



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:54 PM UTC

PDB ID : 4ZGH / pdb_00004zgh
Title : Structure of Sugar Binding Protein Pneumolysin
Authors : Parker, M.W.; Feil, S.C.; Morton, C.
Deposited on : 2015-04-23
Resolution : 2.90 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

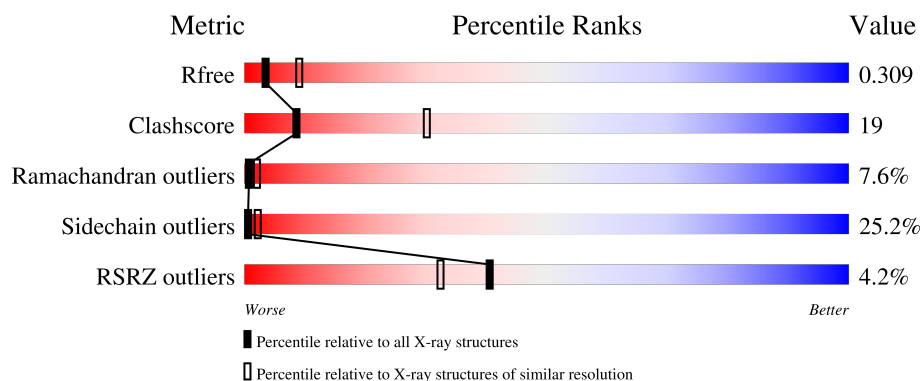
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	477	 4% 47% 38% 13% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7542 atoms, of which 3730 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 Pneumolysin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	473	Total	C	H	N	O	S	0	0	0
			7424	2359	3680	639	740	6			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP Q04IN8
A	-5	HIS	-	expression tag	UNP Q04IN8
A	-4	HIS	-	expression tag	UNP Q04IN8
A	-3	HIS	-	expression tag	UNP Q04IN8
A	-2	HIS	-	expression tag	UNP Q04IN8
A	-1	HIS	-	expression tag	UNP Q04IN8
A	0	GLY	-	expression tag	UNP Q04IN8
A	1	SER	-	expression tag	UNP Q04IN8
A	56	SER	ASN	engineered mutation	UNP Q04IN8
A	208	ARG	LYS	engineered mutation	UNP Q04IN8
A	311	ASP	GLU	engineered mutation	UNP Q04IN8

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



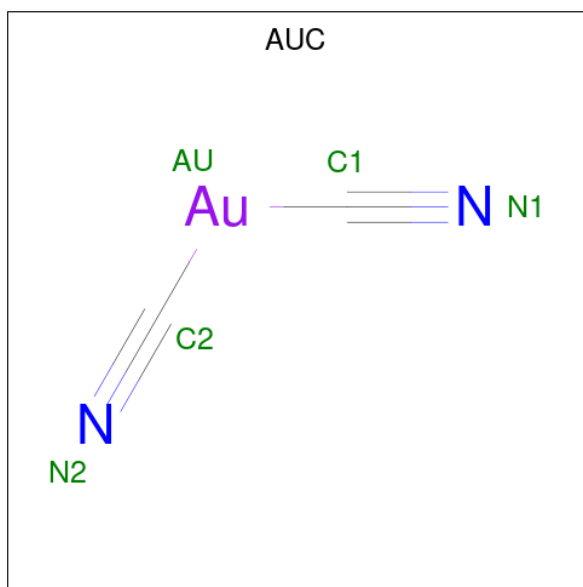
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is GOLD (I) CYANIDE ION (CCD ID: AUC) (formula: C_2AuN_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	Au	C	N	0	0
			3	1	1	1		
4	A	1	Total	Au	C		0	0
			2	1	1			

