



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:56 PM UTC

PDB ID : 8T8D / pdb_00008t8d
Title : Structure of Helicobacter pylori adhesin A, HpaA
Authors : Martini, C.; Calmettes, C.
Deposited on : 2023-06-22
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

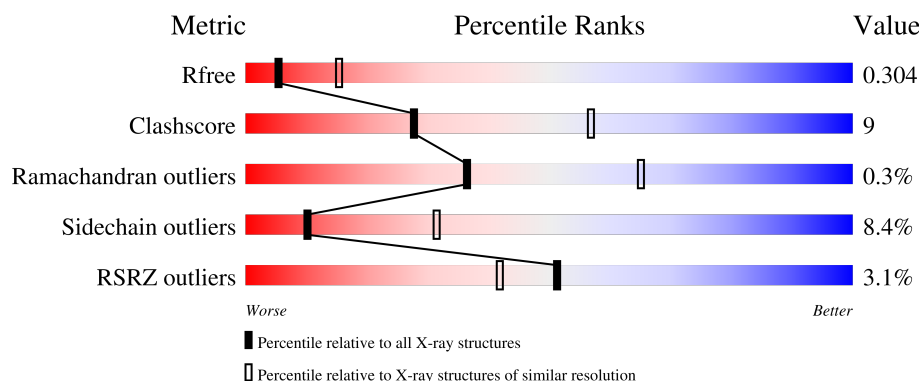
1 Overall quality at a glance

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	215	
1	B	215	
1	C	215	
1	D	215	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	302	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12768 atoms, of which 6400 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 Neuraminyllactose-binding hemagglutinin.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	0	0	0
			3394	1059	1710	290	329	6			
1	B	189	Total	C	H	N	O	S	0	1	0
			3016	952	1514	244	301	5			
1	C	205	Total	C	H	N	O	S	0	0	0
			3247	1013	1643	265	320	6			
1	D	188	Total	C	H	N	O	S	0	0	0
			3002	941	1513	244	299	5			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	MET	-	initiating methionine	UNP P55969
A	234	HIS	-	expression tag	UNP P55969
A	235	HIS	-	expression tag	UNP P55969
A	236	HIS	-	expression tag	UNP P55969
A	237	HIS	-	expression tag	UNP P55969
A	238	HIS	-	expression tag	UNP P55969
A	239	HIS	-	expression tag	UNP P55969
B	25	MET	-	initiating methionine	UNP P55969
B	234	HIS	-	expression tag	UNP P55969
B	235	HIS	-	expression tag	UNP P55969
B	236	HIS	-	expression tag	UNP P55969
B	237	HIS	-	expression tag	UNP P55969
B	238	HIS	-	expression tag	UNP P55969
B	239	HIS	-	expression tag	UNP P55969
C	25	MET	-	initiating methionine	UNP P55969
C	234	HIS	-	expression tag	UNP P55969
C	235	HIS	-	expression tag	UNP P55969
C	236	HIS	-	expression tag	UNP P55969
C	237	HIS	-	expression tag	UNP P55969
C	238	HIS	-	expression tag	UNP P55969
C	239	HIS	-	expression tag	UNP P55969

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Chain	Residue	Modelled	Actual	Comment	Reference
D	25	MET	-	initiating methionine	UNP P55969
D	234	HIS	-	expression tag	UNP P55969
D	235	HIS	-	expression tag	UNP P55969
D	236	HIS	-	expression tag	UNP P55969
D	237	HIS	-	expression tag	UNP P55969
D	238	HIS	-	expression tag	UNP P55969
D	239	HIS	-	expression tag	UNP P55969

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	A	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		
2	B	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

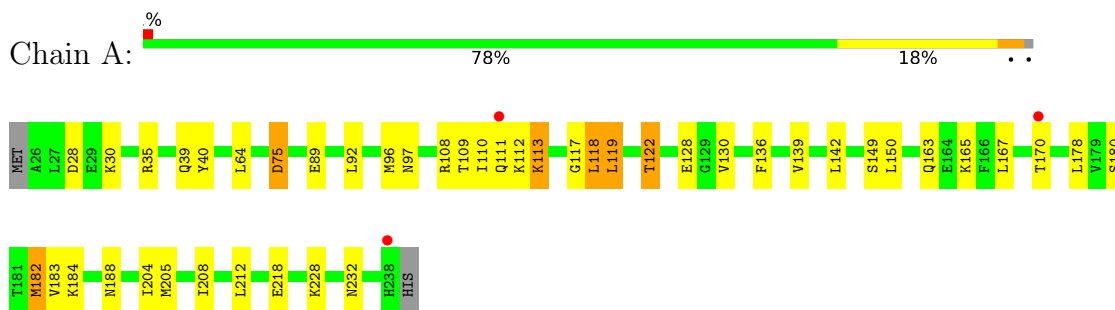
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	15	Total	O	0	0
			15	15		
4	C	17	Total	O	0	0
			17	17		
4	D	9	Total	O	0	0
			9	9		

