



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2025 – 12:55 PM EDT

PDB ID : 9MS4 / pdb_00009ms4
Title : Crystal structure of an expansin (Xa_EXLX1) from Xanthomonas sacchari
Authors : Smith, C.A.; Buchko, G.W.; Momeni, M.H.; Master, E.R.
Deposited on : 2025-01-09
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

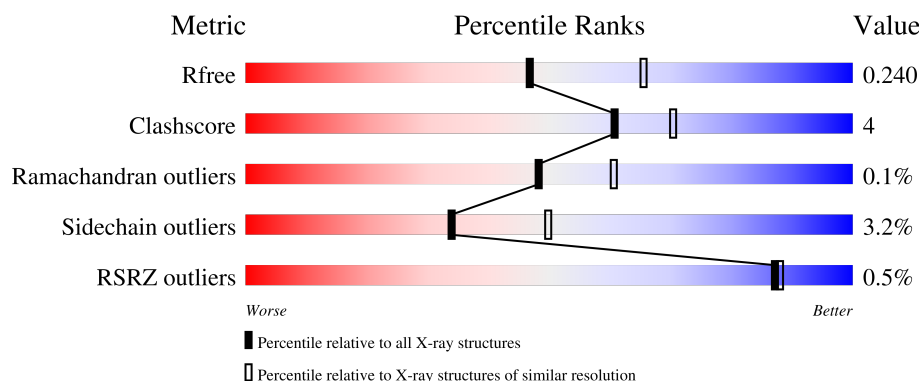
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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	209	<div> <div>88%</div> <div>11%</div> </div>
1	B	209	<div> <div>86%</div> <div>14%</div> </div>
1	C	209	<div> <div>88%</div> <div>12%</div> </div>
1	D	209	<div> <div>91%</div> <div>8%</div> </div>
1	E	209	<div> <div>%</div> <div>89%</div> <div>10%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	209	<div><div></div><div>88%</div><div>11%</div><div></div></div>
1	G	209	<div>%<div><div></div><div>85%</div><div>12%</div><div></div></div>..</div>
1	H	209	<div>%<div><div></div><div>86%</div><div>12%</div><div></div></div>.</div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12995 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 Expansin (Peptidoglycan-binding protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1586	1007	274	301	4			
1	B	209	Total	C	N	O	S	0	0	0
			1586	1007	274	301	4			
1	C	209	Total	C	N	O	S	0	0	0
			1586	1007	274	301	4			
1	D	209	Total	C	N	O	S	0	0	0
			1586	1007	274	301	4			
1	E	207	Total	C	N	O	S	0	0	0
			1575	1001	272	298	4			
1	F	207	Total	C	N	O	S	0	0	0
			1575	1001	272	298	4			
1	G	207	Total	C	N	O	S	0	0	0
			1575	1001	272	298	4			
1	H	207	Total	C	N	O	S	0	0	0
			1575	1001	272	298	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASN	ALA	conflict	UNP A0A7X0FIU8
A	93	MET	THR	conflict	UNP A0A7X0FIU8
A	104	GLU	ASP	conflict	UNP A0A7X0FIU8
A	140	THR	SER	conflict	UNP A0A7X0FIU8
A	215	LEU	ILE	conflict	UNP A0A7X0FIU8
B	60	ASN	ALA	conflict	UNP A0A7X0FIU8
B	93	MET	THR	conflict	UNP A0A7X0FIU8
B	104	GLU	ASP	conflict	UNP A0A7X0FIU8
B	140	THR	SER	conflict	UNP A0A7X0FIU8
B	215	LEU	ILE	conflict	UNP A0A7X0FIU8
C	60	ASN	ALA	conflict	UNP A0A7X0FIU8
C	93	MET	THR	conflict	UNP A0A7X0FIU8
C	104	GLU	ASP	conflict	UNP A0A7X0FIU8

