



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:49 AM UTC

PDB ID : 3QWN / pdb_00003qwn
Title : Crystal structure of a NigD-like immunity protein (BACCAC_03262) from *Bacteroides caccae* ATCC 43185 at 2.42 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2011-02-28
Resolution : 2.42 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 Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

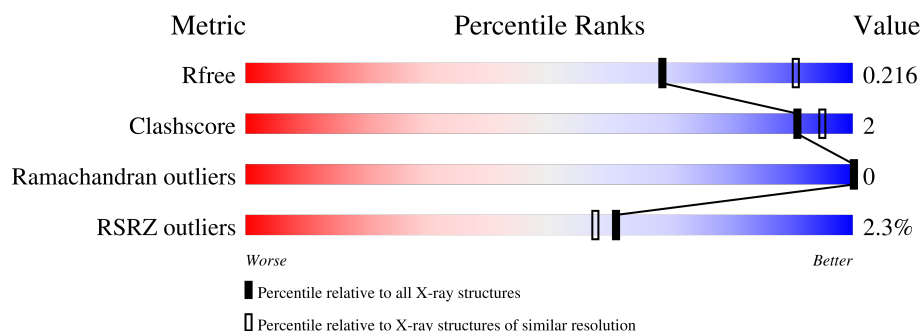
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	214	2% 93% 8% 5%
1	B	214	2% 88% 8% 5%
1	C	214	% 89% 6% 5%
1	D	214	% 91% 5%
1	E	214	3% 92% 5%
1	F	214	% 92% 5%

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Mol	Chain	Length	Quality of chain
1	G	214	2% 93% • •
1	H	214	5% 90% 7% •
1	I	214	3% 90% 6% •
1	J	214	2% 93% 5% •
1	K	214	2% 91% • 5%
1	L	214	2% 90% 5% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20253 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 Hypothetical nigD-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	Se	0	0	0
			1585	1000	264	317	1	3			
1	B	207	Total	C	N	O	S	Se	0	0	0
			1606	1015	262	325	1	3			
1	C	203	Total	C	N	O	S	Se	0	0	0
			1572	991	261	316	1	3			
1	D	204	Total	C	N	O	S	Se	0	1	0
			1578	995	264	315	1	3			
1	E	205	Total	C	N	O	S	Se	0	0	0
			1574	994	260	316	1	3			
1	F	205	Total	C	N	O	S	Se	0	0	0
			1580	996	262	318	1	3			
1	G	207	Total	C	N	O	S	Se	0	0	0
			1595	1010	261	320	1	3			
1	H	206	Total	C	N	O	S	Se	0	1	0
			1576	991	263	318	1	3			
1	I	205	Total	C	N	O	S	Se	0	0	0
			1576	996	259	317	1	3			
1	J	208	Total	C	N	O	S	Se	0	0	0
			1598	1010	262	322	1	3			
1	K	204	Total	C	N	O	S	Se	0	0	0
			1577	995	260	318	1	3			
1	L	203	Total	C	N	O	S	Se	0	0	0
			1561	987	255	315	1	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A5ZK25
B	0	GLY	-	expression tag	UNP A5ZK25
C	0	GLY	-	expression tag	UNP A5ZK25
D	0	GLY	-	expression tag	UNP A5ZK25
E	0	GLY	-	expression tag	UNP A5ZK25

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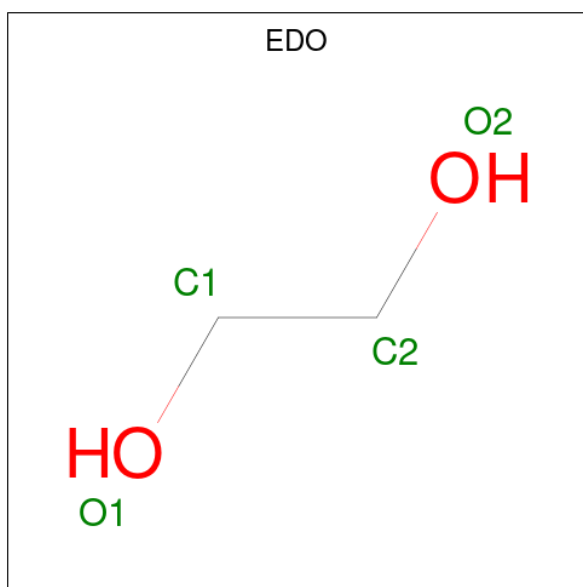
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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	GLY	-	expression tag	UNP A5ZK25
G	0	GLY	-	expression tag	UNP A5ZK25
H	0	GLY	-	expression tag	UNP A5ZK25
I	0	GLY	-	expression tag	UNP A5ZK25
J	0	GLY	-	expression tag	UNP A5ZK25
K	0	GLY	-	expression tag	UNP A5ZK25
L	0	GLY	-	expression tag	UNP A5ZK25

