



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 11:06 AM EDT

PDB ID : 5LGJ
Title : THE CRYSTAL STRUCTURE OF IGE FC MUTANT - P333C
Authors : Dhaliwal, B.; Pang, M.O.Y.; Sutton, B.J.
Deposited on : unknown
Resolution : 2.60 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 ⓘ 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 : rb-20029824
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) : rb-20029824

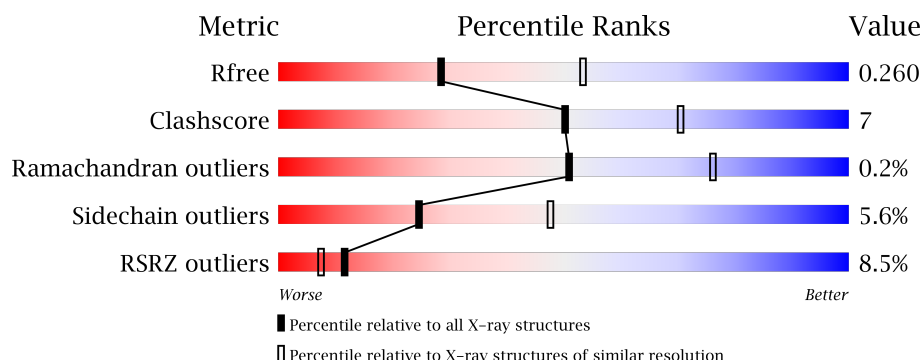
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	319	<div> <div>8%</div> <div>87%</div> <div>10%</div> <div>..</div> </div>
2	B	320	<div> <div>8%</div> <div>81%</div> <div>13%</div> <div>..</div> </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
3	NAG	A	601	-	-	-	X
6	SO4	A	606	-	-	-	X
6	SO4	A	607	-	-	-	X
6	SO4	B	609	-	-	-	X
7	PG4	A	609	-	-	-	X
7	PG4	A	610	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5305 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 epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	315	Total	C	N	O	S	0	0	0
			2465	1539	438	476	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLN	ASN	conflict	UNP P01854
A	333	CYS	PRO	engineered mutation	UNP P01854
A	371	GLN	ASN	conflict	UNP P01854

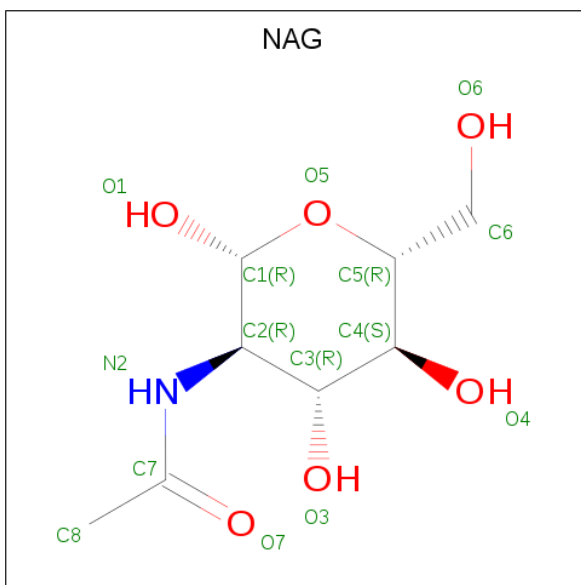
- Molecule 2 is a protein called Ig epsilon chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	309	Total	C	N	O	S	0	0	0
			2410	1506	428	465	11			

There are 3 discrepancies between the modelled and reference sequences:

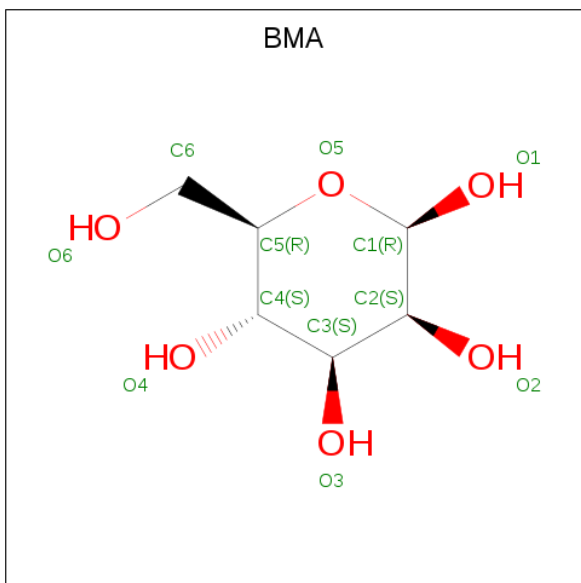
Chain	Residue	Modelled	Actual	Comment	Reference
B	265	GLN	ASN	conflict	UNP P01854
B	333	CYS	PRO	engineered mutation	UNP P01854
B	371	GLN	ASN	conflict	UNP P01854

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



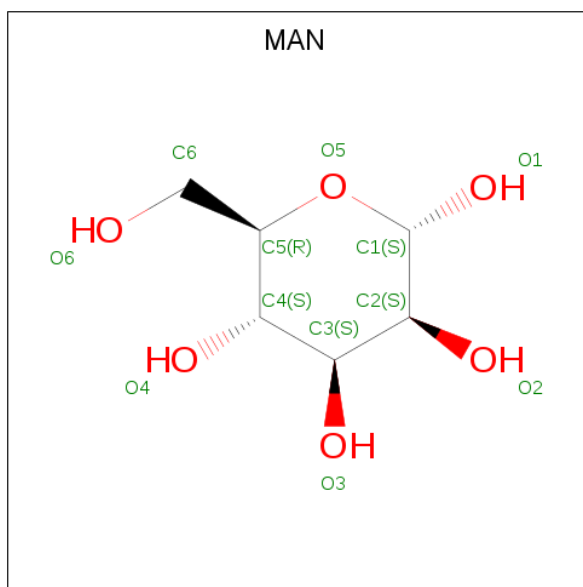
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



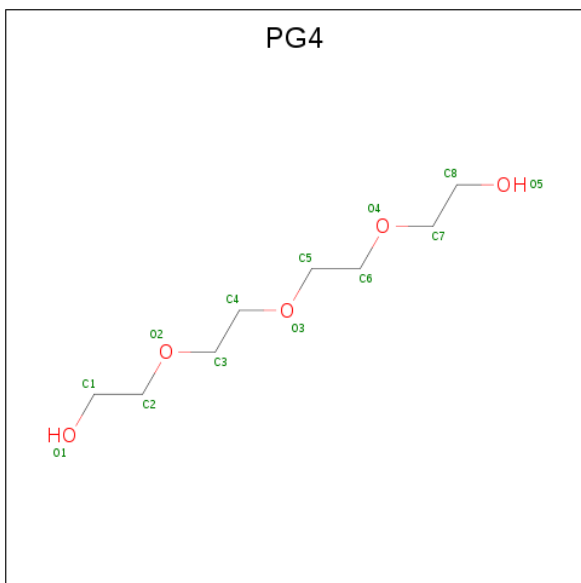
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



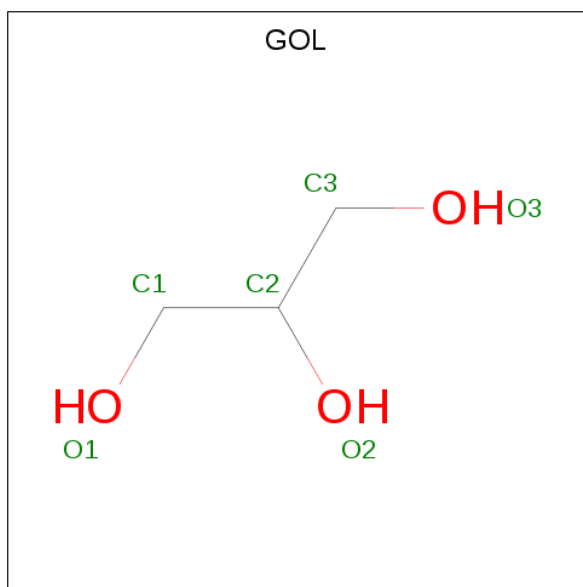
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		
7	A	1	Total	C	O	0	0
			12	8	4		