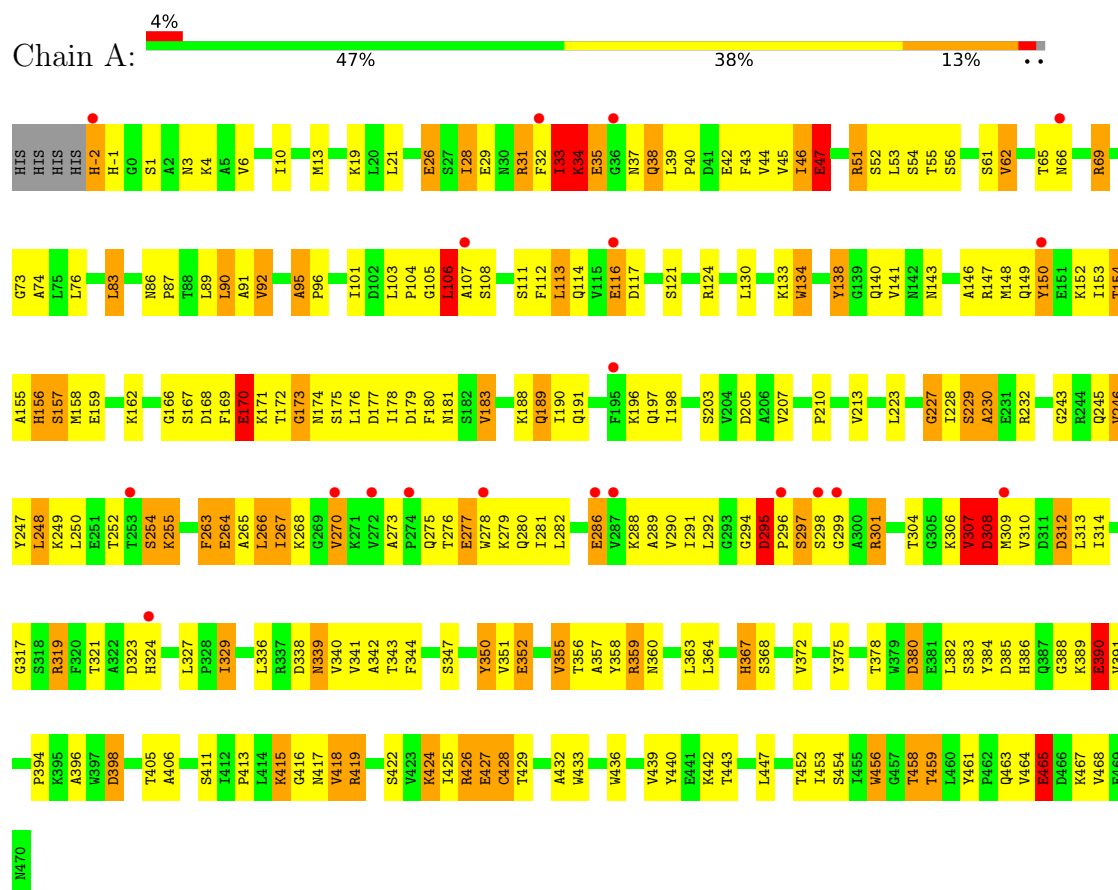
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		

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: Pneumolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	24.86Å 133.62Å 220.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.51 – 2.90 42.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.51-2.90) 99.8 (42.51-2.90)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.307 0.219 , 0.309	Depositor DCC
R_{free} test set	883 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 74.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7542	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: PEG, AUC, 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	1.26	16/3819 (0.4%)	1.24	28/5191 (0.5%)

