



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:16 am GMT

PDB ID : 2YL5
Title : INHIBITION OF THE PNEUMOCOCCAL VIRULENCE FACTOR STRH AND MOLECULAR INSIGHTS INTO N-GLYCAN RECOGNITION AND HYDROLYSIS
Authors : Pluvinage, B.; Higgins, M.A.; Abbott, D.W.; Robb, C.; Dalia, A.B.; Deng, L.; Weiser, J.N.; Parsons, T.B.; Fairbanks, A.J.; Vocadlo, D.J.; Boraston, A.B.
Deposited on : 2011-05-31
Resolution : 2.15 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 : 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

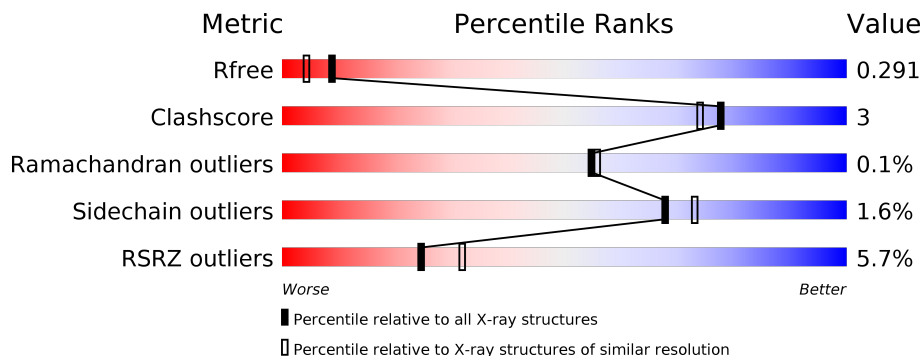
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1170 (2.16-2.16)
Clashscore	112137	1278 (2.16-2.16)
Ramachandran outliers	110173	1256 (2.16-2.16)
Sidechain outliers	110143	1255 (2.16-2.16)
RSRZ outliers	101464	1175 (2.16-2.16)

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	442	<div> <div>4%</div> <div>84% 8% 7%</div> </div>
1	B	442	<div> <div>6%</div> <div>87% 7% 7%</div> </div>
1	C	442	<div> <div>5%</div> <div>85% 8% 6%</div> </div>
1	D	442	<div> <div>6%</div> <div>83% 10% 8%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	2048[B]	-	-	-	X
3	EDO	A	2049	-	-	-	X
3	EDO	B	2043	-	-	-	X
3	EDO	D	2040	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15664 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 BETA-N-ACETYLHEXOSAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	4	8	0
			3320	2133	539	635	13			
1	B	413	Total	C	N	O	S	15	7	0
			3340	2139	546	643	12			
1	C	414	Total	C	N	O	S	11	7	0
			3343	2146	543	642	12			
1	D	408	Total	C	N	O	S	22	4	0
			3282	2107	532	631	12			

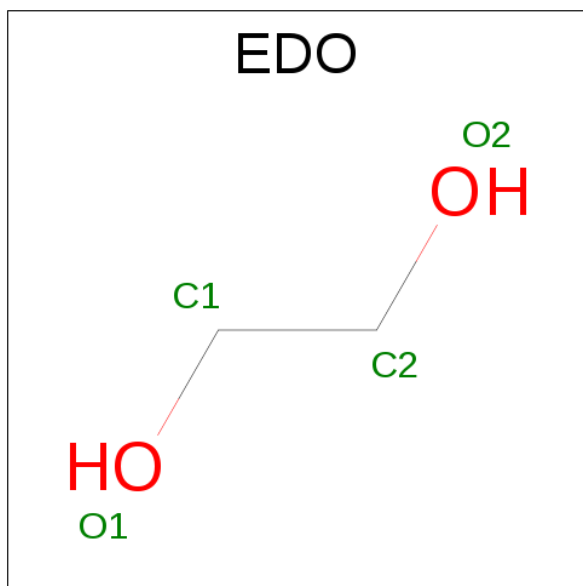
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	623	GLY	-	EXPRESSION TAG	UNP P49610
A	624	SER	-	EXPRESSION TAG	UNP P49610
A	625	HIS	-	EXPRESSION TAG	UNP P49610
A	626	MET	-	EXPRESSION TAG	UNP P49610
B	623	GLY	-	EXPRESSION TAG	UNP P49610
B	624	SER	-	EXPRESSION TAG	UNP P49610
B	625	HIS	-	EXPRESSION TAG	UNP P49610
B	626	MET	-	EXPRESSION TAG	UNP P49610
C	623	GLY	-	EXPRESSION TAG	UNP P49610
C	624	SER	-	EXPRESSION TAG	UNP P49610
C	625	HIS	-	EXPRESSION TAG	UNP P49610
C	626	MET	-	EXPRESSION TAG	UNP P49610
D	623	GLY	-	EXPRESSION TAG	UNP P49610
D	624	SER	-	EXPRESSION TAG	UNP P49610
D	625	HIS	-	EXPRESSION TAG	UNP P49610
D	626	MET	-	EXPRESSION TAG	UNP P49610