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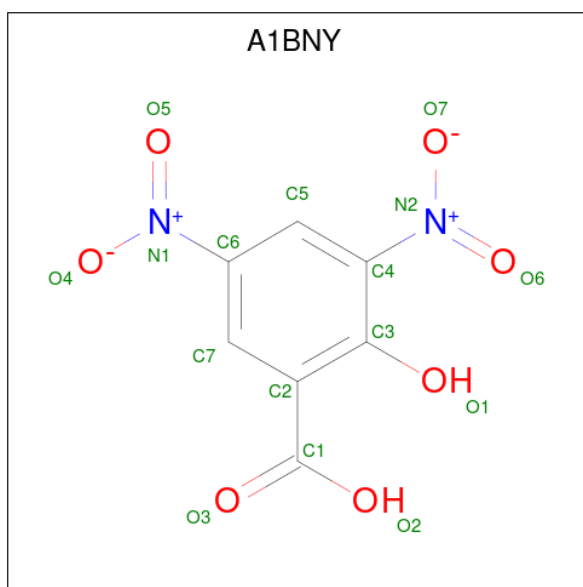
Chain	Residue	Modelled	Actual	Comment	Reference
C	140	THR	SER	conflict	UNP A0A7X0FIU8
C	215	LEU	ILE	conflict	UNP A0A7X0FIU8
D	60	ASN	ALA	conflict	UNP A0A7X0FIU8
D	93	MET	THR	conflict	UNP A0A7X0FIU8
D	104	GLU	ASP	conflict	UNP A0A7X0FIU8
D	140	THR	SER	conflict	UNP A0A7X0FIU8
D	215	LEU	ILE	conflict	UNP A0A7X0FIU8
E	60	ASN	ALA	conflict	UNP A0A7X0FIU8
E	93	MET	THR	conflict	UNP A0A7X0FIU8
E	104	GLU	ASP	conflict	UNP A0A7X0FIU8
E	140	THR	SER	conflict	UNP A0A7X0FIU8
E	215	LEU	ILE	conflict	UNP A0A7X0FIU8
F	60	ASN	ALA	conflict	UNP A0A7X0FIU8
F	93	MET	THR	conflict	UNP A0A7X0FIU8
F	104	GLU	ASP	conflict	UNP A0A7X0FIU8
F	140	THR	SER	conflict	UNP A0A7X0FIU8
F	215	LEU	ILE	conflict	UNP A0A7X0FIU8
G	60	ASN	ALA	conflict	UNP A0A7X0FIU8
G	93	MET	THR	conflict	UNP A0A7X0FIU8
G	104	GLU	ASP	conflict	UNP A0A7X0FIU8
G	140	THR	SER	conflict	UNP A0A7X0FIU8
G	215	LEU	ILE	conflict	UNP A0A7X0FIU8
H	60	ASN	ALA	conflict	UNP A0A7X0FIU8
H	93	MET	THR	conflict	UNP A0A7X0FIU8
H	104	GLU	ASP	conflict	UNP A0A7X0FIU8
H	140	THR	SER	conflict	UNP A0A7X0FIU8
H	215	LEU	ILE	conflict	UNP A0A7X0FIU8

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 2-hydroxy-3,5-dinitrobenzoic acid (CCD ID: A1BNY) (formula: $C_7H_4N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	7	2	7		
3	D	1	Total	C	N	O	0	0
			16	7	2	7		
3	F	1	Total	C	N	O	0	0
			16	7	2	7		
3	G	1	Total	C	N	O	0	0
			16	7	2	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	51	Total	O	0	0
			51	51		
4	C	35	Total	O	0	0
			35	35		
4	D	42	Total	O	0	0
			42	42		
4	E	35	Total	O	0	0
			35	35		
4	F	24	Total	O	0	1
			25	25		
4	G	23	Total	O	0	0
			23	23		
4	H	32	Total	O	0	0
			32	32		

3 Residue-property plots [i](#)


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: Expansin (Peptidoglycan-binding protein)

Chain A: 



- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain B: 



- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain C: 




- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain D: 




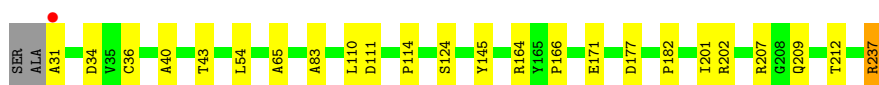
- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain E: 




- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain F:  88% 11% •




- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain G:  85% 12% ••



- Molecule 1: Expansin (Peptidoglycan-binding protein)

Chain H:  86% 12% •



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.21Å 47.88Å 201.44Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	90.11 – 2.30 90.11 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.9 (90.11-2.30) 99.0 (90.11-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419: ???)	Depositor
R, R_{free}	0.188 , 0.240 0.189 , 0.240	Depositor DCC
R_{free} test set	4473 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12995	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 51.18 % 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 5.8175e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: A1BNY, 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	0.35	0/1625	0.57	0/2218
1	B	0.42	0/1625	0.63	0/2218
1	C	0.38	0/1625	0.61	0/2218
1	D	0.37	0/1625	0.58	0/2218
1	E	0.32	0/1614	0.51	0/2203
1	F	0.38	0/1614	0.58	0/2203
1	G	0.36	0/1614	0.56	0/2203
1	H	0.35	0/1614	0.54	0/2203
All	All	0.37	0/12956	0.57	0/17684

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	G	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	237	ARG	Sidechain

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	1586	0	1546	14	0
1	B	1586	0	1546	15	0
1	C	1586	0	1546	11	0
1	D	1586	0	1546	8	0
1	E	1575	0	1536	11	0
1	F	1575	0	1536	12	0
1	G	1575	0	1536	13	0
1	H	1575	0	1536	14	0
2	A	8	0	12	0	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
2	G	4	0	6	0	0
2	H	4	0	6	0	0
3	A	16	0	0	2	0
3	D	16	0	0	2	0
3	F	16	0	0	2	0
3	G	16	0	0	1	0
4	A	20	0	0	0	0
4	B	51	0	0	0	0
4	C	35	0	0	0	0
4	D	42	0	0	0	0
4	E	35	0	0	0	0
4	F	25	0	0	0	0
4	G	23	0	0	0	0
4	H	32	0	0	1	0
All	All	12995	0	12364	102	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 (102) 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:40:ALA:HB2	1:C:130:ILE:HD13	1.64	0.79
1:A:40:ALA:HB2	1:A:130:ILE:HD13	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:ALA:HB2	1:G:166:PRO:HG3	1.82	0.61
1:B:91:ARG:HH22	1:B:122:ASP:HB2	1.67	0.59
3:A:303:A1BNY:O1	3:A:303:A1BNY:O6	2.21	0.58
1:E:117:PHE:HE1	1:E:123:THR:HA	1.70	0.57
1:F:31:ALA:HA	1:F:34:ASP:OD2	2.05	0.55