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	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	74	ALA	CA-CB	-8.37	1.39	1.53
1	A	406	ALA	CA-C	-6.91	1.44	1.53
1	A	74	ALA	C-O	-6.28	1.16	1.23
1	A	339	ASN	CA-C	-5.98	1.45	1.52
1	A	396	ALA	CA-CB	-5.97	1.44	1.53
1	A	456	TRP	CA-C	5.75	1.59	1.53
1	A	342	ALA	CA-CB	-5.63	1.45	1.53
1	A	427	GLU	CA-C	-5.62	1.46	1.52
1	A	6	VAL	N-CA	-5.55	1.39	1.46
1	A	341	VAL	CA-CB	-5.54	1.47	1.54
1	A	146	ALA	CA-CB	-5.48	1.45	1.53
1	A	207	VAL	CA-CB	-5.47	1.47	1.53
1	A	246	VAL	CA-CB	-5.42	1.47	1.54
1	A	76	LEU	C-O	-5.32	1.17	1.24
1	A	95	ALA	CA-CB	-5.30	1.45	1.53
1	A	418	VAL	CA-CB	5.04	1.59	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	ALA	CA-C-N	-7.58	112.88	120.31
1	A	95	ALA	C-N-CA	-7.58	112.88	120.31
1	A	52	SER	N-CA-C	7.52	120.81	107.80
1	A	26	GLU	N-CA-C	7.14	118.99	108.14
1	A	329	ILE	CB-CA-C	-6.80	104.78	111.30
1	A	295	ASP	CA-C-N	-6.73	111.43	119.84
1	A	295	ASP	C-N-CA	-6.73	111.43	119.84
1	A	433	TRP	N-CA-C	6.44	120.40	112.54
1	A	307	VAL	N-CA-C	-6.42	104.90	110.74
1	A	294	GLY	N-CA-C	6.29	120.31	111.00
1	A	254	SER	N-CA-C	6.07	117.88	110.41
1	A	467	LYS	N-CA-C	6.07	118.57	108.20
1	A	464	VAL	N-CA-C	5.89	117.37	107.18
1	A	465	GLU	N-CA-C	5.83	118.22	108.96
1	A	306	LYS	N-CA-C	-5.78	100.91	109.86
1	A	281	ILE	N-CA-C	-5.77	105.11	110.53
1	A	291	ILE	N-CA-C	5.51	115.88	108.17
1	A	53	LEU	N-CA-C	5.43	117.49	108.20
1	A	227	GLY	N-CA-C	5.35	122.74	115.30
1	A	92	VAL	N-CA-C	-5.30	98.32	109.34
1	A	188	LYS	N-CA-C	5.28	119.71	112.68
1	A	398	ASP	N-CA-C	-5.23	105.64	112.23
1	A	181	ASN	N-CA-C	-5.14	106.11	112.38
1	A	73	GLY	N-CA-C	-5.13	108.09	113.58
1	A	154	THR	N-CA-C	-5.10	102.73	110.28
1	A	286	GLU	N-CA-C	5.09	117.70	109.40
1	A	432	ALA	N-CA-C	5.06	116.48	111.07
1	A	134	TRP	N-CA-C	-5.04	106.82	113.12

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	VAL	Peptide
1	A	405	THR	Peptide

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	3744	3680	3682	142	0
2	A	20	30	30	2	0
3	A	14	20	20	0	0
4	A	5	0	0	0	0
5	A	29	0	0	3	0
All	All	3812	3730	3732	142	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 19.