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cl 4 4	0	0
2	B	4	Total Cl 4 4	0	0
2	C	2	Total Cl 2 2	0	0
2	D	6	Total Cl 6 6	0	0
2	E	5	Total Cl 5 5	0	0
2	F	2	Total Cl 2 2	0	0
2	G	5	Total Cl 5 5	0	0
2	H	2	Total Cl 2 2	0	0
2	I	3	Total Cl 3 3	0	0
2	J	3	Total Cl 3 3	0	0
2	K	3	Total Cl 3 3	0	0
2	L	2	Total Cl 2 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	110	Total	O	0	0
			110	110		
4	C	148	Total	O	0	0
			148	148		
4	D	153	Total	O	0	0
			153	153		
4	E	67	Total	O	0	0
			67	67		
4	F	81	Total	O	0	0
			81	81		
4	G	100	Total	O	0	0
			100	100		
4	H	73	Total	O	0	0
			73	73		
4	I	104	Total	O	0	0
			104	104		

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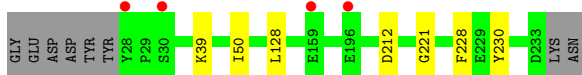
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	80	Total 80	O 80	0	0
4	K	105	Total 105	O 105	0	0
4	L	103	Total 103	O 103	0	0

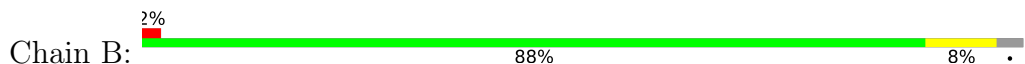
3 Residue-property plots [i](#)

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.

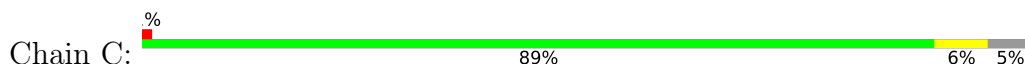
- Molecule 1: Hypothetical nigD-like protein



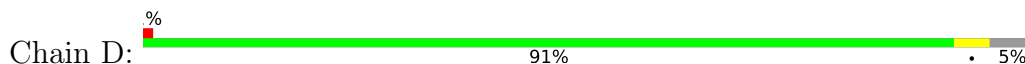
- Molecule 1: Hypothetical nigD-like protein



- Molecule 1: Hypothetical nigD-like protein



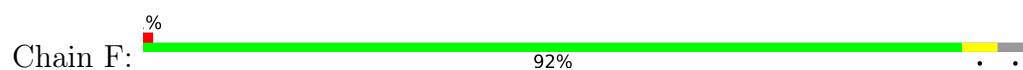
- Molecule 1: Hypothetical nigD-like protein



- Molecule 1: Hypothetical nigD-like protein



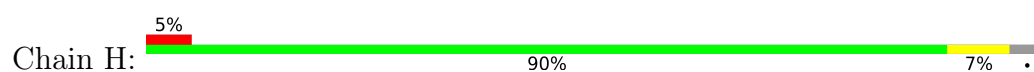
- Molecule 1: Hypothetical nigD-like protein



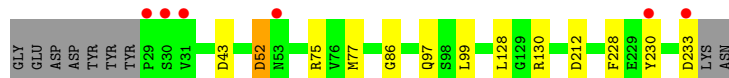
- Molecule 1: Hypothetical nigD-like protein



