



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2020 – 04:29 AM EST

PDB ID : 7JTV
Title : Structure of IMPa from *Pseudomonas aeruginosa* in complex with an O-glycopeptide
Authors : Noach, I.; Boraston, A.B.
Deposited on : 2020-08-18
Resolution : 2.45 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 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 : 2.15.1
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) : 2.15.1

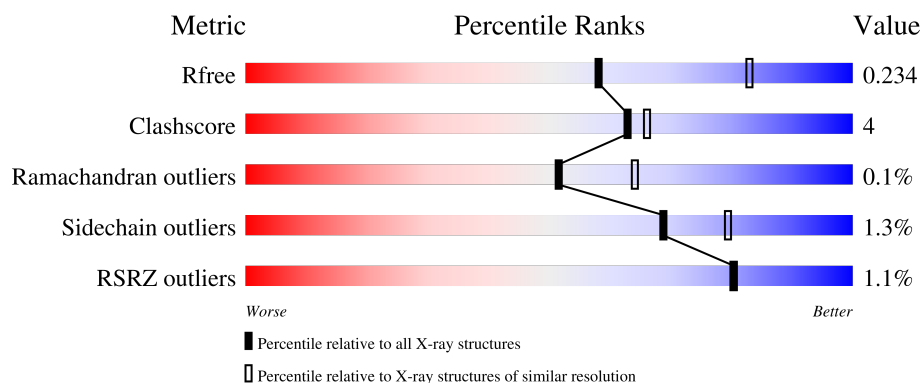
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	885	<div> <div>89%</div> <div>11%</div> </div>
1	B	885	<div> <div>89%</div> <div>10%</div> </div>
2	E	15	<div> <div>13%</div> <div>27%</div> <div>7%</div> <div>67%</div> </div>
2	H	15	<div> <div>13%</div> <div>20%</div> <div>7%</div> <div>73%</div> </div>
3	D	2	<div> <div>100%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	2	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14379 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 Immunomodulating metalloprotease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	883	Total	C	N	O	S	0	0	0
			6777	4242	1214	1307	14			
1	A	884	Total	C	N	O	S	0	1	0
			6790	4250	1215	1311	14			

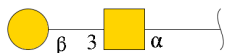
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	MET	-	initiating methionine	UNP Q9I5W4
B	697	GLN	GLU	engineered mutation	UNP Q9I5W4
B	924	LEU	-	expression tag	UNP Q9I5W4
B	925	GLU	-	expression tag	UNP Q9I5W4
A	41	MET	-	initiating methionine	UNP Q9I5W4
A	697	GLN	GLU	engineered mutation	UNP Q9I5W4
A	924	LEU	-	expression tag	UNP Q9I5W4
A	925	GLU	-	expression tag	UNP Q9I5W4

- Molecule 2 is a protein called GLU-ALA-PRO-SER-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	5	Total	C	N	O	0	0	0
			32	19	5	8			
2	H	4	Total	C	N	O	0	0	0
			23	14	4	5			

- Molecule 3 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose.

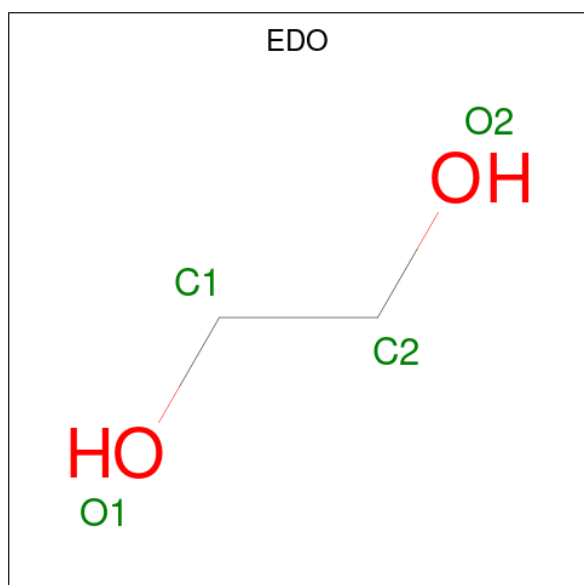


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	2	Total	C	N	O	0	0	0
			25	14	1	10			
3	G	2	Total	C	N	O	0	0	0
			25	14	1	10			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