3:G:301:A1BNY:O1	3:G:301:A1BNY:O6	2.25	0.55
1:H:130:ILE:HD12	1:H:132:TRP:HD1	1.72	0.55
1:H:43:THR:O	1:H:114:PRO:HD3	2.06	0.54
1:B:32:TRP:CE2	1:B:207:ARG:HG2	2.43	0.54
1:D:146:ARG:HB3	1:D:159:GLN:HB3	1.89	0.53
1:B:65:ALA:HB3	1:B:111:ASP:HB3	1.90	0.53
3:D:302:A1BNY:O1	3:D:302:A1BNY:O6	2.26	0.53
1:H:83:ALA:HB2	1:H:166:PRO:HG3	1.91	0.52
1:C:91:ARG:NH2	1:C:122:ASP:HB2	2.25	0.51
1:E:40:ALA:HB2	1:E:130:ILE:HD13	1.92	0.51
1:A:91:ARG:NH2	1:A:122:ASP:HB2	2.26	0.51
1:G:68:PRO:HD3	1:G:102:TYR:O	2.11	0.50
3:F:301:A1BNY:O1	3:F:301:A1BNY:O3	2.28	0.50
1:A:62:THR:HB	1:A:116:ALA:HB2	1.93	0.50
1:B:83:ALA:HB2	1:B:166:PRO:HG3	1.94	0.50
1:C:65:ALA:HB3	1:C:111:ASP:HB3	1.93	0.49
1:F:171:GLU:OE1	1:F:202:ARG:HD2	2.11	0.49
1:B:40:ALA:HB2	1:B:130:ILE:HD13	1.94	0.49
1:G:62:THR:HB	1:G:116:ALA:HB2	1.94	0.49
1:D:53:LEU:HD12	1:D:188:HIS:CE1	2.48	0.48
1:G:78:ALA:HB1	1:G:81:ALA:HB2	1.95	0.48
1:E:117:PHE:CE1	1:E:123:THR:HA	2.48	0.48
1:F:65:ALA:HB3	1:F:111:ASP:HB3	1.96	0.48
1:G:36:CYS:O	1:G:131:ARG:HA	2.14	0.47
1:A:83:ALA:HB2	1:A:166:PRO:HG3	1.95	0.47
1:F:83:ALA:HB2	1:F:166:PRO:HG3	1.96	0.47
1:H:130:ILE:HD12	1:H:132:TRP:CD1	2.49	0.47
1:E:68:PRO:HG3	1:E:101:LEU:HD11	1.96	0.47
1:D:101:LEU:O	1:D:103:PRO:HD3	2.14	0.47
1:D:36:CYS:O	1:D:131:ARG:HA	2.15	0.47
1:G:169:LYS:HB3	1:G:204:THR:HB	1.97	0.47
1:H:199:LEU:HD11	4:H:404:HOH:O	2.15	0.47
1:A:223:ASP:OD1	1:A:223:ASP:N	2.48	0.46
1:A:91:ARG:HH22	1:A:122:ASP:HB2	1.81	0.46
1:G:43:THR:O	1:G:114:PRO:HD3	2.15	0.46
1:E:173:LYS:HB3	1:E:173:LYS:HE3	1.76	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ARG:NH2	1:F:209:GLN:HG3	2.31	0.46
1:B:91:ARG:O	1:B:91:ARG:HG3	2.16	0.46
1:C:215:LEU:HD12	1:C:216:GLY:H	1.80	0.46
1:H:171:GLU:HA	1:H:179:VAL:O	2.16	0.46
1:B:93:MET:HE3	1:B:93:MET:HB2	1.73	0.46
1:D:32:TRP:CE2	1:D:207:ARG:HG2	2.52	0.45
1:F:164:ARG:NH2	1:F:237:ARG:CZ	2.78	0.45
1:H:68:PRO:HD3	1:H:102:TYR:O	2.17	0.45
1:B:145:TYR:CZ	1:B:201:ILE:HD11	2.51	0.45
1:A:36:CYS:O	1:A:131:ARG:HA	2.18	0.44
1:H:101:LEU:O	1:H:103:PRO:HD3	2.17	0.44
1:A:227:TYR:CD1	1:G:182:PRO:HB3	2.53	0.44
3:A:303:A1BNY:O1	3:A:303:A1BNY:O3	2.31	0.44
1:F:54:LEU:HA	1:F:54:LEU:HD23	1.71	0.44
1:A:63:ILE:HG12	1:A:113:SER:HB3	1.98	0.44
1:E:83:ALA:HB2	1:E:166:PRO:HG3	2.01	0.43
1:E:97:TYR:O	1:E:99:THR:HG23	2.18	0.43
3:F:301:A1BNY:O1	3:F:301:A1BNY:O6	2.37	0.43
