



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:29 am GMT

PDB ID : 2J6E
Title : CRYSTAL STRUCTURE OF AN AUTOIMMUNE COMPLEX BETWEEN
A HUMAN IGM RHEUMATOID FACTOR AND IGG1 FC REVEALS A
NOVEL FC EPITOPE AND EVIDENCE FOR AFFINITY MATURATION
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Casali, P.; Vaney, M.-C.; Rey, F.A.; Sutton, B.J.; Taussig, M.J.
Deposited on : 2006-09-28
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

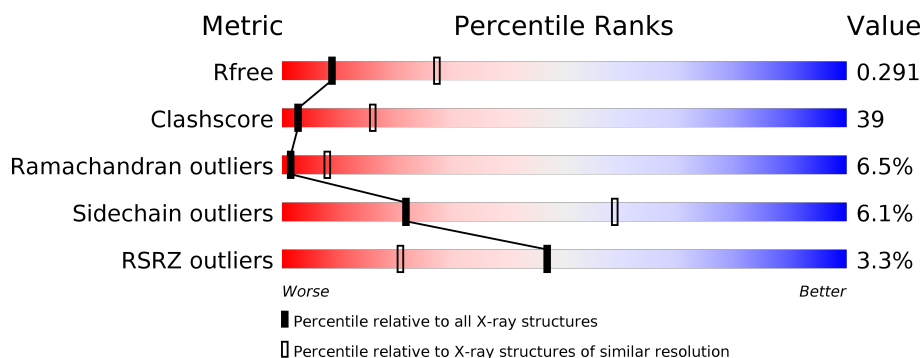
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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 $\leq 5\%$. 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	232	<div> <div>53%</div> <div>34%</div> <div>•</div> <div>9%</div> </div>
1	B	232	<div>2%</div> <div>48%</div> <div>38%</div> <div>5%</div> <div>10%</div>

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
7	MPD	A	1448	-	-	X	X
7	MPD	A	1449	-	-	-	X
7	MPD	A	1450	-	-	-	X
7	MPD	M	1212	-	-	-	X
8	ACT	A	1452	-	-	-	X
8	ACT	B	1449	-	-	-	X
9	GAL	A	1459	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 10195 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 IG GAMMA-1 CHAIN C REGION.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	210	Total	C	N	O	S	0	0	1
			1670	1062	282	320	6			
1	B	209	Total	C	N	O	S	0	0	1
			1667	1061	281	319	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	270	GLU	ASP	CONFLICT	UNP P01857
B	270	GLU	ASP	CONFLICT	UNP P01857

- Molecule 2 is a protein called IGM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1633	1029	275	323	6			
2	I	220	Total	C	N	O	S	0	0	0
			1660	1043	279	331	7			

- Molecule 3 is a protein called IGM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	1
			1587	993	270	320	4			
3	M	215	Total	C	N	O	S	0	0	0
			1602	1001	271	325	5			

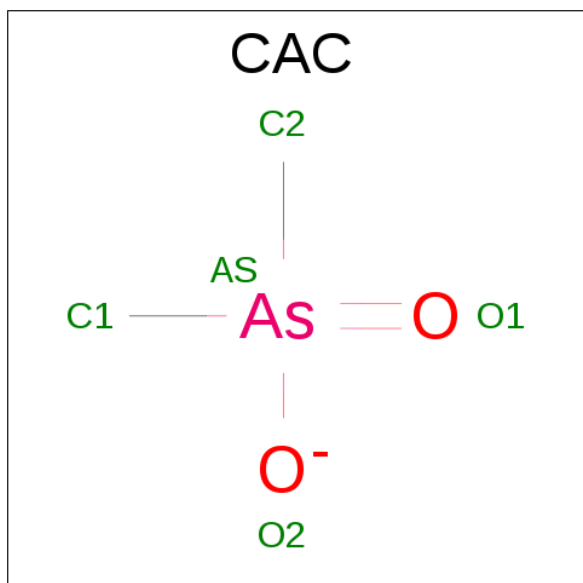
- Molecule 4 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is CACODYLATE ION (three-letter code: CAC) (formula: C₂H₆AsO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	As	C	O	0	0
			5	1	2	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		
7	M	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	H	1	Total	C	O	0	0
			4	2	2		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	A	9	Total	C	N	O	0	0
			110	62	4	44		