- Molecule 1: Hypothetical nigD-like protein



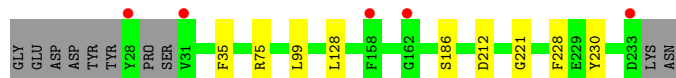
- Molecule 1: Hypothetical nigD-like protein



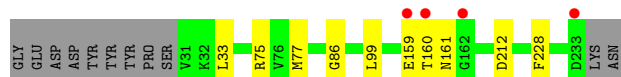
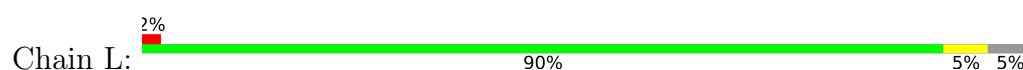
- Molecule 1: Hypothetical nigD-like protein



- Molecule 1: Hypothetical nigD-like protein



- Molecule 1: Hypothetical nigD-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	132.31Å 132.31Å 163.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.71 – 2.42 29.71 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (29.71-2.42) 99.9 (29.71-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.42Å)	Xtriage
Refinement program	BUSTER-TNT 2.8.0, BUSTER 2.8.0	Depositor
R, R_{free}	0.175 , 0.213 (Not available) , 0.216	Depositor DCC
R_{free} test set	6123 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.038 for h,-h-k,-l 0.120 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20253	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.05% 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: CL, 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	0.81	0/1618	1.08	3/2201 (0.1%)
1	B	0.83	0/1641	1.06	1/2233 (0.0%)
1	C	0.95	1/1604 (0.1%)	1.14	5/2180 (0.2%)
1	D	0.92	1/1613 (0.1%)	1.06	1/2193 (0.0%)
1	E	0.75	0/1607	1.06	3/2186 (0.1%)
1	F	0.77	0/1613	1.05	3/2194 (0.1%)
1	G	0.83	0/1628	1.08	5/2214 (0.2%)
1	H	0.81	1/1608 (0.1%)	1.08	6/2191 (0.3%)
1	I	0.80	0/1609	1.07	4/2188 (0.2%)
1	J	0.78	0/1632	1.05	1/2222 (0.0%)
1	K	0.82	1/1609 (0.1%)	1.05	4/2188 (0.2%)
1	L	0.84	0/1593	1.07	3/2166 (0.1%)
All	All	0.83	4/19375 (0.0%)	1.07	39/26356 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	204	ILE	CG1-CD1	-5.68	1.29	1.51
1	C	151	ILE	CG1-CD1	5.39	1.72	1.51
1	H	50	ILE	CA-C	5.31	1.58	1.52
1	K	186	SER	CA-C	-5.09	1.47	1.53

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	ASP	CA-CB-CG	6.01	118.61	112.60
1	H	29	PRO	CA-C-N	5.97	128.28	120.28
1	H	29	PRO	C-N-CA	5.97	128.28	120.28
1	C	212	ASP	CA-CB-CG	5.93	118.53	112.60
1	A	212	ASP	CA-CB-CG	5.81	118.41	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	221	GLY	CA-C-N	5.74	128.25	120.38
1	C	221	GLY	C-N-CA	5.74	128.25	120.38
1	G	221	GLY	CA-C-N	5.72	128.22	120.38
1	G	221	GLY	C-N-CA	5.72	128.22	120.38
1	H	212	ASP	CA-CB-CG	5.71	118.31	112.60
1	I	233	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	212	ASP	CA-CB-CG	5.69	118.29	112.60
1	L	212	ASP	CA-CB-CG	5.62	118.22	112.60
1	K	35	PHE	CA-CB-CG	5.62	119.42	113.80
1	E	212	ASP	CA-CB-CG	5.61	118.21	112.60
1	G	25	ASP	CA-C-N	5.60	129.65	121.31
1	G	25	ASP	C-N-CA	5.60	129.65	121.31
1	I	43	ASP	CA-CB-CG	5.57	118.17	112.60
1	K	221	GLY	CA-C-N	5.52	127.94	120.38
1	K	221	GLY	C-N-CA	5.52	127.94	120.38
1	I	52	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	221	GLY	CA-C-N	5.42	127.80	120.38
1	A	221	GLY	C-N-CA	5.42	127.80	120.38
1	G	212	ASP	CA-CB-CG	5.41	118.01	112.60
1	F	212	ASP	CA-CB-CG	5.40	118.00	112.60
1	J	212	ASP	CA-CB-CG	5.36	117.96	112.60
1	L	159	GLU	CA-C-N	5.36	127.73	120.44
1	L	159	GLU	C-N-CA	5.36	127.73	120.44
1	D	212	ASP	CA-CB-CG	5.31	117.91	112.60
1	H	29	PRO	N-CA-C	5.31	119.43	111.14
1	I	212	ASP	CA-CB-CG	5.27	117.87	112.60
1	H	221	GLY	CA-C-N	5.17	127.46	120.38
1	H	221	GLY	C-N-CA	5.17	127.46	120.38
1	F	221	GLY	CA-C-N	5.16	127.44	120.38
1	F	221	GLY	C-N-CA	5.16	127.44	120.38
1	K	212	ASP	CA-CB-CG	5.16	117.76	112.60
1	E	221	GLY	CA-C-N	5.12	127.40	120.38
1	E	221	GLY	C-N-CA	5.12	127.40	120.38
1	C	35	PHE	CA-CB-CG	5.09	118.89	113.80