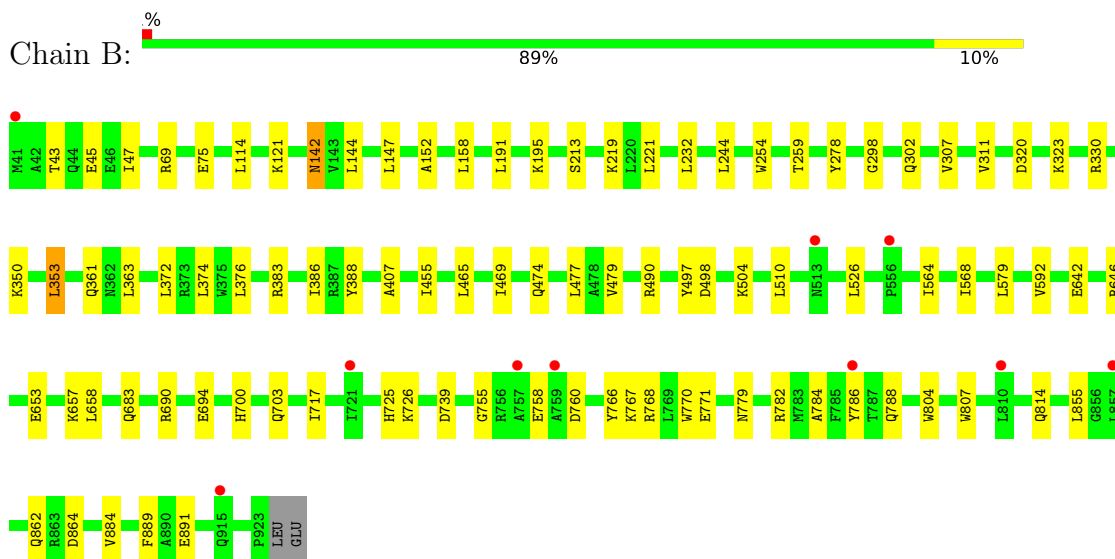
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	365	Total	O	0	0
			365	365		
6	A	300	Total	O	0	0
			300	300		