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total 2	Mg 2	0	0
2	A	5	Total 5	Mg 5	0	0
2	C	3	Total 3	Mg 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

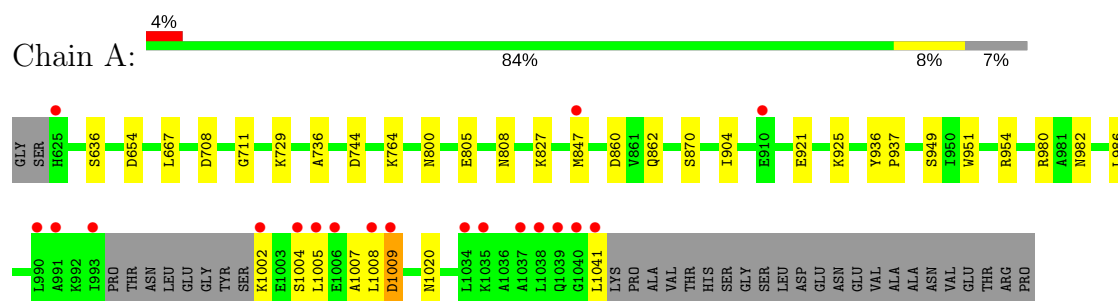
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	673	Total	O	0	0
			673	673		
4	B	542	Total	O	0	0
			542	542		
4	C	613	Total	O	0	0
			613	613		
4	D	489	Total	O	0	0
			489	489		

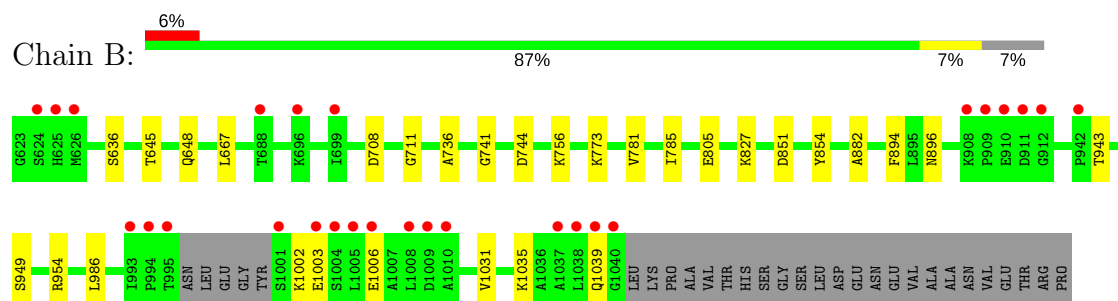
3 Residue-property plots [i](#)

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.