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		

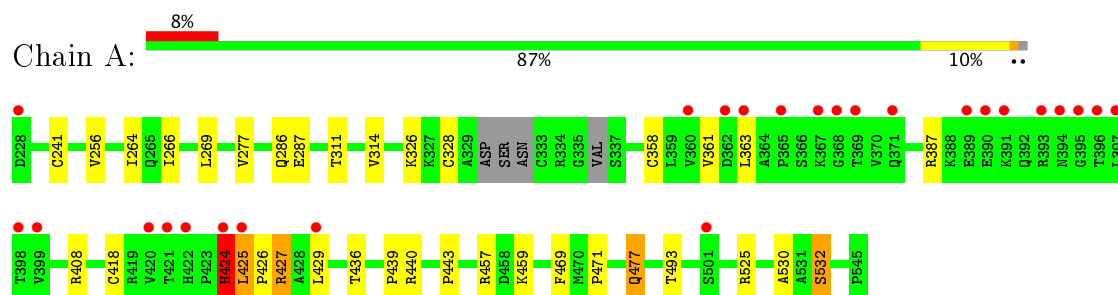
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	113	Total	O	0	0
			113	113		
9	B	122	Total	O	0	0
			122	122		

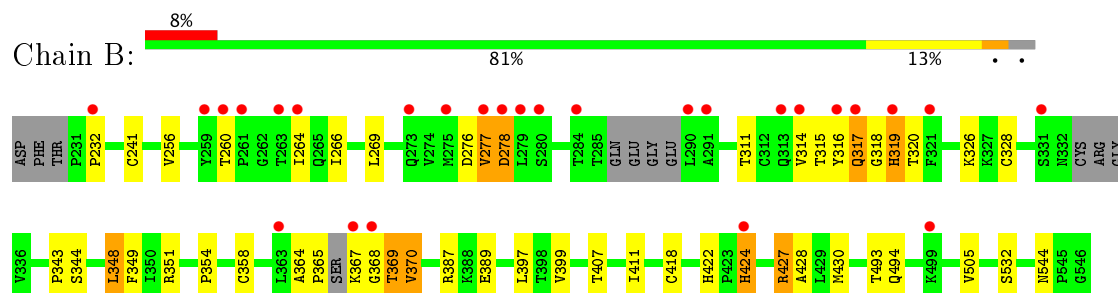
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 epsilon chain C region



- Molecule 2: Ig epsilon chain C region



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	129.45Å 74.91Å 79.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.49 – 2.60 67.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.49-2.60) 98.9 (67.47-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.62Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0	Depositor
R, R_{free}	0.188 , 0.248 0.201 , 0.260	Depositor DCC
R_{free} test set	1223 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5305	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, PG4, SO4, 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	0.61	2/2524 (0.1%)	0.75	6/3436 (0.2%)
2	B	0.42	0/2467	0.69	0/3360
All	All	0.52	2/4991 (0.0%)	0.72	6/6796 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	425	LEU	C-N	-20.94	0.94	1.34
1	A	424	HIS	C-N	10.63	1.58	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	LEU	O-C-N	12.25	144.38	121.10
1	A	425	LEU	C-N-CD	11.72	153.01	128.40
1	A	424	HIS	O-C-N	-8.96	108.36	122.70
1	A	425	LEU	CA-C-N	-8.79	92.48	117.10
1	A	425	LEU	C-N-CA	-7.33	91.20	122.00
1	A	424	HIS	C-N-CA	5.68	135.90	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	424	HIS	Mainchain