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	1585	0	1513	4	0
1	B	1606	0	1527	16	0
1	C	1572	0	1506	6	0
1	D	1578	0	1508	6	0
1	E	1574	0	1501	3	0
1	F	1580	0	1505	6	0
1	G	1595	0	1507	5	0
1	H	1576	0	1485	11	0
1	I	1576	0	1503	8	0
1	J	1598	0	1510	7	0
1	K	1577	0	1494	3	0
1	L	1561	0	1487	7	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	2	0	0	0	0
2	D	6	0	0	0	0
2	E	5	0	0	0	0
2	F	2	0	0	0	0
2	G	5	0	0	0	0
2	H	2	0	0	0	0
2	I	3	0	0	0	0
2	J	3	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
3	D	4	0	6	0	0
3	I	4	0	6	0	0
3	L	4	0	6	0	0
4	A	98	0	0	0	0
4	B	110	0	0	0	0
4	C	148	0	0	1	0
4	D	153	0	0	1	0
4	E	67	0	0	1	0
4	F	81	0	0	0	0
4	G	100	0	0	1	0
4	H	73	0	0	0	0
4	I	104	0	0	0	0
4	J	80	0	0	0	0
4	K	105	0	0	0	0
4	L	103	0	0	0	0
All	All	20253	0	18064	64	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 2.