- Molecule 10 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	9	Total	C	N	O	0	0
			110	62	4	44		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	32	Total	O	0	0
			32	32		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	16	Total 16	O 16	0	0
11	H	9	Total 9	O 9	0	0
11	I	20	Total 20	O 20	0	0
11	L	4	Total 4	O 4	0	0
11	M	3	Total 3	O 3	0	0

3 Residue-property plots

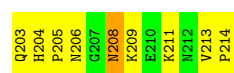
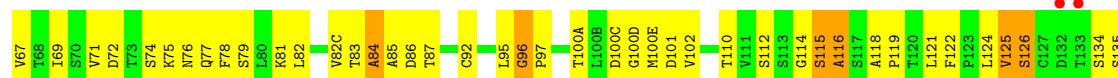
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: IG GAMMA-1 CHAIN C REGION

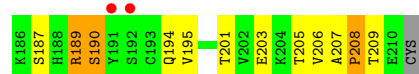
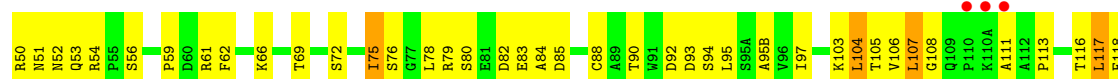




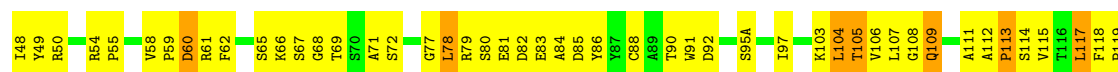
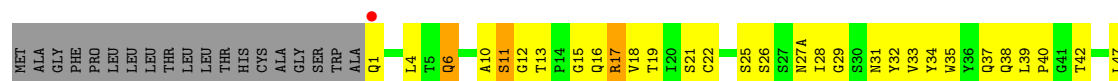
• Molecule 2: IGM

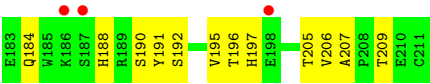


• Molecule 3: IGM



• Molecule 3: IGM





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	241.98Å 75.61Å 102.40Å 90.00° 91.13° 90.00°	Depositor
Resolution (Å)	25.00 – 3.00 24.72 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.00-3.00) 97.9 (24.72-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.99Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.288 0.225 , 0.291	Depositor DCC
R_{free} test set	2601 reflections (7.66%)	DCC
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10195	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: MPD, BMA, NAG, ZN, NDG, CD, GAL, ACT, CAC, FUL, 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	0.51	0/1716	0.68	0/2338
1	B	0.43	0/1713	0.65	1/2335 (0.0%)
2	H	0.34	0/1672	0.62	0/2275
2	I	0.38	0/1699	0.69	1/2312 (0.0%)
3	L	0.35	0/1626	0.60	0/2220
3	M	0.34	0/1641	0.62	0/2238
All	All	0.40	0/10067	0.65	2/13718 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	PRO	N-CA-CB	5.66	110.09	103.30
2	I	92	CYS	CA-CB-SG	5.06	123.11	114.00

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	1670	0	1635	84	0
1	B	1667	0	1631	93	0
2	H	1633	0	1596	179	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	1660	0	1617	129	0
3	L	1587	0	1548	147	0
3	M	1602	0	1559	155	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
7	A	24	0	42	17	0
7	B	16	0	28	0	0
7	M	8	0	14	2	0
8	A	8	0	6	0	0
8	B	4	0	3	0	0
8	H	4	0	3	0	0
9	A	110	0	94	14	0
10	B	110	0	94	15	0
11	A	32	0	0	0	0
11	B	16	0	0	1	0
11	H	9	0	0	0	0
11	I	20	0	0	1	0
11	L	4	0	0	0	0
11	M	3	0	0	0	0
All	All	10195	0	9870	772	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 39.