1:B:117:PHE:CE1	1:B:123:THR:HA	2.54	0.43
1:F:43:THR:O	1:F:114:PRO:HD3	2.18	0.43
1:E:183:LYS:HB2	1:E:189:PHE:CE1	2.54	0.43
1:C:227:TYR:CD1	1:F:182:PRO:HB3	2.54	0.42
3:D:302:A1BNY:O1	3:D:302:A1BNY:O3	2.37	0.42
1:B:164:ARG:HG2	1:B:165:TYR:CD2	2.54	0.42
1:E:101:LEU:O	1:E:103:PRO:HD3	2.19	0.42
1:B:42:TYR:HB3	1:B:117:PHE:CD2	2.54	0.42
1:B:183:LYS:HE3	1:B:189:PHE:CZ	2.54	0.42
1:G:42:TYR:HB3	1:G:117:PHE:CD2	2.54	0.42
1:C:122:ASP:OD1	1:C:124:SER:OG	2.33	0.42
1:A:32:TRP:CE2	1:A:207:ARG:HG2	2.55	0.42
1:C:145:TYR:CZ	1:C:201:ILE:HD11	2.55	0.42
1:H:117:PHE:HE1	1:H:123:THR:HA	1.84	0.42
1:B:43:THR:O	1:B:114:PRO:HD3	2.20	0.41
1:F:145:TYR:CZ	1:F:201:ILE:HD11	2.55	0.41
1:D:169:LYS:HB3	1:D:204:THR:HB	2.01	0.41
1:C:172:TYR:HE1	1:C:181:LEU:HD21	1.85	0.41
1:G:93:MET:HE2	1:G:93:MET:HB2	1.72	0.41
1:A:65:ALA:HB3	1:A:111:ASP:HB3	2.01	0.41
1:A:125:ALA:O	1:A:127:ARG:N	2.44	0.41
1:B:101:LEU:O	1:B:103:PRO:HD3	2.20	0.41
1:D:182:PRO:HB3	1:H:227:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:CD1	1:B:194:MET:HE3	2.56	0.41
1:E:223:ASP:OD1	1:E:224:LYS:NZ	2.46	0.41
1:C:78:ALA:HB1	1:C:81:ALA:HB2	2.03	0.41
1:G:101:LEU:O	1:G:103:PRO:HD3	2.21	0.41
1:H:62:THR:HB	1:H:116:ALA:HB2	2.02	0.41
1:A:115:ASN:OD1	1:A:115:ASN:N	2.53	0.41
1:C:139:VAL:HG21	1:C:164:ARG:HB2	2.03	0.41
1:E:145:TYR:CZ	1:E:201:ILE:HD11	2.55	0.41
1:H:67:ASN:OD1	1:H:69:LYS:HB3	2.21	0.41
1:H:172:TYR:CE2	1:H:174:LYS:HB2	2.56	0.41
1:D:130:ILE:HD12	1:D:132:TRP:HD1	1.87	0.40
1:F:40:ALA:HA	1:F:110:LEU:O	2.21	0.40
1:G:215:LEU:HD12	1:G:216:GLY:H	1.85	0.40
1:A:149:GLU:HB2	1:A:225:GLY:HA2	2.03	0.40
1:F:164:ARG:NE	1:F:237:ARG:HG3	2.36	0.40
1:C:36:CYS:O	1:C:131:ARG:HA	2.20	0.40
1:G:215:LEU:HD12	1:G:216:GLY:N	2.36	0.40
1:H:171:GLU:OE1	1:H:202:ARG:HD2	2.21	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	207/209 (99%)	202 (98%)	4 (2%)	1 (0%)	25	32
1	B	207/209 (99%)	204 (99%)	3 (1%)	0	100	100
1	C	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
1	D	207/209 (99%)	204 (99%)	3 (1%)	0	100	100
1	E	205/209 (98%)	199 (97%)	5 (2%)	1 (0%)	25	32
1	F	205/209 (98%)	200 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	205/209 (98%)	199 (97%)	6 (3%)	0	100	100
1	H	205/209 (98%)	199 (97%)	6 (3%)	0	100	100
All	All	1648/1672 (99%)	1608 (98%)	38 (2%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	175	ASN
1	A	126	GLY