All (64) 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:B:195:ALA:HB2	1:H:225:ASN:HB3	1.49	0.94
1:A:228:PHE:HE1	1:D:86:GLY:HA3	1.41	0.83
1:B:130:ARG:HH22	1:H:160:THR:HG21	1.44	0.82
1:F:228:PHE:HE1	1:G:86:GLY:HA3	1.49	0.77
1:B:52:ASP:HA	1:B:130:ARG:HD2	1.65	0.77
1:A:228:PHE:CE1	1:D:86:GLY:HA3	2.22	0.74
1:C:47:GLN:HG2	4:C:476:HOH:O	1.88	0.73
1:J:27:TYR:HE2	1:J:182:ARG:HG3	1.52	0.72
1:F:228:PHE:CE1	1:G:86:GLY:HA3	2.27	0.69
1:I:228:PHE:HE1	1:L:86:GLY:HA3	1.59	0.66
1:J:75:ARG:HG3	1:J:99:LEU:HD11	1.80	0.63
1:D:202:ILE:HD12	1:D:232:PRO:HG3	1.81	0.62
1:D:75:ARG:HG3	1:D:99:LEU:HD11	1.81	0.61
1:A:39:LYS:HE3	1:A:50:ILE:HD11	1.83	0.60
1:L:75:ARG:HG3	1:L:99:LEU:HD11	1.84	0.60
1:I:75:ARG:HG2	1:I:99:LEU:HD11	1.83	0.60
1:I:228:PHE:CE1	1:L:86:GLY:HA3	2.38	0.58
1:G:75:ARG:HG3	1:G:99:LEU:HD11	1.85	0.57
1:B:75:ARG:HG3	1:B:99:LEU:HD11	1.87	0.56
1:B:52:ASP:HA	1:B:130:ARG:CD	2.35	0.56
1:J:27:TYR:CE2	1:J:182:ARG:HG3	2.36	0.56
1:G:128:LEU:HD13	1:G:230:TYR:HB3	1.88	0.55
1:H:75:ARG:HG3	1:H:99:LEU:HD11	1.91	0.53
1:K:75:ARG:HG3	1:K:99:LEU:HD11	1.91	0.52
1:I:86:GLY:HA3	1:L:228:PHE:CE1	2.46	0.51
1:J:86:GLY:HA3	1:K:228:PHE:CE1	2.45	0.51
1:C:146:GLN:HB2	1:D:146:GLN:HB2	1.94	0.50
1:L:33:LEU:HB3	1:L:77:MSE:HE3	1.94	0.50
1:B:27:TYR:CE2	1:B:182:ARG:HG3	2.48	0.49
1:F:56:ALA:HB2	1:L:160:THR:HG23	1.95	0.48
1:I:52:ASP:HA	1:I:130:ARG:HD2	1.95	0.48
1:B:78:SER:HB2	1:B:96:LEU:HD23	1.95	0.48
1:B:130:ARG:HH22	1:H:160:THR:CG2	2.21	0.48
1:B:42:THR:HG23	1:H:197:ASN:ND2	2.29	0.47
1:C:194:ASP:HB3	1:C:197:ASN:HB2	1.96	0.47
1:D:47:GLN:HG2	4:D:562:HOH:O	2.13	0.47
1:H:128:LEU:HD13	1:H:230:TYR:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:LYS:HE2	1:J:63:ARG:HE	1.80	0.47
1:K:128:LEU:HD13	1:K:230:TYR:HB3	1.96	0.47
1:F:39:LYS:CE	1:L:161:ASN:HA	2.45	0.46
1:B:42:THR:CG2	1:H:197:ASN:HA	2.46	0.46
1:H:77:MSE:SE	1:H:99:LEU:HD23	2.66	0.46
1:B:86:GLY:HA3	1:C:228:PHE:CE1	2.51	0.45
1:E:128:LEU:HD13	1:E:230:TYR:HB3	1.97	0.45
1:B:42:THR:HG21	1:H:197:ASN:HA	1.98	0.45
1:F:128:LEU:HD13	1:F:230:TYR:HB3	2.00	0.44
1:B:132:TYR:CD1	1:B:186:SER:HB3	2.53	0.44
1:I:128:LEU:HD13	1:I:230:TYR:HB3	2.01	0.43
1:E:145:LYS:HG2	1:E:173:ASN:O	2.19	0.43
1:E:75:ARG:HG3	1:E:99:LEU:HD11	2.01	0.42
1:H:194:ASP:HB3	1:H:197:ASN:HB3	2.02	0.42
1:I:77:MSE:HB2	1:I:97:GLN:HG2	2.02	0.42
1:A:128:LEU:HD13	1:A:230:TYR:HB3	2.01	0.42
1:J:128:LEU:HD13	1:J:230:TYR:HB3	2.02	0.42
1:G:55:GLU:HB2	4:G:1108:HOH:O	2.19	0.42
4:E:1369:HOH:O	1:H:87:HIS:HE1	2.02	0.42
1:C:131:GLY:HA2	1:C:230:TYR:OH	2.20	0.41
1:B:145:LYS:HG2	1:B:173:ASN:O	2.21	0.41
1:C:99:LEU:C	1:C:99:LEU:HD12	2.46	0.41
1:J:61:LYS:HE2	1:J:63:ARG:NE	2.35	0.41
1:B:225:ASN:HA	1:B:226:PRO:HA	1.97	0.41
1:B:27:TYR:HE2	1:B:182:ARG:HG3	1.86	0.40
1:F:75:ARG:HG3	1:F:99:LEU:HD11	2.03	0.40
1:I:77:MSE:HB2	1:I:97:GLN:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/214 (95%)	198 (97%)	6 (3%)	0	100	100
1	B	205/214 (96%)	197 (96%)	8 (4%)	0	100	100
1	C	201/214 (94%)	193 (96%)	8 (4%)	0	100	100
1	D	203/214 (95%)	198 (98%)	5 (2%)	0	100	100
1	E	203/214 (95%)	197 (97%)	6 (3%)	0	100	100
1	F	203/214 (95%)	197 (97%)	6 (3%)	0	100	100
1	G	203/214 (95%)	196 (97%)	7 (3%)	0	100	100
1	H	205/214 (96%)	197 (96%)	8 (4%)	0	100	100
1	I	203/214 (95%)	194 (96%)	9 (4%)	0	100	100
1	J	206/214 (96%)	200 (97%)	6 (3%)	0	100	100
1	K	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
1	L	201/214 (94%)	196 (98%)	5 (2%)	0	100	100
All	All	2438/2568 (95%)	2359 (97%)	79 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 44 ligands modelled in this entry, 41 are monoatomic - leaving 3 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	I	277	-	3,3,3	0.48	0	2,2,2	0.22	0
3	EDO	D	278	-	3,3,3	0.36	0	2,2,2	0.50	0
3	EDO	L	279	-	3,3,3	0.58	0	2,2,2	0.14	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	I	277	-	-	1/1/1/1	-
3	EDO	D	278	-	-	1/1/1/1	-
3	EDO	L	279	-	-	1/1/1/1	-