All (142) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:O	1:A:310:VAL:N	2.11	0.84
1:A:296:PRO:O	1:A:301:ARG:NH2	2.12	0.82
1:A:275:GLN:O	1:A:277:GLU:N	2.15	0.80
1:A:106:LEU:O	1:A:108:SER:N	2.18	0.77
1:A:246:VAL:HG22	1:A:292:LEU:HD22	1.68	0.76
1:A:295:ASP:HB3	1:A:296:PRO:HD3	1.71	0.73
1:A:301:ARG:N	1:A:301:ARG:HD3	2.09	0.68
1:A:416:GLY:O	1:A:419:ARG:NH2	2.30	0.65
1:A:263:PHE:O	1:A:266:LEU:N	2.31	0.64
1:A:360:ASN:HB2	1:A:415:LYS:HA	1.80	0.63
1:A:157:SER:OG	1:A:159:GLU:OE1	2.17	0.62
1:A:173:GLY:O	1:A:175:SER:N	2.34	0.61
1:A:106:LEU:HG	1:A:111:SER:HB3	1.82	0.61
1:A:166:GLY:O	1:A:168:ASP:N	2.34	0.60
1:A:338:ASP:OD1	1:A:340:VAL:HG23	2.01	0.60
1:A:424:LYS:NZ	5:A:602:HOH:O	2.34	0.60
1:A:382:LEU:HD23	1:A:383:SER:N	2.19	0.58
1:A:266:LEU:HD21	1:A:307:VAL:HG11	1.84	0.58
1:A:273:ALA:HB3	1:A:280:GLN:CD	2.29	0.58
1:A:278:TRP:C	1:A:280:GLN:H	2.12	0.58
1:A:312:ASP:HA	1:A:314:ILE:HD12	1.85	0.57
1:A:112:PHE:C	1:A:113:LEU:HD23	2.30	0.57
1:A:166:GLY:C	1:A:168:ASP:H	2.12	0.56
1:A:33:ILE:CG1	1:A:34:LYS:H	2.17	0.56
1:A:13:MET:HE2	1:A:230:ALA:N	2.20	0.56
1:A:169:PHE:HE2	1:A:247:TYR:CE2	2.24	0.56
1:A:169:PHE:O	1:A:172:THR:OG1	2.12	0.56
1:A:170:GLU:N	1:A:170:GLU:OE1	2.38	0.56
1:A:360:ASN:CB	1:A:415:LYS:HA	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HD13	1:A:134:TRP:NE1	2.21	0.55
1:A:106:LEU:N	1:A:106:LEU:CD2	2.70	0.55
1:A:288:LYS:NZ	1:A:307:VAL:HG13	2.21	0.55
1:A:299:GLY:O	1:A:301:ARG:NH1	2.40	0.54
1:A:363:LEU:C	1:A:364:LEU:HD23	2.34	0.53
1:A:301:ARG:N	1:A:301:ARG:CD	2.71	0.53
1:A:155:ALA:O	1:A:156:HIS:CG	2.61	0.53
1:A:458:THR:HG23	2:A:503:EDO:H22	1.91	0.53
1:A:288:LYS:HE3	1:A:307:VAL:HG22	1.91	0.52
1:A:103:LEU:HD12	1:A:106:LEU:HD21	1.91	0.52
1:A:313:LEU:C	1:A:313:LEU:HD12	2.35	0.52
1:A:312:ASP:OD2	1:A:314:ILE:HD13	2.10	0.52
1:A:250:LEU:CD2	1:A:288:LYS:HE2	2.41	0.51
1:A:440:TYR:C	1:A:440:TYR:CD1	2.88	0.51
1:A:266:LEU:HD22	1:A:266:LEU:O	2.09	0.51
1:A:295:ASP:HB3	1:A:296:PRO:CD	2.41	0.51
1:A:196:LYS:HD3	1:A:329:ILE:HG21	1.93	0.49
1:A:364:LEU:HD22	1:A:411:SER:CB	2.42	0.49
1:A:62:VAL:HG13	1:A:329:ILE:C	2.38	0.49
1:A:183:VAL:HG13	1:A:189:GLN:H	1.76	0.49
1:A:-2:HIS:N	1:A:3:ASN:OD1	2.45	0.48
1:A:307:VAL:C	1:A:309:MET:N	2.70	0.48
1:A:43:PHE:HB3	1:A:416:GLY:HA3	1.95	0.48
1:A:428:CYS:HB2	1:A:436:TRP:CZ3	2.47	0.48
1:A:43:PHE:O	1:A:358:TYR:HB2	2.13	0.48
1:A:95:ALA:HB1	1:A:96:PRO:HD2	1.97	0.47
1:A:33:ILE:HD13	1:A:34:LYS:H	1.79	0.47
1:A:34:LYS:O	1:A:35:GLU:HB2	2.14	0.47
1:A:273:ALA:HB3	1:A:280:GLN:CG	2.44	0.47
1:A:388:GLY:O	1:A:390:GLU:N	2.48	0.47
1:A:154:THR:HA	1:A:191:GLN:HA	1.97	0.47
1:A:266:LEU:HD22	1:A:266:LEU:C	2.39	0.47
1:A:250:LEU:HD22	1:A:288:LYS:HE2	1.95	0.47
1:A:103:LEU:HB2	1:A:104:PRO:CD	2.46	0.46
1:A:31:ARG:HG3	1:A:31:ARG:O	2.15	0.46
1:A:162:LYS:NZ	1:A:170:GLU:OE2	2.34	0.46
1:A:254:SER:HB3	1:A:282:LEU:HD23	1.97	0.46
1:A:339:ASN:ND2	5:A:604:HOH:O	2.39	0.46
1:A:458:THR:HG22	1:A:461:TYR:H	1.80	0.46
1:A:386:HIS:C	1:A:388:GLY:N	2.73	0.46
1:A:190:ILE:HG22	1:A:191:GLN:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:ARG:NH1	5:A:603:HOH:O	2.36	0.45