The worst 5 of 772 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)
3:L:16:GLN:HG2	3:L:17:ARG:H	1.18	1.09
1:A:346:PRO:HB3	1:A:372:PHE:HB3	1.35	1.06
3:M:79:ARG:HB3	3:M:79:ARG:NH1	1.82	0.95
3:L:80:SER:HA	3:L:106:VAL:HG11	1.48	0.94
2:I:96:GLY:HA3	2:I:100(A):THR:HG21	1.49	0.94

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	208/232 (90%)	194 (93%)	11 (5%)	3 (1%)	13	49
1	B	207/232 (89%)	173 (84%)	26 (13%)	8 (4%)	3	20
2	H	212/231 (92%)	152 (72%)	40 (19%)	20 (9%)	1	3
2	I	216/231 (94%)	171 (79%)	23 (11%)	22 (10%)	1	3
3	L	212/234 (91%)	152 (72%)	45 (21%)	15 (7%)	1	6
3	M	213/234 (91%)	153 (72%)	45 (21%)	15 (7%)	1	7
All	All	1268/1394 (91%)	995 (78%)	190 (15%)	83 (6%)	1	8

5 of 83 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	43	LYS
2	H	86	ASP
2	H	96	GLY
2	H	149	SER
2	H	156	TYR

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	194/215 (90%)	181 (93%)	13 (7%)	19	54
1	B	194/215 (90%)	185 (95%)	9 (5%)	31	70
2	H	185/198 (93%)	176 (95%)	9 (5%)	29	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	189/198 (96%)	177 (94%)	12 (6%)	21	57
3	L	177/193 (92%)	165 (93%)	12 (7%)	18	54
3	M	179/193 (93%)	166 (93%)	13 (7%)	16	50
All	All	1118/1212 (92%)	1050 (94%)	68 (6%)	22	59

5 of 68 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	208	ASN
2	I	150	ILE
3	M	117	LEU
2	I	1	GLN
2	I	59	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	208	ASN
2	I	56	ASN
3	M	169	ASN
2	H	212	ASN
2	I	77	GLN

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 ⓘ

18 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	$\# Z > 2$
9	NAG	A	1453	1,9	14,14,15	0.59	0	15,19,21	1.01	0
9	FUL	A	1454	9	9,10,11	0.48	0	13,14,16	0.95	0
9	NAG	A	1455	9	14,14,15	0.54	0	15,19,21	0.99	0
9	BMA	A	1456	9	11,11,12	0.68	0	13,15,17	0.80	0
9	MAN	A	1457	9	11,11,12	0.47	0	13,15,17	0.59	0
9	NDG	A	1458	9	14,14,15	0.66	0	15,19,21	1.13	1 (6%)
9	GAL	A	1459	9	11,11,12	0.43	0	13,15,17	0.55	0
9	BMA	A	1460	9	11,11,12	0.72	0	13,15,17	0.96	1 (7%)
9	NAG	A	1461	9	14,14,15	0.69	0	15,19,21	0.99	1 (6%)
10	NAG	B	1450	1,10	14,14,15	0.65	0	15,19,21	0.80	0
10	FUL	B	1451	10	9,10,11	0.44	0	13,14,16	0.62	0
10	NAG	B	1452	10	14,14,15	0.68	0	15,19,21	0.72	0
10	BMA	B	1453	10	11,11,12	0.58	0	13,15,17	0.48	0
10	MAN	B	1454	10	11,11,12	0.57	0	13,15,17	0.89	1 (7%)
10	NAG	B	1455	10	14,14,15	0.54	0	15,19,21	1.07	2 (13%)
10	GAL	B	1456	10	11,11,12	0.48	0	13,15,17	0.40	0
10	BMA	B	1457	10	11,11,12	0.74	0	13,15,17	0.80	0
10	NAG	B	1458	10	14,14,15	0.57	0	15,19,21	0.68	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
9	NAG	A	1453	1,9	-	0/6/23/26	0/1/1/1
9	FUL	A	1454	9	-	0/0/17/20	0/1/1/1
9	NAG	A	1455	9	-	0/6/23/26	0/1/1/1
9	BMA	A	1456	9	-	0/2/19/22	0/1/1/1
9	MAN	A	1457	9	-	0/2/19/22	1/1/1/1
9	NDG	A	1458	9	-	0/6/23/26	0/1/1/1
9	GAL	A	1459	9	-	0/2/19/22	0/1/1/1
9	BMA	A	1460	9	-	0/2/19/22	0/1/1/1
9	NAG	A	1461	9	-	0/6/23/26	0/1/1/1
10	NAG	B	1450	1,10	-	0/6/23/26	0/1/1/1
10	FUL	B	1451	10	-	0/0/17/20	0/1/1/1
10	NAG	B	1452	10	-	1/6/23/26	0/1/1/1
10	BMA	B	1453	10	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MAN	B	1454	10	-	0/2/19/22	1/1/1/1
10	NAG	B	1455	10	-	0/6/23/26	0/1/1/1
10	GAL	B	1456	10	-	0/2/19/22	0/1/1/1
10	BMA	B	1457	10	-	0/2/19/22	0/1/1/1
10	NAG	B	1458	10	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1458	NDG	C2-N2-C7	-2.82	118.83	122.94
10	B	1455	NAG	C4-C3-C2	-2.51	107.34	111.02
9	A	1461	NAG	C2-N2-C7	-2.34	119.52	122.94
10	B	1455	NAG	C2-N2-C7	-2.25	119.65	122.94
9	A	1460	BMA	C3-C4-C5	-2.22	106.31	110.22

