:OG1	2.07	0.55
1:G:18:SER:HB3	1:G:51:PHE:CB	2.37	0.54
1:E:29:GLN:HG3	1:E:43:ASN:HA	1.89	0.54
1:G:113:ILE:HD13	1:G:131:LEU:CD2	2.38	0.54
1:G:63:GLU:HB2	1:G:90:LYS:HE3	1.92	0.52
1:G:108:ILE:HD11	1:G:113:ILE:HD11	1.91	0.51
1:G:20:ASN:HB3	1:G:23:THR:OG1	2.10	0.50
1:A:29:GLN:HG3	1:A:43:ASN:CA	2.32	0.49
1:E:18:SER:HB3	1:E:51:PHE:CB	2.43	0.49
1:G:113:ILE:HD13	1:G:131:LEU:HD23	1.95	0.48
1:C:113:ILE:HG21	1:C:129:MET:HE2	1.95	0.47
1:C:8:ALA:H	1:G:35:ASN:ND2	2.12	0.47
1:C:35:ASN:ND2	4:C:508:HOH:O	2.45	0.47
1:E:18:SER:HB2	1:E:27:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ILE:HD11	1:A:113:ILE:HD11	1.97	0.46
1:E:42:GLN:HG2	1:E:44:HIS:CE1	2.51	0.46
1:E:54:VAL:HG11	1:E:96:TYR:CE1	2.51	0.46
1:E:20:ASN:HB3	1:E:23:THR:OG1	2.16	0.46
1:A:16:ASN:ND2	1:A:55:LYS:HG3	2.32	0.45
1:C:113:ILE:HD12	1:C:129:MET:CE	2.47	0.45
2:F:9:THR:HG22	2:F:10:VAL:O	2.17	0.45
1:A:35:ASN:ND2	1:E:8:ALA:H	2.15	0.45
1:C:91:LYS:HE2	1:C:93:TYR:CE2	2.52	0.44
1:C:14:GLU:HB3	1:C:31:VAL:HB	1.99	0.44
1:E:32:TYR:CE1	1:E:115:GLY:HA2	2.53	0.43
1:C:56:ILE:HG22	1:C:58:LEU:HD13	2.01	0.43
1:E:18:SER:HB3	1:E:51:PHE:HB3	2.00	0.43
1:A:8:ALA:H	1:E:35:ASN:HD21	1.67	0.42
1:C:35:ASN:HD21	1:G:8:ALA:H	1.67	0.42
1:E:83:SER:HB2	1:E:98:VAL:O	2.20	0.41
2:D:9:THR:HG22	2:D:10:VAL:O	2.20	0.41
1:G:60:PHE:HA	1:G:61:PRO:HA	1.82	0.41
1:A:14:GLU:HB3	1:A:31:VAL:HB	2.02	0.41
1:C:108:ILE:HD11	1:C:113:ILE:CD1	2.44	0.41
1:A:117:LYS:HG3	1:A:128:SER:HB2	2.02	0.41
1:C:17:LEU:HD12	1:C:17:LEU:C	2.41	0.41
1:C:113:ILE:HD13	1:C:131:LEU:CD1	2.51	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	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
1	C	131/133 (98%)	126 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	131/133 (98%)	127 (97%)	4 (3%)	0	100	100
1	G	131/133 (98%)	126 (96%)	5 (4%)	0	100	100
2	B	13/20 (65%)	13 (100%)	0	0	100	100
2	D	13/20 (65%)	13 (100%)	0	0	100	100
2	F	13/20 (65%)	13 (100%)	0	0	100	100
2	H	13/20 (65%)	13 (100%)	0	0	100	100
All	All	576/612 (94%)	557 (97%)	19 (3%)	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	113/113 (100%)	103 (91%)	10 (9%)	10	19
1	C	113/113 (100%)	104 (92%)	9 (8%)	12	23
1	E	113/113 (100%)	104 (92%)	9 (8%)	12	23
1	G	113/113 (100%)	103 (91%)	10 (9%)	10	19
2	B	11/16 (69%)	11 (100%)	0	100	100
2	D	11/16 (69%)	9 (82%)	2 (18%)	1	3
2	F	11/16 (69%)	10 (91%)	1 (9%)	9	18
2	H	11/16 (69%)	11 (100%)	0	100	100
All	All	496/516 (96%)	455 (92%)	41 (8%)	11	22