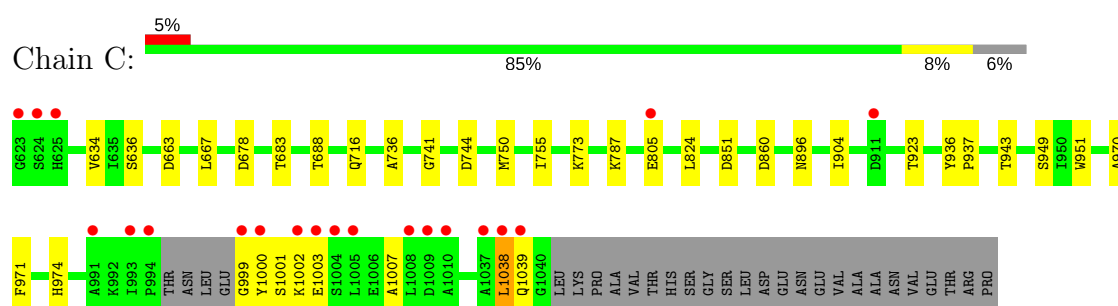
• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE



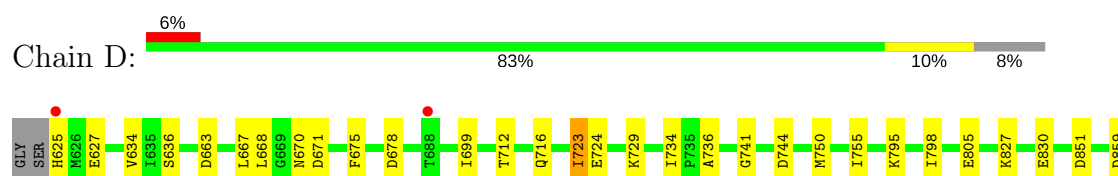
• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE

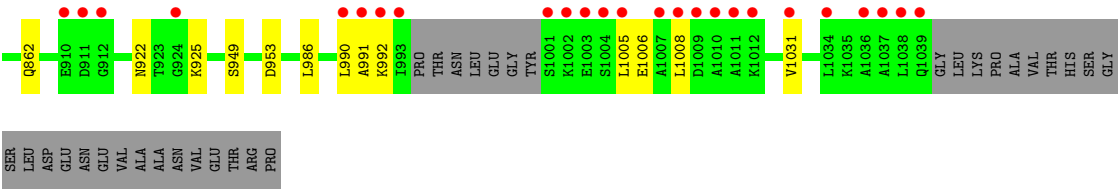


• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE



• Molecule 1: BETA-N-ACETYLHEXOSAMINIDASE





SER
LEU
ASP
GLU
ASN
GLU
VAL
ALA
ALA
ASN
VAL
GLU
THR
ARG
PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.25Å 115.86Å 132.26Å 90.00° 99.62° 90.00°	Depositor
Resolution (Å)	38.25 – 2.15 38.25 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.0 (38.25-2.15) 97.0 (38.25-2.15)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.44 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.237 , 0.293 0.237 , 0.291	Depositor DCC
R_{free} test set	5261 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 53.3	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	0.91	EDS
Total number of atoms	15664	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.0551e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: MG, EDO