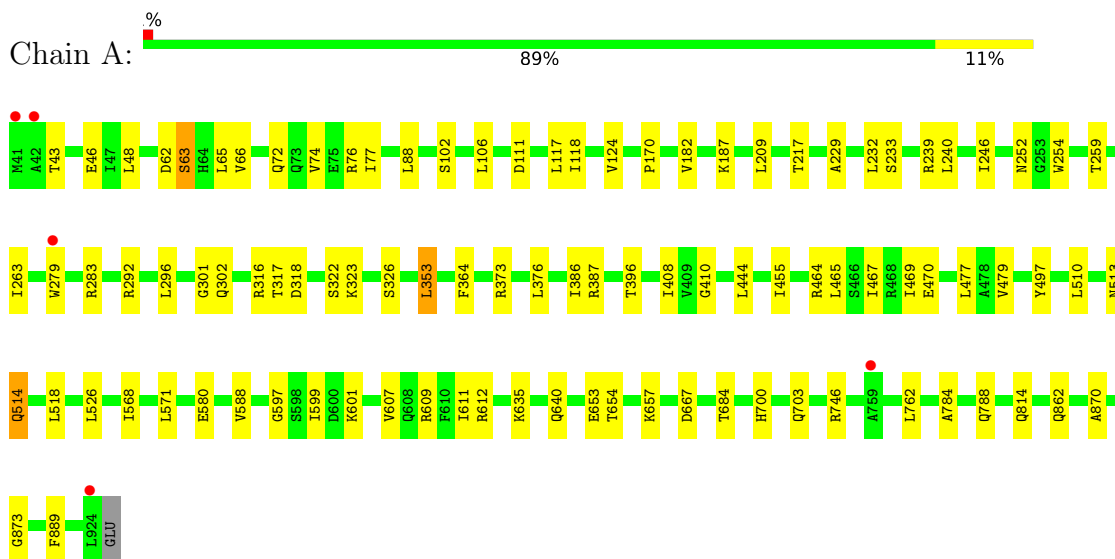
3 Residue-property plots

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.

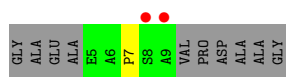
- Molecule 1: Immunomodulating metalloprotease



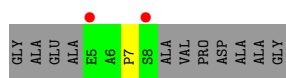
- Molecule 1: Immunomodulating metalloprotease



- Molecule 2: GLU-ALA-PRO-SER-ALA



- Molecule 2: GLU-ALA-PRO-SER-ALA



- Molecule 3: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose



- Molecule 3: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-alpha-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.34Å 156.50Å 95.68Å 90.00° 114.31° 90.00°	Depositor
Resolution (Å)	29.96 – 2.45 29.96 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.96-2.45) 94.3 (29.96-2.45)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.180 , 0.234 0.180 , 0.234	Depositor DCC
R_{free} test set	4347 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14379	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: ZN, GAL, EDO, A2G

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	0.42	0/6938	0.58	0/9445
1	B	0.41	0/6925	0.57	1/9426 (0.0%)
2	E	0.33	0/32	0.52	0/43
2	H	0.32	0/23	0.59	0/31
All	All	0.41	0/13918	0.58	1/18945 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	LEU	CA-CB-CG	-6.16	101.14	115.30

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	6790	0	6584	61	0
1	B	6777	0	6579	56	0
2	E	32	0	26	2	0
2	H	23	0	17	1	0
3	D	25	0	21	0	0
3	G	25	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	36	0	54	4	0
5	B	4	0	6	1	0
6	A	300	0	0	2	0
6	B	365	0	0	3	0
All	All	14379	0	13308	116	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 4.