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	2465	0	2414	26	1
2	B	2410	0	2360	41	0
3	A	28	0	24	1	0
3	B	28	0	24	0	0
4	A	11	0	9	0	0
4	B	11	0	8	0	0
5	A	22	0	19	0	0
5	B	44	0	38	1	0
6	A	15	0	0	0	0
6	B	5	0	0	0	0
7	A	25	0	33	0	0
8	B	6	0	8	1	0
9	A	113	0	0	0	0
9	B	122	0	0	0	0
All	All	5305	0	4937	61	1

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 7.

All (61) 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)
2:B:260:THR:O	2:B:316:TYR:OH	1.53	1.27
1:A:424:HIS:CD2	1:A:425:LEU:CD2	2.35	1.08
2:B:317:GLN:HG3	2:B:318:GLY:N	1.65	1.08
2:B:364:ALA:O	2:B:367:LYS:HA	1.55	1.06
1:A:439:PRO:HG2	2:B:278:ASP:HB3	1.34	1.04
2:B:318:GLY:O	2:B:319:HIS:HB3	1.64	0.96
2:B:317:GLN:CG	2:B:318:GLY:H	1.79	0.95
2:B:317:GLN:CG	2:B:318:GLY:N	2.30	0.93
1:A:424:HIS:CD2	1:A:425:LEU:HD21	2.06	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:CYS:HG	2:B:418:CYS:HG	0.90	0.88
2:B:368:GLY:HA3	2:B:422:HIS:NE2	1.94	0.81
2:B:369:THR:O	2:B:370:VAL:HB	1.82	0.78
1:A:424:HIS:CD2	1:A:425:LEU:HD22	2.20	0.77
2:B:315:THR:HG22	2:B:319:HIS:C	2.05	0.77
1:A:439:PRO:HG2	2:B:278:ASP:CB	2.12	0.76
1:A:328:CYS:HG	2:B:241:CYS:HG	0.76	0.75
1:A:424:HIS:NE2	1:A:425:LEU:HD21	2.05	0.72
2:B:318:GLY:O	2:B:319:HIS:CB	2.35	0.72
2:B:427:ARG:HD2	2:B:428:ALA:H	1.59	0.68
2:B:348:LEU:HD13	2:B:354:PRO:HB3	1.79	0.65
2:B:364:ALA:O	2:B:367:LYS:CA	2.42	0.61
1:A:477:GLN:HG2	1:A:525:ARG:HB3	1.85	0.59
1:A:425:LEU:O	1:A:426:PRO:C	2.27	0.59
2:B:422:HIS:HD1	2:B:424:HIS:H	1.51	0.58
2:B:315:THR:HG22	2:B:320:THR:N	2.19	0.57
2:B:407:THR:H	8:B:608:GOL:H32	1.72	0.55
2:B:317:GLN:HG2	2:B:318:GLY:H	1.68	0.53
2:B:343:PRO:HB2	2:B:348:LEU:HD22	1.90	0.53
2:B:369:THR:O	2:B:370:VAL:CB	2.49	0.53
1:A:241:CYS:SG	2:B:328:CYS:SG	3.04	0.51
2:B:358:CYS:CB	2:B:418:CYS:HG	2.23	0.50
1:A:425:LEU:N	1:A:425:LEU:HD22	2.25	0.50
2:B:370:VAL:HG22	2:B:422:HIS:HB2	1.94	0.50
2:B:368:GLY:CA	2:B:422:HIS:NE2	2.71	0.49
1:A:425:LEU:HD13	1:A:426:PRO:HD2	1.95	0.49
1:A:241:CYS:HG	2:B:328:CYS:HG	1.48	0.49
1:A:424:HIS:CD2	1:A:425:LEU:HD23	2.43	0.48
1:A:443:PRO:HB3	1:A:469:PHE:HB3	1.96	0.48
2:B:277:VAL:O	2:B:277:VAL:CG2	2.61	0.48
2:B:266:ILE:HG12	2:B:314:VAL:HG22	1.95	0.48
2:B:365:PRO:HG3	2:B:397:LEU:HB2	1.95	0.47
1:A:425:LEU:CD1	1:A:426:PRO:HD2	2.45	0.47
1:A:436:THR:HG21	1:A:471:PRO:HG3	1.96	0.46
2:B:232:PRO:HD3	2:B:316:TYR:CD2	2.51	0.46
1:A:493:THR:HG21	2:B:493:THR:HG21	1.98	0.45
2:B:232:PRO:HD3	2:B:316:TYR:HD2	1.82	0.45
2:B:344:SER:HB3	5:B:606:MAN:H61	1.98	0.45
2:B:349:PHE:HE1	2:B:411:ILE:HD11	1.83	0.43
1:A:425:LEU:HD13	1:A:425:LEU:HA	1.84	0.43
1:A:256:VAL:HG11	1:A:264:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ILE:HG12	1:A:314:VAL:HG22	2.00	0.43
2:B:256:VAL:HG11	2:B:264:ILE:HD11	2.01	0.42
2:B:269:LEU:HB2	2:B:311:THR:HB	2.01	0.42
1:A:424:HIS:C	1:A:425:LEU:HD22	2.40	0.41
1:A:269:LEU:HB2	1:A:311:THR:HB	2.03	0.40
1:A:358:CYS:CB	1:A:418:CYS:HG	2.35	0.40
2:B:389:GLU:HG2	2:B:399:VAL:HG22	2.03	0.40
1:A:361:VAL:HG11	3:A:602:NAG:H2	2.03	0.40
2:B:260:THR:O	2:B:316:TYR:CZ	2.61	0.40
2:B:348:LEU:HD13	2:B:354:PRO:CB	2.50	0.40
1:A:440:ARG:HB3	1:A:530:ALA:HB2	2.03	0.40