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
3	I	277	EDO	O1-C1-C2-O2
3	L	279	EDO	O1-C1-C2-O2
3	D	278	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

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	203/214 (94%)	-0.20	4 (1%) 65 61	31, 54, 111, 142	0
1	B	204/214 (95%)	-0.31	4 (1%) 65 61	31, 50, 89, 121	0
1	C	200/214 (93%)	-0.48	2 (1%) 79 77	26, 41, 83, 111	0
1	D	201/214 (93%)	-0.60	2 (0%) 79 77	23, 40, 72, 119	1 (0%)
1	E	202/214 (94%)	-0.02	6 (2%) 52 49	45, 63, 110, 142	0
1	F	202/214 (94%)	-0.17	3 (1%) 72 69	37, 58, 101, 145	0
1	G	204/214 (95%)	-0.16	5 (2%) 58 55	36, 56, 89, 137	0
1	H	203/214 (94%)	0.17	10 (4%) 35 31	36, 64, 118, 167	1 (0%)
1	I	202/214 (94%)	-0.21	6 (2%) 52 49	38, 57, 94, 113	0
1	J	205/214 (95%)	-0.11	5 (2%) 59 56	36, 58, 108, 138	0
1	K	201/214 (93%)	-0.26	5 (2%) 58 55	33, 50, 95, 143	0
1	L	200/214 (93%)	-0.21	4 (2%) 65 61	33, 52, 111, 152	0
All	All	2427/2568 (94%)	-0.21	56 (2%) 61 57	23, 55, 103, 167	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	28	TYR	5.8
1	H	162	GLY	3.6
1	K	233	ASP	3.4
1	B	27	TYR	3.4
1	J	26	TYR	3.3
1	G	233	ASP	3.3
1	G	27	TYR	3.0
1	D	30	SER	2.9
1	J	31	VAL	2.9
1	E	53	ASN	2.9
1	L	160	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	L	233	ASP	2.8
1	K	158	PHE	2.8
1	B	230	TYR	2.7
1	F	233	ASP	2.7
1	H	29	PRO	2.7
1	H	159	GLU	2.7
1	H	161	ASN	2.6
1	E	233	ASP	2.6
1	G	25	ASP	2.6
1	I	31	VAL	2.6
1	G	30	SER	2.6
1	E	31	VAL	2.5
1	C	201	LYS	2.5
1	E	230	TYR	2.5
1	I	230	TYR	2.5
1	I	233	ASP	2.5
1	H	30	SER	2.5
1	F	31	VAL	2.5
1	A	30	SER	2.5
1	B	233	ASP	2.4
1	C	233	ASP	2.4
1	H	158	PHE	2.4
1	B	53	ASN	2.4
1	A	159	GLU	2.4
1	H	233	ASP	2.3
1	A	28	TYR	2.3
1	K	162	GLY	2.3
1	G	26	TYR	2.3
1	L	162	GLY	2.3
1	F	30	SER	2.3
1	A	196	GLU	2.3
1	E	196	GLU	2.2
1	D	233	ASP	2.2
1	I	53	ASN	2.1
1	E	30	SER	2.1
1	K	31	VAL	2.1
1	J	195	ALA	2.1
1	J	30	SER	2.1
1	I	29	PRO	2.1
1	H	31	VAL	2.1
1	H	111	THR	2.1
1	I	30	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	27	TYR	2.0
1	K	28	TYR	2.0
1	L	159	GLU	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](#)