All (116) 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:479:VAL:HG23	1:A:510:LEU:HD11	1.49	0.91
1:B:469:ILE:HG21	1:B:477:LEU:HD12	1.59	0.83
1:A:469:ILE:HG21	1:A:477:LEU:HD13	1.67	0.77
1:A:316:ARG:HE	1:A:318:ASP:HB3	1.52	0.75
1:B:700:HIS:HD1	1:B:703:GLN:HE22	1.36	0.72
1:B:700:HIS:HD1	1:B:703:GLN:NE2	1.88	0.69
1:A:353:LEU:HD13	1:A:408:ILE:HG23	1.73	0.69
1:A:77:ILE:HD11	1:A:111:ASP:HA	1.75	0.69
1:A:48:LEU:HD13	1:A:66:VAL:HG22	1.75	0.67
1:A:444:LEU:HD11	1:A:455:ILE:HA	1.79	0.62
1:A:43:THR:HG23	1:A:46:GLU:H	1.64	0.62
1:B:383:ARG:HA	1:B:386:ILE:HD12	1.81	0.62
1:A:464:ARG:HH12	5:A:1008:EDO:H21	1.66	0.60
1:A:232:LEU:HD21	1:A:259:THR:HG23	1.83	0.60
1:A:209:LEU:O	1:A:239:ARG:NH1	2.33	0.60
1:B:254:TRP:NE1	6:B:1105:HOH:O	2.29	0.59
1:A:118:ILE:HD12	5:A:1003:EDO:H21	1.85	0.58
1:A:386:ILE:O	1:A:387:ARG:NH2	2.34	0.57
1:A:653:GLU:O	1:A:657:LYS:HB2	2.05	0.56
1:B:864:ASP:HB3	1:B:891:GLU:HA	1.87	0.55
1:B:363:LEU:HD13	1:B:372:LEU:HB3	1.88	0.55
1:A:240:LEU:HD13	1:A:246:ILE:HD12	1.87	0.55
1:A:607:VAL:O	1:A:611:ILE:HG12	2.06	0.55
1:A:317:THR:HG22	1:A:396:THR:HG21	1.89	0.55
1:B:767:LYS:HA	1:B:771:GLU:HB2	1.89	0.54
1:B:43:THR:O	1:B:47:ILE:HG12	2.07	0.54
1:B:653:GLU:O	1:B:657:LYS:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:690:ARG:HA	1:B:726:LYS:HE3	1.89	0.54
1:B:784:ALA:O	1:B:788:GLN:HG2	2.08	0.54
1:A:479:VAL:CG2	1:A:510:LEU:HD11	2.31	0.53
1:B:254:TRP:CE3	2:E:7:PRO:HG3	2.44	0.53
1:B:232:LEU:HD21	1:B:259:THR:HG23	1.91	0.53
1:B:142:ASN:HD21	1:B:144:LEU:HB2	1.73	0.53
1:B:469:ILE:HG12	1:B:510:LEU:HD13	1.91	0.52
1:A:254:TRP:NE1	6:A:1105:HOH:O	2.30	0.52
1:B:320:ASP:OD2	1:B:323:LYS:HD3	2.10	0.52
1:B:121:LYS:NZ	6:B:1101:HOH:O	2.20	0.52
1:A:229:ALA:HB3	1:A:232:LEU:HD13	1.91	0.52
1:B:142:ASN:HD22	1:B:142:ASN:C	2.12	0.52
1:A:301:GLY:O	1:A:302:GLN:NE2	2.42	0.51
1:A:74:VAL:O	1:A:77:ILE:HG22	2.11	0.51
1:A:762:LEU:HD23	1:A:870:ALA:HA	1.93	0.51
1:B:298:GLY:O	1:B:302:GLN:NE2	2.42	0.51
1:B:855:LEU:HD23	1:B:884:VAL:HG23	1.93	0.51
1:B:758:GLU:HG2	1:B:760:ASP:H	1.76	0.51
1:A:609:ARG:HG3	1:A:612:ARG:NH1	2.25	0.51
1:B:465:LEU:HD11	1:B:526:LEU:HD11	1.92	0.49
1:B:717:ILE:HD11	1:B:779:ASN:HA	1.94	0.49
1:A:609:ARG:HG3	1:A:612:ARG:HH12	1.77	0.49
1:A:77:ILE:CD1	1:A:111:ASP:HA	2.43	0.48
1:A:252:ASN:ND2	5:A:1007:EDO:H11	2.28	0.48
1:A:72:GLN:HG3	1:A:76:ARG:NH2	2.29	0.48
1:A:182:VAL:HB	1:A:187:LYS:HG3	1.96	0.47
1:A:784:ALA:O	1:A:788:GLN:HG2	2.14	0.47
1:A:470:GLU:HG2	1:A:513:ASN:OD1	2.14	0.47
1:A:106:LEU:HD22	1:A:124:VAL:HB	1.96	0.47
1:A:376:LEU:HD21	1:A:410:GLY:HA3	1.97	0.46
1:B:717:ILE:HD12	1:B:782:ARG:HB2	1.98	0.46
1:B:642:GLU:O	1:B:646:ARG:HG3	2.14	0.46
1:B:725:HIS:HD2	1:B:804:TRP:CG	2.33	0.46
1:B:221:LEU:HB2	1:B:244:LEU:HD21	1.97	0.46