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	0.50	3/3398 (0.1%)	0.46	1/4584 (0.0%)
1	B	0.86	5/3416 (0.1%)	0.61	4/4610 (0.1%)
1	C	0.44	2/3423 (0.1%)	0.48	4/4619 (0.1%)
1	D	0.42	5/3357 (0.1%)	0.55	5/4532 (0.1%)
All	All	0.58	15/13594 (0.1%)	0.53	14/18345 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	756	LYS	CE-NZ	-38.99	0.51	1.49
1	A	764	LYS	CE-NZ	-20.01	0.99	1.49
1	B	1003	GLU	CB-CG	-15.22	1.23	1.52
1	C	1003	GLU	CG-CD	-15.20	1.29	1.51
1	B	1035	LYS	CG-CD	-12.99	1.08	1.52
1	B	1006	GLU	CD-OE2	-12.24	1.12	1.25
1	B	1006	GLU	CD-OE1	10.97	1.37	1.25
1	C	1038	LEU	CB-CG	-9.39	1.25	1.52
1	A	1007	ALA	CA-CB	-9.30	1.32	1.52
1	D	1008	LEU	CB-CG	-8.25	1.28	1.52
1	D	990	LEU	CG-CD1	-6.98	1.26	1.51
1	D	1005	LEU	CB-CG	-5.75	1.35	1.52
1	D	1006	GLU	CB-CG	5.60	1.62	1.52
1	D	991	ALA	CA-CB	5.30	1.63	1.52
1	A	827	LYS	CD-CE	5.28	1.64	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	756	LYS	CD-CE-NZ	25.23	169.73	111.70
1	D	1008	LEU	CB-CG-CD2	-11.06	92.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1008	LEU	CA-CB-CG	-10.14	91.98	115.30
1	D	992	LYS	CD-CE-NZ	9.54	133.65	111.70
1	B	1003	GLU	CB-CG-CD	-8.57	91.06	114.20
1	B	1003	GLU	CA-CB-CG	-7.97	95.86	113.40
1	D	1008	LEU	CB-CG-CD1	7.43	123.62	111.00
1	C	1003	GLU	CG-CD-OE1	5.85	130.00	118.30
1	C	1003	GLU	CG-CD-OE2	-5.67	106.95	118.30
1	D	1005	LEU	CA-CB-CG	5.59	128.16	115.30
1	A	827	LYS	CD-CE-NZ	5.56	124.48	111.70
1	B	1006	GLU	CG-CD-OE1	-5.39	107.52	118.30
1	C	1038	LEU	CA-CB-CG	-5.29	103.13	115.30
1	C	1007	ALA	N-CA-CB	5.12	117.27	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3320	0	3265	26	0
1	B	3340	0	3272	18	0
1	C	3343	0	3282	24	0
1	D	3282	0	3216	21	0
2	A	5	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
3	A	16	0	24	3	0
3	B	4	0	6	0	0
3	C	16	0	24	0	0
3	D	16	0	24	0	0
4	A	673	0	0	0	0
4	B	542	0	0	0	0
4	C	613	0	0	0	0
4	D	489	0	0	0	0
All	All	15664	0	13113	89	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 3.