There are no oligosaccharides 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	CL	E	275	1/1	0.85	0.13	92,92,92,92	0
2	CL	A	238	1/1	0.86	0.15	81,81,81,81	0
3	EDO	L	279	4/4	0.86	0.13	53,56,57,59	0
2	CL	L	246	1/1	0.87	0.14	78,78,78,78	0
2	CL	D	276	1/1	0.88	0.11	94,94,94,94	0
2	CL	A	241	1/1	0.89	0.11	65,65,65,65	0
2	CL	G	244	1/1	0.90	0.12	84,84,84,84	0
2	CL	J	247	1/1	0.90	0.10	73,73,73,73	0
2	CL	B	240	1/1	0.90	0.10	60,60,60,60	0
2	CL	D	249	1/1	0.90	0.14	73,73,73,73	0
2	CL	E	245	1/1	0.91	0.11	71,71,71,71	0
2	CL	G	243	1/1	0.91	0.11	76,76,76,76	0
2	CL	J	236	1/1	0.92	0.12	65,65,65,65	0
2	CL	F	266	1/1	0.92	0.10	87,87,87,87	0
2	CL	E	253	1/1	0.92	0.10	71,71,71,71	0
3	EDO	I	277	4/4	0.92	0.10	54,55,60,65	0
2	CL	B	239	1/1	0.92	0.11	71,71,71,71	0
2	CL	I	256	1/1	0.93	0.09	69,69,69,69	0
2	CL	D	272	1/1	0.93	0.09	67,67,67,67	0
2	CL	G	274	1/1	0.93	0.11	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	D	261	1/1	0.94	0.11	73,73,73,73	0
2	CL	C	259	1/1	0.94	0.14	67,67,67,67	0
2	CL	G	260	1/1	0.94	0.12	74,74,74,74	0
2	CL	B	251	1/1	0.94	0.08	63,63,63,63	0
2	CL	E	242	1/1	0.94	0.08	73,73,73,73	0
2	CL	A	250	1/1	0.95	0.08	66,66,66,66	0
2	CL	I	269	1/1	0.95	0.08	78,78,78,78	0
2	CL	D	252	1/1	0.95	0.09	63,63,63,63	0
2	CL	G	267	1/1	0.95	0.09	75,75,75,75	0
2	CL	K	257	1/1	0.95	0.08	76,76,76,76	0
2	CL	K	270	1/1	0.95	0.08	85,85,85,85	0
2	CL	E	265	1/1	0.95	0.14	75,75,75,75	0
2	CL	L	258	1/1	0.95	0.09	71,71,71,71	0
3	EDO	D	278	4/4	0.95	0.07	45,47,49,54	0
2	CL	H	268	1/1	0.95	0.09	82,82,82,82	0
2	CL	I	237	1/1	0.95	0.11	64,64,64,64	0
2	CL	B	263	1/1	0.96	0.10	78,78,78,78	0
2	CL	F	254	1/1	0.96	0.08	70,70,70,70	0
2	CL	H	255	1/1	0.96	0.12	72,72,72,72	0
2	CL	D	271	1/1	0.96	0.07	65,65,65,65	0
2	CL	K	273	1/1	0.97	0.06	68,68,68,68	0
2	CL	A	262	1/1	0.97	0.07	73,73,73,73	0
2	CL	J	248	1/1	0.97	0.07	57,57,57,57	0
2	CL	C	264	1/1	0.98	0.05	65,65,65,65	0

6.5 Other polymers

There are no such residues in this entry.