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1452	NAG	O7-C7-N2-C2

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	B	1454	MAN	C1-C2-C3-C4-C5-O5
9	A	1457	MAN	C1-C2-C3-C4-C5-O5

15 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1453	NAG	2	0
9	A	1454	FUL	2	0
9	A	1455	NAG	4	0
9	A	1458	NDG	3	0
9	A	1459	GAL	5	0
9	A	1460	BMA	2	0
9	A	1461	NAG	2	0
10	B	1450	NAG	2	0
10	B	1451	FUL	1	0
10	B	1452	NAG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	1454	MAN	3	0
10	B	1455	NAG	4	0
10	B	1456	GAL	3	0
10	B	1457	BMA	2	0
10	B	1458	NAG	2	0

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 3 are monoatomic - leaving 11 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	$\# Z > 2$
6	CAC	A	1447	5	0,4,4	0.00	-	0,6,6	0.00	-
7	MPD	A	1448	-	7,7,7	0.52	0	9,10,10	0.47	0
7	MPD	A	1449	-	7,7,7	0.60	0	9,10,10	0.52	0
7	MPD	A	1450	-	7,7,7	0.70	0	9,10,10	0.60	0
8	ACT	A	1451	-	1,3,3	0.85	0	0,3,3	0.00	-
8	ACT	A	1452	-	1,3,3	1.25	0	0,3,3	0.00	-
7	MPD	B	1447	-	7,7,7	0.46	0	9,10,10	0.43	0
7	MPD	B	1448	-	7,7,7	0.53	0	9,10,10	0.44	0
8	ACT	B	1449	-	1,3,3	0.42	0	0,3,3	0.00	-
8	ACT	H	1215	-	1,3,3	1.33	0	0,3,3	0.00	-
7	MPD	M	1212	-	7,7,7	0.48	0	9,10,10	0.47	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
6	CAC	A	1447	5	-	0/0/0/0	0/0/0/0
7	MPD	A	1448	-	-	0/5/5/5	0/0/0/0
7	MPD	A	1449	-	-	0/5/5/5	0/0/0/0
7	MPD	A	1450	-	-	0/5/5/5	0/0/0/0
8	ACT	A	1451	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	ACT	A	1452	-	-	0/0/0/0	0/0/0/0
7	MPD	B	1447	-	-	0/5/5/5	0/0/0/0
7	MPD	B	1448	-	-	0/5/5/5	0/0/0/0
8	ACT	B	1449	-	-	0/0/0/0	0/0/0/0
8	ACT	H	1215	-	-	0/0/0/0	0/0/0/0
7	MPD	M	1212	-	-	0/5/5/5	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1448	MPD	13	0
7	A	1449	MPD	2	0
7	A	1450	MPD	4	0
7	M	1212	MPD	2	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	210/232 (90%)	-0.68	0 100 100	24, 39, 56, 68	0
1	B	209/232 (90%)	-0.28	4 (1%) 67 37	23, 56, 131, 140	0
2	H	216/231 (93%)	0.18	18 (8%) 12 4	32, 77, 151, 152	0
2	I	220/231 (95%)	-0.31	3 (1%) 75 49	24, 56, 133, 146	0
3	L	214/234 (91%)	0.20	14 (6%) 20 7	36, 89, 151, 152	0
3	M	215/234 (91%)	0.00	4 (1%) 67 37	45, 95, 138, 141	0
All	All	1284/1394 (92%)	-0.15	43 (3%) 47 21	23, 67, 148, 152	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	194	THR	4.9
1	B	324	SER	4.7
2	H	184	LEU	4.7
2	H	146	LEU	4.5
3	L	183	GLU	3.3