All (89) 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:C:999:GLY:HA2	1:C:1000:TYR:HB2	1.26	1.10
1:C:787[B]:LYS:HA	1:C:787[B]:LYS:HE2	1.50	0.93
1:C:999:GLY:CA	1:C:1000:TYR:HB2	1.99	0.91
1:B:773[A]:LYS:HD3	1:B:827[A]:LYS:HZ2	1.41	0.86
1:D:625:HIS:HD2	1:D:627:GLU:H	1.26	0.83
1:B:773[A]:LYS:CD	1:B:827[A]:LYS:HZ2	1.93	0.82
1:A:925[A]:LYS:NZ	1:A:925[A]:LYS:HB3	1.95	0.81
1:C:999:GLY:HA2	1:C:1000:TYR:CB	2.02	0.81
1:D:859:ASP:HB2	1:D:862:GLN:HE22	1.55	0.71
1:A:925[A]:LYS:HZ3	1:A:925[A]:LYS:HB3	1.57	0.69
1:B:773[A]:LYS:CD	1:B:827[A]:LYS:NZ	2.56	0.68
1:A:986[A]:LEU:O	1:A:986[A]:LEU:HD12	1.96	0.66
1:B:741:GLY:HA3	1:B:805:GLU:HG3	1.79	0.64
1:A:654[A]:ASP:CG	1:A:729[A]:LYS:HZ3	2.02	0.63
1:D:859:ASP:HB2	1:D:862:GLN:NE2	2.14	0.62
1:B:773[A]:LYS:HG2	1:B:827[A]:LYS:NZ	2.15	0.62
1:C:923:THR:HG23	1:C:971:PHE:HA	1.81	0.61
1:D:625:HIS:CD2	1:D:627:GLU:H	2.14	0.59
1:A:805:GLU:HB3	3:A:2049:EDO:H11	1.85	0.58
1:D:723[A]:ILE:O	1:D:723[A]:ILE:HG12	2.04	0.58
1:B:773[A]:LYS:CG	1:B:827[A]:LYS:HZ2	2.17	0.57
1:C:787[B]:LYS:HA	1:C:787[B]:LYS:CE	2.30	0.57
1:A:654[A]:ASP:CG	1:A:729[A]:LYS:NZ	2.57	0.57
1:D:723[A]:ILE:HD12	1:D:795:LYS:HB3	1.90	0.54
1:A:980:ARG:HA	1:A:1020:ASN:HA	1.89	0.54
1:C:896:ASN:HB2	1:C:943:THR:HG21	1.90	0.53
1:D:667:LEU:HA	1:D:736:ALA:HB3	1.88	0.53
1:D:827[A]:LYS:NZ	1:D:830:GLU:OE2	2.36	0.53
1:B:773[A]:LYS:HD3	1:B:827[A]:LYS:NZ	2.15	0.52
1:A:667:LEU:HA	1:A:736:ALA:HB3	1.91	0.52
1:B:773[A]:LYS:CG	1:B:827[A]:LYS:NZ	2.74	0.51
1:A:982:ASN:HD21	3:A:2047:EDO:H22	1.75	0.51
1:A:925[A]:LYS:NZ	1:A:925[A]:LYS:CB	2.72	0.51
1:A:808:ASN:HB2	3:A:2049:EDO:H22	1.93	0.51
1:C:741:GLY:HA3	1:C:805[A]:GLU:HG3	1.92	0.50
1:A:986[B]:LEU:C	1:A:986[B]:LEU:HD23	2.31	0.50
1:B:773[A]:LYS:HG2	1:B:827[A]:LYS:HZ3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:636:SER:HB3	1:D:949:SER:HA	1.93	0.50
1:C:904:ILE:HG13	1:C:951:TRP:HB2	1.93	0.49
1:C:923:THR:HG22	1:C:974:HIS:CD2	2.47	0.49
1:D:741:GLY:HA3	1:D:805:GLU:HG3	1.94	0.49
1:B:667:LEU:HA	1:B:736:ALA:HB3	1.94	0.49
1:A:654[A]:ASP:OD1	1:A:729[A]:LYS:NZ	2.46	0.49
1:C:936:TYR:CG	1:C:937:PRO:HA	2.48	0.49
1:B:645:THR:H	1:B:648:GLN:HE21	1.60	0.48
1:C:667:LEU:HA	1:C:736:ALA:HB3	1.95	0.48