1:B:700:HIS:HA	1:B:703:GLN:NE2	2.31	0.46
1:B:683:GLN:HE22	1:B:694:GLU:HG3	1.81	0.46
1:B:579:LEU:HD23	1:B:592:VAL:HG22	1.98	0.45
1:B:786:TYR:HD2	1:B:807:TRP:CZ2	2.34	0.45
1:A:762:LEU:HD22	1:A:873:GLY:HA2	1.98	0.45
1:B:330:ARG:HG3	1:B:490:ARG:CZ	2.47	0.45
1:A:467:ILE:HD13	1:A:479:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:GLY:O	1:A:601:LYS:HG2	2.17	0.44
1:B:147:LEU:O	1:B:152:ALA:HA	2.17	0.44
1:B:469:ILE:CG2	1:B:477:LEU:HD12	2.40	0.44
1:B:755:GLY:HA2	1:B:768:ARG:NH1	2.32	0.44
1:A:364:PHE:HA	1:A:373:ARG:CZ	2.48	0.44
1:A:580:GLU:HA	1:A:588:VAL:O	2.17	0.44
1:A:259:THR:O	1:A:263:ILE:HG13	2.18	0.44
1:B:766:TYR:CD1	1:B:770:TRP:HB2	2.53	0.44
1:B:862:GLN:HA	1:B:889:PHE:CE2	2.52	0.44
1:A:292:ARG:O	1:A:296:LEU:HG	2.18	0.44
1:A:514:GLN:HG3	1:A:514:GLN:O	2.17	0.44
1:B:657:LYS:HG3	1:B:658:LEU:O	2.18	0.44
1:A:635:LYS:HB2	1:A:640:GLN:HG3	2.00	0.43
1:B:142:ASN:HD22	1:B:144:LEU:H	1.65	0.43
1:B:504:LYS:NZ	6:B:1121:HOH:O	2.50	0.43
1:A:568:ILE:HG12	1:A:607:VAL:HG11	2.00	0.43
1:A:469:ILE:HG12	1:A:510:LEU:HD13	2.01	0.43
1:B:361:GLN:O	5:B:1002:EDO:H12	2.19	0.43
1:A:465:LEU:CD2	1:A:518:LEU:HB2	2.49	0.43
1:A:62:ASP:O	1:A:63:SER:HB3	2.19	0.43
1:A:667:ASP:O	1:A:684:THR:HA	2.19	0.43
1:B:350:LYS:HB2	1:B:407:ALA:HB1	2.01	0.43
1:B:374:LEU:HA	1:B:374:LEU:HD23	1.88	0.42
1:A:117:LEU:HA	5:A:1003:EDO:H12	2.02	0.42
1:B:474:GLN:HG3	1:A:654:THR:HG21	2.00	0.42
1:A:700:HIS:HA	1:A:703:GLN:OE1	2.20	0.42
1:A:279:TRP:CZ2	2:H:7:PRO:HB2	2.55	0.42
1:A:316:ARG:HG2	1:A:318:ASP:H	1.84	0.42
1:B:219:LYS:HD3	1:B:219:LYS:HA	1.89	0.41
1:B:307:VAL:O	1:B:311:VAL:HG23	2.20	0.41
1:B:388:TYR:CD1	1:B:498:ASP:HA	2.55	0.41
1:B:564:ILE:O	1:B:568:ILE:HG13	2.20	0.41
1:A:316:ARG:NE	1:A:318:ASP:HB3	2.27	0.41
1:B:191:LEU:O	1:B:195:LYS:HG3	2.21	0.41
1:A:599:ILE:HD13	1:A:607:VAL:HG22	2.03	0.41
1:A:48:LEU:HD22	1:A:65:LEU:HD23	2.03	0.41
1:B:455:ILE:HD12	1:B:526:LEU:HB3	2.03	0.41
1:A:88:LEU:HD23	1:A:170:PRO:HB3	2.03	0.41
1:B:479:VAL:HB	1:B:510:LEU:HD11	2.02	0.41
1:A:217:THR:OG1	6:A:1101:HOH:O	2.22	0.40
1:B:147:LEU:HD11	1:B:158:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:OE1	1:B:69:ARG:NH2	2.47	0.40
1:A:455:ILE:HD12	1:A:526:LEU:HB3	2.03	0.40
1:A:862:GLN:HA	1:A:889:PHE:CE2	2.57	0.40
1:B:278:TYR:CD2	2:E:7:PRO:HD2	2.57	0.40
1:B:353:LEU:HD22	1:B:376:LEU:HD21	2.02	0.40
1:A:571:LEU:HA	1:A:571:LEU:HD23	1.82	0.40
1:A:72:GLN:HE21	1:A:76:ARG:HH22	1.70	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	883/885 (100%)	857 (97%)	25 (3%)	1 (0%)	51	64
1	B	881/885 (100%)	855 (97%)	26 (3%)	0	100	100
2	E	3/15 (20%)	3 (100%)	0	0	100	100
2	H	2/15 (13%)	2 (100%)	0	0	100	100
All	All	1769/1800 (98%)	1717 (97%)	51 (3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	LYS