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](#)

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(\AA^2)	Q<0.9
9	GAL	A	1459	11/12	0.88	0.24	2.21	53,56,61,61	0
10	GAL	B	1456	11/12	0.85	0.23	0.57	108,108,109,110	0
10	NAG	B	1450	14/15	0.84	0.21	-0.57	118,122,123,123	0
9	NDG	A	1458	14/15	0.93	0.15	-1.85	50,51,57,59	0
9	NAG	A	1455	14/15	0.97	0.12	-	34,36,39,40	0
9	NAG	A	1461	14/15	0.85	0.23	-	88,91,92,92	0
9	BMA	A	1460	11/12	0.89	0.19	-	71,78,82,83	0
10	BMA	B	1457	11/12	0.82	0.27	-	112,117,118,119	0
9	FUL	A	1454	10/11	0.95	0.14	-	45,48,51,51	0
10	NAG	B	1458	14/15	0.80	0.25	-	119,121,122,122	0
9	MAN	A	1457	11/12	0.93	0.11	-	49,50,52,54	0
10	MAN	B	1454	11/12	0.84	0.32	-	108,109,110,110	0
9	BMA	A	1456	11/12	0.95	0.11	-	45,47,51,62	0
9	NAG	A	1453	14/15	0.96	0.15	-	32,34,40,45	0
10	BMA	B	1453	11/12	0.88	0.23	-	112,117,119,120	0
10	NAG	B	1452	14/15	0.83	0.19	-	120,122,126,126	0
10	NAG	B	1455	14/15	0.85	0.17	-	106,107,108,109	0
10	FUL	B	1451	10/11	0.80	0.25	-	119,119,120,120	0

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
7	MPD	A	1449	8/8	0.77	0.58	19.55	81,83,85,86	0
7	MPD	A	1448	8/8	0.73	0.48	12.66	92,95,96,98	0
7	MPD	A	1450	8/8	0.73	0.49	11.70	81,81,81,81	0
8	ACT	A	1452	4/4	0.86	0.32	5.43	85,85,85,85	0
7	MPD	M	1212	8/8	0.88	0.30	2.58	81,81,81,81	0
8	ACT	B	1449	4/4	0.94	0.22	2.15	81,81,81,81	0
8	ACT	A	1451	4/4	0.97	0.21	0.98	64,65,65,66	0
4	CD	A	1445	1/1	0.99	0.06	-4.04	57,57,57,57	0
8	ACT	H	1215	4/4	0.77	0.29	-	81,81,81,81	0
5	ZN	A	1446	1/1	0.98	0.04	-	43,43,43,43	0
6	CAC	A	1447	5/5	0.98	0.09	-	83,84,84,87	0
7	MPD	B	1448	8/8	0.77	0.52	-	82,83,84,84	0
7	MPD	B	1447	8/8	0.82	0.17	-	81,83,83,84	0
5	ZN	B	1446	1/1	0.78	0.15	-	143,143,143,143	0

6.5 Other polymers [i](#)

There are no such residues in this entry.