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	163/163 (100%)	161 (99%)	2 (1%)	67	81
1	B	163/163 (100%)	159 (98%)	4 (2%)	42	60
1	C	163/163 (100%)	156 (96%)	7 (4%)	25	36
1	D	163/163 (100%)	157 (96%)	6 (4%)	29	43
1	E	162/163 (99%)	158 (98%)	4 (2%)	42	60
1	F	162/163 (99%)	157 (97%)	5 (3%)	35	51
1	G	162/163 (99%)	153 (94%)	9 (6%)	17	26
1	H	162/163 (99%)	157 (97%)	5 (3%)	35	51
All	All	1300/1304 (100%)	1258 (97%)	42 (3%)	34	50

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	36	CYS
1	B	29	SER
1	B	36	CYS
1	B	161	ARG

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Mol	Chain	Res	Type
1	B	212	THR
1	C	34	ASP
1	C	36	CYS
1	C	37	SER
1	C	161	ARG
1	C	174	LYS
1	C	193	GLN
1	C	212	THR
1	D	34	ASP
1	D	36	CYS
1	D	64	THR
1	D	124	SER
1	D	130	ILE
1	D	215	LEU
1	E	36	CYS
1	E	80	LEU
1	E	123	THR
1	E	193	GLN
1	F	36	CYS
1	F	124	SER
1	F	177	ASP
1	F	212	THR
1	F	237	ARG
1	G	36	CYS
1	G	88	GLN
1	G	101	LEU
1	G	123	THR
1	G	140	THR
1	G	177	ASP
1	G	212	THR
1	G	220	SER
1	G	237	ARG
1	H	36	CYS
1	H	44	SER
1	H	48	SER
1	H	177	ASP
1	H	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	175	ASN
1	A	221	GLN
1	B	142	ASN
1	C	193	GLN
1	D	142	ASN
1	E	88	GLN
1	F	209	GLN
1	G	77	GLN
1	G	175	ASN
1	H	77	GLN
1	H	133	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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
2	EDO	G	302	-	3,3,3	0.26	0	2,2,2	0.63	0
3	A1BNY	G	301	-	16,16,16	4.81	5 (31%)	17,23,23	1.96	4 (23%)
2	EDO	D	301	-	3,3,3	0.27	0	2,2,2	0.41	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	301	-	3,3,3	0.26	0	2,2,2	0.22	0
3	A1BNY	F	301	-	16,16,16	4.68	6 (37%)	17,23,23	2.86	6 (35%)
3	A1BNY	A	303	-	16,16,16	5.00	5 (31%)	17,23,23	1.92	4 (23%)
2	EDO	A	302	-	3,3,3	0.28	0	2,2,2	0.16	0
2	EDO	H	301	-	3,3,3	0.34	0	2,2,2	0.14	0
3	A1BNY	D	302	-	16,16,16	5.92	5 (31%)	17,23,23	1.59	3 (17%)
2	EDO	C	301	-	3,3,3	0.27	0	2,2,2	0.28	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
2	EDO	G	302	-	-	0/1/1/1	-
3	A1BNY	G	301	-	-	0/8/12/12	0/1/1/1
2	EDO	D	301	-	-	1/1/1/1	-
2	EDO	A	301	-	-	1/1/1/1	-
3	A1BNY	F	301	-	-	0/8/12/12	0/1/1/1
3	A1BNY	A	303	-	-	0/8/12/12	0/1/1/1
2	EDO	A	302	-	-	0/1/1/1	-
2	EDO	H	301	-	-	0/1/1/1	-
3	A1BNY	D	302	-	-	0/8/12/12	0/1/1/1
2	EDO	C	301	-	-	0/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	A1BNY	O5-N1	17.33	1.52	1.22
3	D	302	A1BNY	O6-N2	13.32	1.45	1.22
3	G	301	A1BNY	O6-N2	13.01	1.45	1.22
3	A	303	A1BNY	O6-N2	12.35	1.44	1.22
3	F	301	A1BNY	O6-N2	11.83	1.43	1.22
3	A	303	A1BNY	O5-N1	11.82	1.43	1.22
3	F	301	A1BNY	O5-N1	10.24	1.40	1.22
3	G	301	A1BNY	O5-N1	9.90	1.39	1.22
3	A	303	A1BNY	C4-N2	-6.46	1.33	1.45
3	G	301	A1BNY	C4-N2	-6.10	1.34	1.45
3	D	302	A1BNY	C4-N2	-6.03	1.34	1.45
3	F	301	A1BNY	C4-N2	-5.96	1.34	1.45