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	699/701 (100%)	688 (98%)	11 (2%)	62	74
1	B	698/701 (100%)	691 (99%)	7 (1%)	76	84
2	E	3/7 (43%)	3 (100%)	0	100	100
2	H	2/7 (29%)	2 (100%)	0	100	100
All	All	1402/1416 (99%)	1384 (99%)	18 (1%)	69	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	75	GLU
1	B	114	LEU
1	B	142	ASN
1	B	213	SER
1	B	497	TYR
1	B	739	ASP
1	B	814	GLN
1	A	63	SER
1	A	102	SER
1	A	233	SER
1	A	283	ARG
1	A	322	SER
1	A	326	SER
1	A	353	LEU
1	A	497	TYR
1	A	514	GLN
1	A	746	ARG
1	A	814	GLN

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

Mol	Chain	Res	Type
1	B	142	ASN
1	B	683	GLN
1	B	703	GLN
1	A	72	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 ⓘ

4 monosaccharides 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	A2G	D	1	3,2	14,14,15	0.41	0	17,19,21	0.95	1 (5%)
3	GAL	D	2	3	11,11,12	0.31	0	15,15,17	1.08	2 (13%)
3	A2G	G	1	3,2	14,14,15	0.53	0	17,19,21	0.90	0
3	GAL	G	2	3	11,11,12	0.49	0	15,15,17	1.22	1 (6%)

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	A2G	D	1	3,2	-	4/6/23/26	0/1/1/1
3	GAL	D	2	3	-	0/2/19/22	0/1/1/1
3	A2G	G	1	3,2	-	2/6/23/26	0/1/1/1
3	GAL	G	2	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	GAL	C1-C2-C3	3.10	113.47	109.67
3	D	2	GAL	O5-C5-C6	2.46	111.06	107.20
3	D	1	A2G	O5-C1-C2	-2.41	107.47	111.29
3	D	2	GAL	C3-C4-C5	-2.05	106.58	110.24