1:A:636:SER:HB3	1:A:949:SER:HA	1.96	0.48
1:A:904:ILE:HG13	1:A:951:TRP:HB2	1.95	0.48
1:B:781:VAL:O	1:B:785:ILE:HG12	2.12	0.48
1:B:636:SER:HB3	1:B:949:SER:HA	1.96	0.48
1:C:773:LYS:HE2	1:C:824:LEU:HD21	1.96	0.48
1:A:1008:LEU:HD22	1:A:1041:LEU:HD21	1.96	0.48
1:C:636:SER:HB3	1:C:949:SER:HA	1.96	0.47
1:C:936:TYR:CD1	1:C:937:PRO:HA	2.50	0.47
1:C:923:THR:HG22	1:C:974:HIS:HD2	1.80	0.47
1:A:936:TYR:CG	1:A:937:PRO:HA	2.50	0.46
1:D:678:ASP:H	1:D:716:GLN:NE2	2.13	0.46
1:C:923:THR:CG2	1:C:971:PHE:HA	2.46	0.46
1:A:936:TYR:CD1	1:A:937:PRO:HA	2.52	0.45
1:A:1004:SER:HB3	1:A:1041:LEU:HA	1.97	0.45
1:A:1005:LEU:O	1:A:1009:ASP:HB2	2.17	0.45
1:C:683:THR:HG23	1:C:688[A]:THR:HG22	1.99	0.44
1:C:787[A]:LYS:HD2	1:C:787[A]:LYS:HA	1.82	0.44
1:D:734:ILE:HD12	1:D:798:ILE:HD12	2.00	0.44
1:D:750:MET:HB3	1:D:755:ILE:HB	2.00	0.44
1:A:925[A]:LYS:HZ2	1:A:925[A]:LYS:HB3	1.77	0.44
1:B:894:PHE:HB2	1:B:943:THR:HG22	2.00	0.44
1:D:986:LEU:HD13	1:D:1031:VAL:HG22	2.00	0.43
1:D:699:ILE:HG23	1:D:712:THR:HG21	2.00	0.43
1:C:750:MET:HB3	1:C:755:ILE:HB	2.01	0.43
1:D:827[A]:LYS:N	1:D:827[A]:LYS:HD2	2.34	0.43
1:A:708:ASP:HB3	1:A:711:GLY:O	2.17	0.43
1:A:921:GLU:OE2	1:A:925[B]:LYS:CE	2.67	0.43
1:C:678:ASP:H	1:C:716:GLN:NE2	2.17	0.42
1:A:921:GLU:OE2	1:A:925[B]:LYS:HE2	2.19	0.42
1:D:670:ASN:O	1:D:671:ASP:HB2	2.20	0.42
1:C:1001:SER:HA	1:C:1002:LYS:HA	1.73	0.42
1:B:986:LEU:HD13	1:B:1031:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:LEU:HD22	1:D:675:PHE:HB2	2.02	0.42
1:D:678:ASP:H	1:D:716:GLN:HE21	1.66	0.41
1:D:922:ASN:HA	1:D:925:LYS:HB2	2.01	0.41
1:A:800:ASN:HA	1:A:847[B]:MET:HB3	2.01	0.41
1:B:827[B]:LYS:HE2	1:B:827[B]:LYS:HB3	1.84	0.41
1:B:854:TYR:O	1:B:882:ALA:HB2	2.19	0.41
1:D:634:VAL:HG22	1:D:663:ASP:HB2	2.03	0.41
1:B:708:ASP:HB3	1:B:711:GLY:O	2.20	0.41
1:C:634:VAL:HG22	1:C:663:ASP:HB2	2.03	0.40
1:C:923:THR:HG21	1:C:970:ALA:C	2.42	0.40
1:A:847[B]:MET:CE	1:A:870:SER:HB2	2.52	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	413/442 (93%)	400 (97%)	13 (3%)	0	100	100
1	B	416/442 (94%)	400 (96%)	15 (4%)	1 (0%)	51	50
1	C	417/442 (94%)	402 (96%)	15 (4%)	0	100	100
1	D	408/442 (92%)	398 (98%)	10 (2%)	0	100	100
All	All	1654/1768 (94%)	1600 (97%)	53 (3%)	1 (0%)	55	56