All (1) 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)
1:A:427:ARG:NH1	1:A:532:SER:CB[3_556]	1.81	0.39

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	309/319 (97%)	300 (97%)	9 (3%)	0	100	100
2	B	301/320 (94%)	287 (95%)	13 (4%)	1 (0%)	44	70
All	All	610/639 (96%)	587 (96%)	22 (4%)	1 (0%)	51	76

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	370	VAL

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	279/283 (99%)	265 (95%)	14 (5%)	28	53
2	B	273/283 (96%)	256 (94%)	17 (6%)	21	42
All	All	552/566 (98%)	521 (94%)	31 (6%)	25	48

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	VAL
1	A	286	GLN
1	A	287	GLU
1	A	326	LYS
1	A	363	LEU
1	A	387	ARG
1	A	408	ARG
1	A	424	HIS
1	A	427	ARG
1	A	429	LEU
1	A	457	ARG
1	A	459	LYS
1	A	477	GLN
1	A	532	SER
2	B	276	ASP
2	B	277	VAL
2	B	278	ASP
2	B	317	GLN
2	B	319	HIS
2	B	326	LYS
2	B	348	LEU
2	B	351	ARG
2	B	369	THR
2	B	387	ARG
2	B	424	HIS
2	B	427	ARG
2	B	430	MET

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Mol	Chain	Res	Type
2	B	494	GLN
2	B	505	VAL
2	B	532	SER
2	B	544	ASN

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

Mol	Chain	Res	Type
1	A	371	GLN
1	A	424	HIS
1	A	468	ASN
2	B	317	GLN
2	B	468	ASN
2	B	481	ASN
2	B	538	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