3	G	301	A1BNY	C6-N1	-5.54	1.32	1.45
3	F	301	A1BNY	C6-N1	-5.54	1.32	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	301	A1BNY	C2-C1	-5.39	1.38	1.49
3	A	303	A1BNY	C2-C1	-5.38	1.38	1.49
3	A	303	A1BNY	C6-N1	-5.09	1.33	1.45
3	G	301	A1BNY	C2-C1	-5.05	1.38	1.49
3	D	302	A1BNY	C2-C1	-4.41	1.40	1.49
3	D	302	A1BNY	C6-N1	-4.34	1.34	1.45
3	F	301	A1BNY	C2-C3	-2.18	1.38	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	301	A1BNY	C5-C6-N1	7.07	124.83	118.74
3	F	301	A1BNY	C7-C6-N1	-6.62	113.03	118.74
3	A	303	A1BNY	C5-C6-N1	4.47	122.59	118.74
3	D	302	A1BNY	C2-C3-C4	4.14	122.28	117.29
3	G	301	A1BNY	C2-C3-C4	4.11	122.25	117.29
3	G	301	A1BNY	C5-C6-N1	4.00	122.18	118.74
3	F	301	A1BNY	C2-C3-C4	3.94	122.03	117.29
3	A	303	A1BNY	C2-C3-C4	3.73	121.79	117.29
3	G	301	A1BNY	C7-C6-N1	-3.40	115.81	118.74
3	A	303	A1BNY	C7-C6-N1	-3.32	115.88	118.74
3	F	301	A1BNY	C5-C4-C3	-2.96	118.53	121.54
3	F	301	A1BNY	O1-C3-C2	-2.67	116.36	121.11
3	G	301	A1BNY	C5-C4-C3	-2.63	118.87	121.54
3	D	302	A1BNY	C5-C4-C3	-2.62	118.88	121.54
3	D	302	A1BNY	C5-C6-N1	2.48	120.88	118.74
3	F	301	A1BNY	O5-N1-C6	-2.46	115.43	118.82
3	A	303	A1BNY	C5-C4-C3	-2.33	119.17	121.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	301	EDO	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	301	A1BNY	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	A1BNY	2	0
3	A	303	A1BNY	2	0
3	D	302	A1BNY	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	209/209 (100%)	-0.07	0 100 100	35, 44, 63, 77	0
1	B	209/209 (100%)	-0.26	0 100 100	33, 39, 55, 71	0
1	C	209/209 (100%)	-0.17	1 (0%) 87 88	32, 42, 61, 71	0
1	D	209/209 (100%)	-0.17	0 100 100	34, 42, 56, 80	0
1	E	207/209 (99%)	0.08	2 (0%) 79 79	38, 49, 74, 90	0
1	F	207/209 (99%)	-0.03	1 (0%) 87 88	36, 45, 64, 82	0
1	G	207/209 (99%)	0.10	2 (0%) 79 79	37, 47, 72, 89	0
1	H	207/209 (99%)	0.07	3 (1%) 73 74	36, 46, 67, 88	0
All	All	1664/1672 (99%)	-0.06	9 (0%) 87 88	32, 45, 66, 90	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	31	ALA	5.0
1	E	31	ALA	3.5
1	H	32	TRP	3.5
1	G	32	TRP	3.4
1	G	31	ALA	3.3
1	H	33	ASN	2.8
1	F	31	ALA	2.6
1	E	32	TRP	2.1
1	C	139	VAL	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 [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	A	301	4/4	0.80	0.17	51,57,60,63	0
3	A1BNY	D	302	16/16	0.88	0.10	46,49,56,56	0
3	A1BNY	G	301	16/16	0.88	0.11	48,51,56,61	0
3	A1BNY	F	301	16/16	0.89	0.11	42,47,53,58	0
2	EDO	H	301	4/4	0.90	0.18	44,45,46,47	0
2	EDO	D	301	4/4	0.91	0.10	47,47,50,58	0
2	EDO	G	302	4/4	0.91	0.11	51,54,55,55	0
3	A1BNY	A	303	16/16	0.92	0.09	45,49,53,53	0
2	EDO	C	301	4/4	0.93	0.10	44,47,48,48	0
2	EDO	A	302	4/4	0.94	0.10	47,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.