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	896	ASN

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	344/363 (95%)	337 (98%)	7 (2%)	60	64
1	B	346/363 (95%)	340 (98%)	6 (2%)	66	71
1	C	346/363 (95%)	341 (99%)	5 (1%)	71	77
1	D	340/363 (94%)	333 (98%)	7 (2%)	59	62
All	All	1376/1452 (95%)	1351 (98%)	25 (2%)	68	68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	744	ASP
1	A	860	ASP
1	A	862[A]	GLN
1	A	862[B]	GLN
1	A	954	ARG
1	A	1002	LYS
1	A	1009	ASP
1	B	744	ASP
1	B	851	ASP
1	B	954[A]	ARG
1	B	954[B]	ARG
1	B	1002	LYS
1	B	1039	GLN
1	C	744	ASP
1	C	851	ASP
1	C	860	ASP
1	C	1038	LEU
1	C	1039	GLN
1	D	723[A]	ILE
1	D	723[B]	ILE
1	D	724	GLU
1	D	729	LYS
1	D	744	ASP
1	D	851	ASP
1	D	953	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	670	ASN
1	A	742	HIS
1	A	808	ASN
1	A	929	ASN
1	A	1033	ASN
1	B	648	GLN
1	B	670	ASN
1	B	761	HIS
1	B	808	ASN
1	B	1033	ASN
1	B	1039	GLN
1	C	632	ASN
1	C	670	ASN
1	C	716	GLN
1	C	814	GLN
1	C	823	GLN
1	C	929	ASN
1	C	1039	GLN
1	D	625	HIS
1	D	670	ASN
1	D	716	GLN
1	D	808	ASN
1	D	922	ASN
1	D	975	ASN
1	D	982	ASN
1	D	1033	ASN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 23 ligands modelled in this entry, 10 are monoatomic - leaving 13 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
3	EDO	A	2047	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	A	2048[A]	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	A	2048[B]	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	A	2049	-	3,3,3	0.44	0	2,2,2	0.38	0
3	EDO	B	2043	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	C	2044	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	C	2045	-	3,3,3	0.45	0	2,2,2	0.39	0
3	EDO	C	2046	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	C	2047	-	3,3,3	0.45	0	2,2,2	0.36	0
3	EDO	D	2040	-	3,3,3	0.44	0	2,2,2	0.37	0
3	EDO	D	2041	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	D	2042	-	3,3,3	0.46	0	2,2,2	0.34	0
3	EDO	D	2043	-	3,3,3	0.45	0	2,2,2	0.36	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	EDO	A	2047	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2048[A]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2048[B]	-	-	0/1/1/1	0/0/0/0
3	EDO	A	2049	-	-	0/1/1/1	0/0/0/0
3	EDO	B	2043	-	-	0/1/1/1	0/0/0/0
3	EDO	C	2044	-	-	0/1/1/1	0/0/0/0
3	EDO	C	2045	-	-	0/1/1/1	0/0/0/0
3	EDO	C	2046	-	-	0/1/1/1	0/0/0/0
3	EDO	C	2047	-	-	0/1/1/1	0/0/0/0
3	EDO	D	2040	-	-	0/1/1/1	0/0/0/0
3	EDO	D	2041	-	-	0/1/1/1	0/0/0/0
3	EDO	D	2042	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	D	2043	-	-	0/1/1/1	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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2047	EDO	1	0
3	A	2049	EDO	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 ⓘ

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	409/442 (92%)	0.38	19 (4%)	33 41	3, 7, 29, 43	16 (3%)
1	B	413/442 (93%)	0.67	27 (6%)	20 25	13, 18, 34, 47	11 (2%)
1	C	414/442 (93%)	0.44	20 (4%)	31 39	3, 7, 33, 56	21 (5%)
1	D	408/442 (92%)	0.76	27 (6%)	19 24	12, 19, 42, 57	15 (3%)
All	All	1644/1768 (92%)	0.57	93 (5%)	24 32	3, 15, 35, 57	63 (3%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1000	TYR	6.6
1	D	1005	LEU	6.0
1	A	991	ALA	5.9
1	C	1004	SER	5.8
1	C	999	GLY	5.8
1	A	1041	LEU	5.8
1	C	1005	LEU	5.6
1	C	1008	LEU	5.5
1	B	995	THR	5.5
1	B	1005	LEU	5.4
1	A	1038	LEU	5.1
1	B	1008	LEU	4.9
1	D	1038	LEU	4.8
1	D	993	ILE	4.6
1	D	991	ALA	4.6
1	D	1037	ALA	4.6
1	B	994	PRO	4.5
1	C	1002	LYS	4.2
1	B	624	SER	4.2
1	D	1004	SER	4.2
1	A	1039	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1005	LEU	4.1
1	D	1031	VAL	4.1
1	D	1039	GLN	4.1
1	C	993	ILE	4.0
1	A	1008	LEU	3.9
1	C	1038	LEU	3.9
1	B	1004	SER	3.8
1	D	911	ASP	3.8
1	D	1001	SER	3.7
1	A	993	ILE	3.6
1	B	625	HIS	3.6
1	B	910	GLU	3.5
1	B	1038	LEU	3.5
1	D	1007	ALA	3.5
1	C	1037	ALA	3.5
1	A	1037	ALA	3.4
1	D	992	LYS	3.4
1	D	1010	ALA	3.3
1	C	911	ASP	3.3
1	C	625	HIS	3.3
1	D	1034	LEU	3.3
1	A	1040	GLY	3.3
1	A	1006	GLU	3.3
1	B	993	ILE	3.2
1	D	1011	ALA	3.2
1	D	1008	LEU	3.2
1	A	1004	SER	3.1
1	B	909	PRO	3.1
1	C	994	PRO	3.1
1	D	1002	LYS	3.1
1	C	991	ALA	3.0
1	B	908	LYS	3.0
1	B	1040	GLY	3.0
1	C	1039	GLN	3.0
1	D	1003	GLU	2.9
1	D	1009	ASP	2.9
1	D	625	HIS	2.9
1	A	1002	LYS	2.9
1	C	623	GLY	2.8
1	C	1009	ASP	2.8
1	B	1039	GLN	2.8
1	B	1006	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	688	THR	2.5
1	B	911	ASP	2.5
1	A	625	HIS	2.5
1	B	1009	ASP	2.5
1	A	847[A]	MET	2.4
1	B	1001	SER	2.4
1	A	1009	ASP	2.4
1	B	1010	ALA	2.4
1	C	1003	GLU	2.4
1	B	1037	ALA	2.4
1	B	696	LYS	2.4
1	C	624	SER	2.3
1	B	1003	GLU	2.3
1	D	924	GLY	2.3
1	B	626	MET	2.2
1	D	910	GLU	2.2
1	B	942	PRO	2.2
1	A	910	GLU	2.2
1	A	1034	LEU	2.2
1	C	805[A]	GLU	2.2
1	B	688[A]	THR	2.2
1	D	990	LEU	2.1
1	A	990	LEU	2.1
1	D	1012	LYS	2.1
1	A	1035	LYS	2.1
1	B	699	ILE	2.1
1	C	1010	ALA	2.1
1	D	1036	ALA	2.1
1	B	912	GLY	2.1
1	D	912	GLY	2.0