19 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	NAG	A	601	1,3	14,14,15	0.30	0	15,19,21	1.20	1 (6%)
3	NAG	A	602	3,4	14,14,15	0.29	0	15,19,21	0.70	0
4	BMA	A	603	3,5	11,11,12	0.33	0	13,15,17	0.64	0
5	MAN	A	604	5,4	11,11,12	0.38	0	13,15,17	0.87	1 (7%)
5	MAN	A	605	5	11,11,12	0.42	0	13,15,17	1.12	2 (15%)
6	SO4	A	606	-	4,4,4	0.28	0	6,6,6	0.22	0
6	SO4	A	607	-	4,4,4	0.23	0	6,6,6	0.10	0
6	SO4	A	608	-	4,4,4	0.25	0	6,6,6	0.45	0
7	PG4	A	609	-	12,12,12	0.18	0	11,11,11	0.15	0
7	PG4	A	610	-	11,11,12	0.24	0	10,10,11	0.28	0
3	NAG	B	601	3,2	14,14,15	0.24	0	15,19,21	0.84	1 (6%)
3	NAG	B	602	3,4	14,14,15	0.26	0	15,19,21	0.64	0
4	BMA	B	603	3,5	11,11,12	0.29	0	13,15,17	0.58	0
5	MAN	B	604	5,4	11,11,12	0.36	0	13,15,17	0.98	1 (7%)
5	MAN	B	605	4	11,11,12	0.36	0	13,15,17	0.66	0
5	MAN	B	606	5	11,11,12	0.35	0	13,15,17	0.98	2 (15%)
5	MAN	B	607	5	11,11,12	0.37	0	13,15,17	1.00	1 (7%)
8	GOL	B	608	-	5,5,5	0.12	0	5,5,5	0.24	0
6	SO4	B	609	-	4,4,4	0.11	0	6,6,6	0.22	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
3	NAG	A	601	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	602	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	603	3,5	-	0/2/19/22	0/1/1/1
5	MAN	A	604	5,4	-	0/2/19/22	0/1/1/1
5	MAN	A	605	5	-	0/2/19/22	0/1/1/1
6	SO4	A	606	-	-	0/0/0/0	0/0/0/0
6	SO4	A	607	-	-	0/0/0/0	0/0/0/0
6	SO4	A	608	-	-	0/0/0/0	0/0/0/0
7	PG4	A	609	-	-	0/10/10/10	0/0/0/0
7	PG4	A	610	-	-	0/9/9/10	0/0/0/0
3	NAG	B	601	3,2	-	0/6/23/26	0/1/1/1
3	NAG	B	602	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	603	3,5	-	0/2/19/22	0/1/1/1
5	MAN	B	604	5,4	-	0/2/19/22	0/1/1/1
5	MAN	B	605	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MAN	B	606	5	-	0/2/19/22	0/1/1/1
5	MAN	B	607	5	-	0/2/19/22	1/1/1/1
8	GOL	B	608	-	-	0/4/4/4	0/0/0/0
6	SO4	B	609	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	NAG	O5-C1-C2	-4.09	105.78	111.47
3	B	601	NAG	O5-C1-C2	-2.19	108.42	111.47
5	B	606	MAN	C1-C2-C3	2.00	112.19	109.65
5	A	605	MAN	C1-C2-C3	2.64	113.00	109.65
5	A	605	MAN	C1-O5-C5	2.71	115.90	112.17
5	B	606	MAN	C1-O5-C5	2.72	115.92	112.17
5	A	604	MAN	C1-O5-C5	2.73	115.92	112.17
5	B	604	MAN	C1-O5-C5	3.05	116.36	112.17
5	B	607	MAN	C1-O5-C5	3.19	116.56	112.17

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	607	MAN	C1-C2-C3-C4-C5-O5

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	NAG	1	0
5	B	606	MAN	1	0
8	B	608	GOL	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	425:LEU	C	426:PRO	N	0.94