1:A:190:ILE:CG2	1:A:191:GLN:N	2.79	0.45
1:A:307:VAL:HG12	1:A:309:MET:HA	1.99	0.45
1:A:428:CYS:O	1:A:428:CYS:SG	2.70	0.45
1:A:289:ALA:HA	1:A:304:THR:HG22	1.97	0.45
1:A:51:ARG:NH1	1:A:352:GLU:OE1	2.50	0.45
1:A:384:TYR:HB3	1:A:388:GLY:HA2	1.98	0.45
1:A:426:ARG:HD3	1:A:436:TRP:CE3	2.51	0.45
1:A:89:LEU:HG	1:A:90:LEU:N	2.31	0.45
1:A:273:ALA:HB3	1:A:280:GLN:NE2	2.31	0.45
1:A:338:ASP:O	1:A:339:ASN:HB2	2.17	0.45
1:A:314:ILE:HD12	1:A:314:ILE:H	1.81	0.45
1:A:33:ILE:HG23	1:A:34:LYS:N	2.32	0.45
1:A:254:SER:OG	1:A:255:LYS:N	2.49	0.45
1:A:317:GLY:HA2	1:A:319:ARG:HH12	1.81	0.45
1:A:350:TYR:CD1	1:A:350:TYR:N	2.84	0.45
1:A:458:THR:HG22	1:A:461:TYR:HB2	1.99	0.45
1:A:263:PHE:O	1:A:264:GLU:C	2.59	0.45
1:A:170:GLU:O	1:A:172:THR:N	2.50	0.44
1:A:180:PHE:N	1:A:180:PHE:CD1	2.85	0.44
1:A:166:GLY:C	1:A:168:ASP:N	2.76	0.44
1:A:10:ILE:HG21	1:A:210:PRO:HB3	2.00	0.43
1:A:39:LEU:HD23	1:A:43:PHE:HB2	1.99	0.43
1:A:263:PHE:O	1:A:265:ALA:N	2.51	0.43
1:A:46:ILE:O	1:A:47:GLU:HB2	2.18	0.43
1:A:248:LEU:HD12	1:A:290:VAL:CG2	2.48	0.43
1:A:308:ASP:C	1:A:310:VAL:H	2.26	0.43
1:A:255:LYS:N	1:A:255:LYS:HD3	2.34	0.43
1:A:266:LEU:HD13	1:A:267:ILE:N	2.34	0.43
1:A:69:ARG:HH11	1:A:69:ARG:CG	2.32	0.43
1:A:223:LEU:O	1:A:228:ILE:HD12	2.19	0.43
1:A:170:GLU:C	1:A:172:THR:N	2.74	0.43
1:A:456:TRP:HZ3	1:A:465:GLU:H	1.67	0.43
1:A:367:HIS:ND1	1:A:367:HIS:C	2.76	0.42
1:A:-2:HIS:O	1:A:-1:HIS:HB2	2.19	0.42
1:A:375:TYR:CD2	1:A:425:ILE:HG12	2.55	0.42
1:A:386:HIS:C	1:A:388:GLY:H	2.28	0.42
1:A:13:MET:HE2	1:A:229:SER:C	2.44	0.42
1:A:46:ILE:O	1:A:47:GLU:CB	2.67	0.42
1:A:138:TYR:O	1:A:140:GLN:N	2.50	0.42
1:A:158:MET:HE1	1:A:173:GLY:HA3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLY:O	1:A:232:ARG:NH1	2.51	0.42
1:A:359:ARG:HG2	1:A:360:ASN:N	2.34	0.42
1:A:382:LEU:HB3	1:A:417:ASN:HB2	2.01	0.42
1:A:33:ILE:CD1	1:A:34:LYS:H	2.33	0.42
1:A:56:SER:HA	1:A:344:PHE:O	2.20	0.41
1:A:197:GLN:O	1:A:243:GLY:HA3	2.19	0.41
1:A:278:TRP:C	1:A:280:GLN:N	2.76	0.41
1:A:411:SER:O	1:A:413:PRO:HD3	2.21	0.41
1:A:173:GLY:C	1:A:175:SER:H	2.27	0.41
1:A:21:LEU:HA	1:A:83:LEU:HD11	2.03	0.41
1:A:31:ARG:HG2	1:A:33:ILE:HB	2.02	0.41
1:A:69:ARG:NH2	1:A:87:PRO:HD2	2.36	0.41
1:A:147:ARG:HG3	1:A:198:ILE:HB	2.02	0.41
1:A:458:THR:HG23	1:A:459:THR:N	2.35	0.41
1:A:69:ARG:HH22	1:A:86:ASN:HA	1.85	0.41
1:A:91:ALA:HA	2:A:501:EDO:H21	2.02	0.41
1:A:456:TRP:CE2	1:A:463:GLN:HB2	2.56	0.41
1:A:229:SER:O	1:A:230:ALA:CB	2.69	0.41
1:A:355:VAL:CG1	1:A:356:THR:N	2.84	0.41
1:A:385:ASP:CG	1:A:386:HIS:N	2.78	0.41
1:A:105:GLY:C	1:A:106:LEU:HD22	2.46	0.41
1:A:229:SER:O	1:A:230:ALA:HB2	2.21	0.41
1:A:178:ILE:N	1:A:178:ILE:HD12	2.36	0.40
1:A:380:ASP:HA	1:A:394:PRO:HA	2.02	0.40
1:A:288:LYS:HZ2	1:A:307:VAL:HG13	1.86	0.40
1:A:150:TYR:O	1:A:150:TYR:CD1	2.74	0.40
1:A:245:GLN:CD	1:A:247:TYR:HE1	2.29	0.40
1:A:96:PRO:HB3	1:A:116:GLU:HA	2.03	0.40
1:A:228:ILE:HD12	1:A:228:ILE:H	1.87	0.40
1:A:263:PHE:N	1:A:263:PHE:CD1	2.88	0.40
1:A:173:GLY:C	1:A:175:SER:N	2.79	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	471/477 (99%)	368 (78%)	67 (14%)	36 (8%)	1	2