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
3	EDO	A	2048[B]	4/4	0.87	0.29	7.55	2,2,2,2	4
3	EDO	B	2043	4/4	0.93	0.26	6.91	26,26,26,26	0
3	EDO	A	2049	4/4	0.79	0.27	3.14	7,7,7,7	1
3	EDO	D	2040	4/4	0.90	0.23	2.06	22,22,22,22	0
3	EDO	C	2045	4/4	0.87	0.18	0.99	16,16,16,16	0
3	EDO	C	2044	4/4	0.85	0.23	0.92	10,10,10,11	0
2	MG	A	2044	1/1	0.95	0.15	0.80	4,4,4,4	0
3	EDO	A	2047	4/4	0.86	0.21	0.61	36,36,36,36	0
2	MG	C	2041	1/1	0.96	0.15	0.59	2,2,2,2	0
2	MG	C	2043	1/1	0.97	0.05	-2.65	20,20,20,20	0
2	MG	A	2046	1/1	0.96	0.08	-4.23	9,9,9,9	0
3	EDO	C	2046	4/4	0.83	0.23	-	32,32,32,32	0
2	MG	A	2042	1/1	0.99	0.16	-	6,6,6,6	0
2	MG	A	2045	1/1	0.89	0.17	-	27,27,27,27	0
3	EDO	D	2042	4/4	0.83	0.23	-	41,41,41,41	0
3	EDO	A	2048[A]	4/4	0.87	0.29	-	10,10,10,10	4
3	EDO	C	2047	4/4	0.78	0.34	-	34,34,34,34	0
2	MG	B	2041	1/1	0.73	0.22	-	35,35,35,35	0
3	EDO	D	2043	4/4	0.76	0.34	-	50,50,50,50	0
2	MG	A	2043	1/1	0.97	0.07	-	2,2,2,2	0
2	MG	B	2042	1/1	0.99	0.16	-	14,14,14,14	0
3	EDO	D	2041	4/4	0.50	0.33	-	58,58,58,58	0
2	MG	C	2042	1/1	0.98	0.12	-	6,6,6,6	0

6.5 Other polymers ⓘ

There are no such residues in this entry.