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	57	SER
1	A	58	LEU
1	A	62	SER

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Mol	Chain	Res	Type
1	A	74	ASN
1	A	84	LEU
1	A	106	LEU
1	A	112	LEU
1	A	127	PHE
1	A	133	LEU
1	C	21	LYS
1	C	34	LEU
1	C	57	SER
1	C	58	LEU
1	C	84	LEU
1	C	90	LYS
1	C	112	LEU
1	C	127	PHE
1	C	133	LEU
2	D	6	LYS
2	D	7	SER
1	E	17	LEU
1	E	42	GLN
1	E	58	LEU
1	E	84	LEU
1	E	91	LYS
1	E	102	THR
1	E	112	LEU
1	E	131	LEU
1	E	132	SER
2	F	10	VAL
1	G	22	GLU
1	G	57	SER
1	G	58	LEU
1	G	62	SER
1	G	84	LEU
1	G	100	SER
1	G	102	THR
1	G	106	LEU
1	G	112	LEU
1	G	132	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN

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Mol	Chain	Res	Type
1	A	35	ASN
1	C	35	ASN
1	E	35	ASN
1	E	42	GLN
1	G	35	ASN
2	H	8	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	AMG	C	502	-	13,13,13	0.49	0	18,18,18	1.25	3 (16%)
3	AMG	G	504	-	13,13,13	0.44	0	18,18,18	1.26	2 (11%)
3	AMG	A	501	-	13,13,13	0.55	0	18,18,18	1.07	2 (11%)
3	AMG	E	503	-	13,13,13	0.53	0	18,18,18	1.25	2 (11%)

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
3	AMG	C	502	-	-	4/4/24/24	0/1/1/1
3	AMG	G	504	-	-	1/4/24/24	0/1/1/1
3	AMG	A	501	-	-	0/4/24/24	0/1/1/1
3	AMG	E	503	-	-	2/4/24/24	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	AMG	O1-C1-C2	-3.49	104.06	108.15
3	E	503	AMG	O6-C6-C5	2.69	120.50	111.29
3	G	504	AMG	C3-C4-C5	-2.40	105.96	110.24
3	G	504	AMG	O2-C2-C3	-2.30	105.03	110.35
3	A	501	AMG	O2-C2-C1	-2.18	104.76	110.05
3	E	503	AMG	O5-C5-C6	2.12	111.70	106.44
3	C	502	AMG	O4-C4-C3	-2.08	105.53	110.35
3	A	501	AMG	O2-C2-C3	-2.08	105.54	110.35
3	C	502	AMG	O2-C2-C1	-2.00	105.18	110.05

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	503	AMG	C4-C5-C6-O6
3	E	503	AMG	O5-C5-C6-O6
3	C	502	AMG	C4-C5-C6-O6
3	C	502	AMG	O5-C5-C6-O6
3	C	502	AMG	O5-C1-O1-C7
3	C	502	AMG	C2-C1-O1-C7
3	G	504	AMG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	133/133 (100%)	-0.61	0 100 100	34, 42, 52, 63	1 (0%)
1	C	133/133 (100%)	-0.60	0 100 100	32, 41, 50, 56	1 (0%)
1	E	133/133 (100%)	-0.50	0 100 100	36, 46, 58, 65	1 (0%)
1	G	133/133 (100%)	-0.51	0 100 100	34, 45, 57, 65	2 (1%)
2	B	15/20 (75%)	-0.39	0 100 100	32, 41, 53, 64	1 (6%)
2	D	15/20 (75%)	-0.21	0 100 100	33, 41, 59, 62	1 (6%)
2	F	15/20 (75%)	-0.41	0 100 100	35, 43, 59, 64	1 (6%)
2	H	15/20 (75%)	-0.48	0 100 100	34, 45, 56, 67	1 (6%)
All	All	592/612 (96%)	-0.54	0 100 100	32, 44, 56, 67	9 (1%)

There are no RSRZ outliers to report.

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 monosaccharides 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, 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	B-factors(\AA^2)	Q<0.9
3	AMG	C	502	13/13	0.97	0.14	48,50,52,52	0
3	AMG	A	501	13/13	0.98	0.10	41,43,44,46	0
3	AMG	E	503	13/13	0.98	0.13	40,41,42,43	0
3	AMG	G	504	13/13	0.98	0.12	38,41,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.