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	PRO
1	A	46	ILE
1	A	107	ALA
1	A	167	SER
1	A	174	ASN
1	A	230	ALA
1	A	276	THR
1	A	295	ASP
1	A	298	SER
1	A	308	ASP
1	A	357	ALA
1	A	28	ILE
1	A	33	ILE
1	A	38	GLN
1	A	65	THR
1	A	156	HIS
1	A	277	GLU
1	A	297	SER
1	A	42	GLU
1	A	173	GLY
1	A	177	ASP
1	A	189	GLN
1	A	263	PHE
1	A	264	GLU
1	A	270	VAL
1	A	321	THR
1	A	323	ASP
1	A	389	LYS
1	A	390	GLU
1	A	29	GLU
1	A	32	PHE
1	A	106	LEU
1	A	170	GLU
1	A	391	VAL
1	A	47	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	34	LYS

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	417/421 (99%)	312 (75%)	105 (25%)	0 2

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	HIS
1	A	1	SER
1	A	4	LYS
1	A	19	LYS
1	A	26	GLU
1	A	28	ILE
1	A	31	ARG
1	A	33	ILE
1	A	34	LYS
1	A	35	GLU
1	A	37	ASN
1	A	38	GLN
1	A	44	VAL
1	A	45	VAL
1	A	47	GLU
1	A	51	ARG
1	A	54	SER
1	A	55	THR
1	A	61	SER
1	A	62	VAL
1	A	66	ASN
1	A	69	ARG
1	A	83	LEU
1	A	90	LEU
1	A	92	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	101	ILE
1	A	106	LEU
1	A	113	LEU
1	A	114	GLN
1	A	116	GLU
1	A	117	ASP
1	A	121	SER
1	A	130	LEU
1	A	133	LYS
1	A	138	TYR
1	A	141	VAL
1	A	143	ASN
1	A	148	MET
1	A	149	GLN
1	A	150	TYR
1	A	152	LYS
1	A	153	ILE
1	A	157	SER
1	A	170	GLU
1	A	171	LYS
1	A	176	LEU
1	A	179	ASP
1	A	183	VAL
1	A	203	SER
1	A	205	ASP
1	A	213	VAL
1	A	229	SER
1	A	248	LEU
1	A	249	LYS
1	A	252	THR
1	A	255	LYS
1	A	266	LEU
1	A	267	ILE
1	A	268	LYS
1	A	270	VAL
1	A	279	LYS
1	A	286	GLU
1	A	297	SER
1	A	301	ARG
1	A	307	VAL
1	A	308	ASP
1	A	312	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	319	ARG
1	A	324	HIS
1	A	327	LEU
1	A	336	LEU
1	A	343	THR
1	A	347	SER
1	A	350	TYR
1	A	351	VAL
1	A	352	GLU
1	A	355	VAL
1	A	359	ARG
1	A	367	HIS
1	A	368	SER
1	A	372	VAL
1	A	378	THR
1	A	380	ASP
1	A	390	GLU
1	A	398	ASP
1	A	415	LYS
1	A	418	VAL
1	A	419	ARG
1	A	422	SER
1	A	424	LYS
1	A	426	ARG
1	A	427	GLU
1	A	428	CYS
1	A	429	THR
1	A	439	VAL
1	A	442	LYS
1	A	443	THR
1	A	447	LEU
1	A	452	THR
1	A	453	ILE
1	A	454	SER
1	A	458	THR
1	A	459	THR
1	A	465	GLU
1	A	468	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	280	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](#)