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	A2G	O7-C7-N2-C2
3	G	1	A2G	C8-C7-N2-C2
3	D	1	A2G	O7-C7-N2-C2
3	D	1	A2G	C8-C7-N2-C2
3	D	1	A2G	C4-C5-C6-O6
3	D	1	A2G	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
5	EDO	B	1002	-	3,3,3	0.49	0	2,2,2	0.19	0
5	EDO	A	1007	-	3,3,3	0.52	0	2,2,2	0.17	0
5	EDO	A	1003	-	3,3,3	0.51	0	2,2,2	0.16	0
5	EDO	A	1006	-	3,3,3	0.55	0	2,2,2	0.29	0
5	EDO	A	1009	-	3,3,3	0.43	0	2,2,2	0.25	0
5	EDO	A	1002	-	3,3,3	0.46	0	2,2,2	0.29	0
5	EDO	A	1008	-	3,3,3	0.49	0	2,2,2	0.18	0
5	EDO	A	1005	-	3,3,3	0.56	0	2,2,2	0.09	0
5	EDO	A	1004	-	3,3,3	0.51	0	2,2,2	0.31	0
5	EDO	A	1010	-	3,3,3	0.64	0	2,2,2	0.05	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	EDO	B	1002	-	-	0/1/1/1	-
5	EDO	A	1007	-	-	1/1/1/1	-
5	EDO	A	1003	-	-	0/1/1/1	-
5	EDO	A	1006	-	-	0/1/1/1	-
5	EDO	A	1009	-	-	0/1/1/1	-
5	EDO	A	1002	-	-	0/1/1/1	-
5	EDO	A	1008	-	-	1/1/1/1	-
5	EDO	A	1005	-	-	1/1/1/1	-
5	EDO	A	1004	-	-	0/1/1/1	-
5	EDO	A	1010	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1007	EDO	O1-C1-C2-O2
5	A	1008	EDO	O1-C1-C2-O2
5	A	1005	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1002	EDO	1	0
5	A	1007	EDO	1	0
5	A	1003	EDO	2	0
5	A	1008	EDO	1	0

5.7 Other polymers ⓘ

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

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, 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	884/885 (99%)	-0.21	5 (0%) 89 89	21, 37, 58, 92	0
1	B	883/885 (99%)	-0.22	10 (1%) 80 80	22, 35, 56, 84	0
2	E	5/15 (33%)	2.07	2 (40%) 0 0	52, 57, 77, 77	0
2	H	4/15 (26%)	1.64	2 (50%) 0 0	75, 80, 82, 84	0
All	All	1776/1800 (98%)	-0.21	19 (1%) 80 80	21, 36, 58, 92	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	759	ALA	3.8
2	E	9	ALA	3.5
1	B	41	MET	3.3
1	A	41	MET	3.2
1	B	757	ALA	2.5
1	A	759	ALA	2.5
1	A	42	ALA	2.5
1	B	786	TYR	2.4
1	B	556	PRO	2.3
2	E	8	SER	2.3
1	B	915	GLN	2.2
1	A	279	TRP	2.2
2	H	5	GLU	2.2
1	B	513	ASN	2.2
1	B	721	ILE	2.1
2	H	8	SER	2.1
1	A	924	LEU	2.1
1	B	810	LEU	2.0
1	B	857	LEU	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](#)

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	A2G	G	1	14/15	0.75	0.35	86,97,107,111	0
3	GAL	G	2	11/12	0.82	0.38	67,74,79,84	0
3	GAL	D	2	11/12	0.87	0.32	64,67,75,76	0
3	A2G	D	1	14/15	0.87	0.38	79,86,90,94	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. 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
5	EDO	A	1007	4/4	0.79	0.28	53,62,66,66	0
5	EDO	A	1008	4/4	0.85	0.18	46,52,53,53	0
5	EDO	B	1002	4/4	0.87	0.31	54,56,57,58	0
5	EDO	A	1003	4/4	0.92	0.26	57,58,61,61	0
5	EDO	A	1006	4/4	0.93	0.11	42,44,45,50	0
5	EDO	A	1004	4/4	0.95	0.11	30,30,32,35	0
5	EDO	A	1010	4/4	0.95	0.11	30,34,35,37	0
5	EDO	A	1002	4/4	0.96	0.21	48,54,57,62	0
5	EDO	A	1005	4/4	0.96	0.20	30,33,42,45	0
5	EDO	A	1009	4/4	0.98	0.09	42,46,52,53	0
4	ZN	B	1001	1/1	0.98	0.09	33,33,33,33	0
4	ZN	A	1001	1/1	0.99	0.07	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.