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	315/319 (98%)	0.30	26 (8%)	12 8	20, 49, 127, 187	0
2	B	309/320 (96%)	0.42	27 (8%)	11 7	17, 46, 117, 161	0
All	All	624/639 (97%)	0.36	53 (8%)	11 7	17, 48, 125, 187	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	284	THR	9.9
1	A	362	ASP	8.8
2	B	291	ALA	7.9
2	B	278	ASP	6.1
2	B	263	THR	5.7
1	A	363	LEU	5.3
2	B	290	LEU	4.9
1	A	429	LEU	4.9
1	A	393	ARG	4.7
1	A	396	THR	4.5
1	A	399	VAL	4.5
1	A	424	HIS	4.5
2	B	316	TYR	4.4
2	B	277	VAL	4.2
1	A	422	HIS	4.1
1	A	425	LEU	4.1
1	A	365	PRO	4.0
1	A	394	ASN	3.9
1	A	420	VAL	3.7
1	A	421	THR	3.7
1	A	389	GLU	3.7
1	A	395	GLY	3.6
2	B	317	GLN	3.6
1	A	367	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	280	SER	3.5
2	B	232	PRO	3.4
2	B	259	TYR	3.3
2	B	260	THR	3.3
2	B	264	ILE	3.3
2	B	321	PHE	3.1
2	B	314	VAL	3.1
1	A	501	SER	3.0
2	B	313	GLN	2.9
2	B	331	SER	2.8
1	A	368	GLY	2.8
2	B	279	LEU	2.7
2	B	261	PRO	2.7
1	A	360	VAL	2.7
1	A	390	GLU	2.6
2	B	368	GLY	2.6
2	B	319	HIS	2.5
2	B	363	LEU	2.5
2	B	424	HIS	2.5
1	A	228	ASP	2.4
2	B	275	MET	2.4
1	A	398	THR	2.4
2	B	367	LYS	2.3
1	A	391	LYS	2.3
1	A	371	GLN	2.2
1	A	369	THR	2.2
2	B	499	LYS	2.2
1	A	397	LEU	2.1
2	B	273	GLN	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 ⓘ

There are no carbohydrates in this entry.

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(Å ²)	Q<0.9
7	PG4	A	610	12/13	0.67	0.43	9.67	63,65,69,70	0
7	PG4	A	609	13/13	0.58	0.41	7.56	79,81,82,83	0
6	SO4	B	609	5/5	0.71	0.28	6.41	109,110,111,111	0
6	SO4	A	606	5/5	0.95	0.27	4.64	63,64,64,66	0
6	SO4	A	607	5/5	0.93	0.19	3.41	91,93,93,94	0
6	SO4	A	608	5/5	0.94	0.18	0.33	61,64,64,65	0
3	NAG	A	601	14/15	0.77	0.45	0.02	113,116,118,119	0
3	NAG	A	602	14/15	0.66	0.34	-0.21	117,119,120,120	0
3	NAG	B	601	14/15	0.93	0.17	-0.35	52,54,55,56	0
3	NAG	B	602	14/15	0.94	0.17	-0.49	55,58,61,68	0
5	MAN	A	604	11/12	0.75	0.28	-	120,121,123,125	0
4	BMA	A	603	11/12	0.81	0.21	-	113,115,117,119	0
8	GOL	B	608	6/6	0.91	0.16	-	67,68,69,70	0
5	MAN	A	605	11/12	0.60	0.30	-	126,127,128,128	0
5	MAN	B	607	11/12	0.69	0.26	-	105,106,107,107	0
5	MAN	B	606	11/12	0.72	0.39	-	110,112,113,114	0
5	MAN	B	605	11/12	0.72	0.24	-	88,90,92,92	0
5	MAN	B	604	11/12	0.80	0.19	-	96,100,103,107	0
4	BMA	B	603	11/12	0.93	0.13	-	76,83,87,91	0

6.5 Other polymers

There are no such residues in this entry.