9 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	A	501	-	3,3,3	0.51	0	2,2,2	0.14	0
2	EDO	A	502	-	3,3,3	0.76	0	2,2,2	0.43	0
3	PEG	A	507	-	6,6,6	0.71	0	5,5,5	0.52	0
2	EDO	A	505	-	3,3,3	0.75	0	2,2,2	0.21	0
4	AUC	A	508	-	1,2,4	0.27	0	-		
2	EDO	A	504	-	3,3,3	0.47	0	2,2,2	0.15	0
2	EDO	A	503	-	3,3,3	0.99	0	2,2,2	0.89	0
3	PEG	A	506	-	6,6,6	0.80	0	5,5,5	0.59	0
4	AUC	A	509	1	0,1,4	-	-	-		

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	A	501	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
3	PEG	A	507	-	-	3/4/4/4	-
2	EDO	A	505	-	-	1/1/1/1	-
2	EDO	A	504	-	-	1/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
3	PEG	A	506	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	506	PEG	O1-C1-C2-O2
2	A	503	EDO	O1-C1-C2-O2
3	A	507	PEG	O1-C1-C2-O2
3	A	507	PEG	O2-C3-C4-O4
2	A	505	EDO	O1-C1-C2-O2
3	A	506	PEG	C4-C3-O2-C2
2	A	501	EDO	O1-C1-C2-O2
3	A	507	PEG	C1-C2-O2-C3
2	A	504	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	EDO	1	0
2	A	503	EDO	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	473/477 (99%)	0.28	20 (4%) 40 32	24, 69, 131, 165	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	TRP	3.4
1	A	324	HIS	3.2
1	A	270	VAL	3.2
1	A	32	PHE	3.1
1	A	287	VAL	2.7
1	A	36	GLY	2.7
1	A	296	PRO	2.5
1	A	-2	HIS	2.4
1	A	309	MET	2.4
1	A	299	GLY	2.4
1	A	298	SER	2.3
1	A	286	GLU	2.2
1	A	107	ALA	2.2
1	A	253	THR	2.1
1	A	116	GLU	2.1
1	A	66	ASN	2.1
1	A	274	PRO	2.1
1	A	195	PHE	2.1
1	A	272	VAL	2.0
1	A	150	TYR	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($\text{\AA}^2$)	Q<0.9
2	EDO	A	505	4/4	0.83	0.15	40,63,76,76	0
2	EDO	A	503	4/4	0.85	0.14	38,46,55,55	0
3	PEG	A	507	7/7	0.88	0.14	50,74,110,110	0
3	PEG	A	506	7/7	0.90	0.18	38,58,119,119	0
2	EDO	A	502	4/4	0.91	0.19	38,49,84,84	0
2	EDO	A	504	4/4	0.92	0.12	54,86,120,120	0
2	EDO	A	501	4/4	0.95	0.13	41,84,101,101	0
4	AUC	A	509	2/5	0.99	0.07	38,38,38,63	2
4	AUC	A	508	3/5	1.00	0.06	38,38,48,58	3

6.5 Other polymers [i](#)

There are no such residues in this entry.