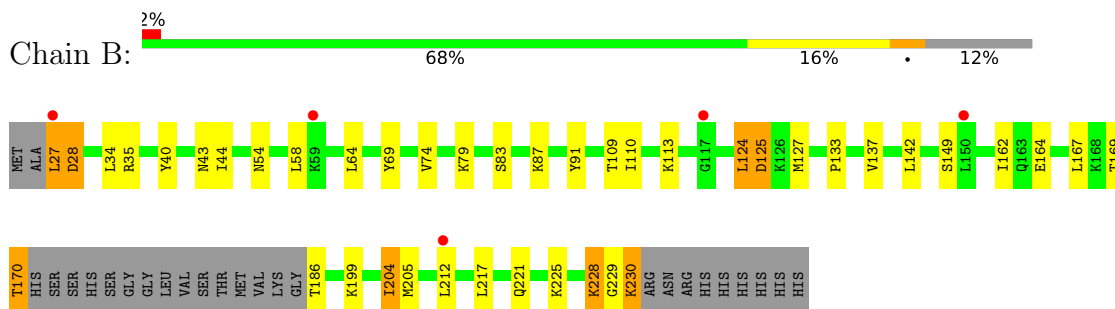
3 Residue-property plots [i](#)

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.

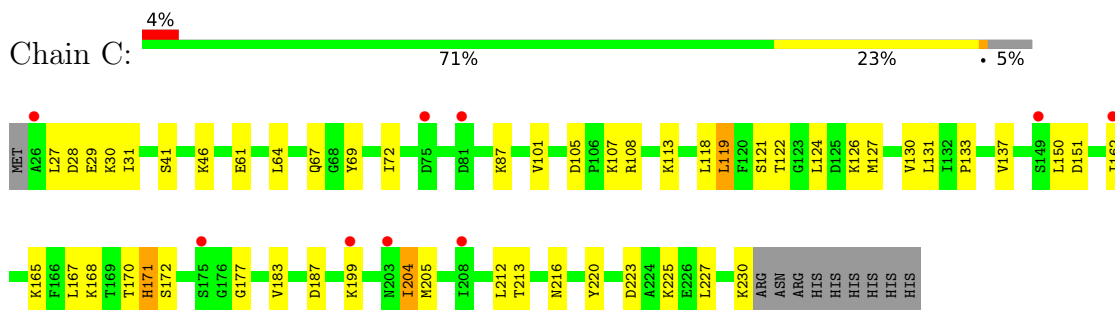
- Molecule 1: Neuraminyllactose-binding hemagglutinin



- Molecule 1: Neuraminyllactose-binding hemagglutinin

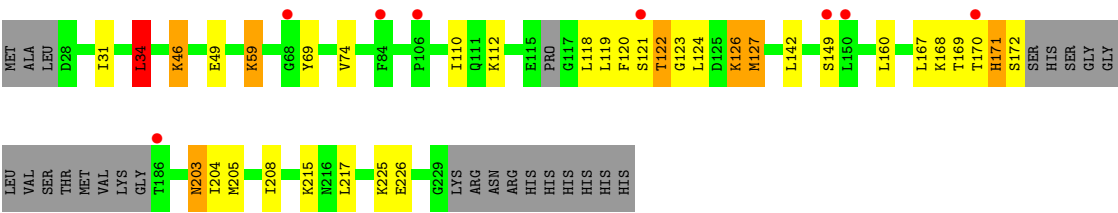


- Molecule 1: Neuraminyllactose-binding hemagglutinin



- Molecule 1: Neuraminyllactose-binding hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.54Å 59.81Å 94.03Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	48.13 – 2.90 48.13 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.13-2.90) 95.0 (48.13-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.241 , 0.306 0.240 , 0.304	Depositor DCC
R_{free} test set	1012 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 60.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12768	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL

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	0.25	0/1709	0.53	0/2291
1	B	0.22	0/1522	0.47	0/2039
1	C	0.29	0/1624	0.55	1/2177 (0.0%)
1	D	0.27	0/1505	0.51	1/2014 (0.0%)
All	All	0.26	0/6360	0.52	2/8521 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	HIS	N-CA-C	-5.35	100.01	108.73
1	D	34	LEU	CA-CB-CG	5.18	134.43	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1684	1710	1710	32	0
1	B	1502	1514	1540	29	0
1	C	1604	1643	1643	34	3
1	D	1489	1513	1516	25	3
2	A	8	6	6	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	6	6	1	0
3	D	6	8	8	0	0
4	A	26	0	0	2	0
4	B	15	0	0	0	0
4	C	17	0	0	3	0
4	D	9	0	0	0	0
All	All	6368	6400	6429	115	3

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 9.

All (115) 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:97:ASN:HB2	2:A:302:ACT:O	1.45	1.14
1:B:164:GLU:OE2	1:B:199:LYS:NZ	1.98	0.94
1:D:127:MET:O	1:D:127:MET:HE3	1.75	0.87
1:C:162:ILE:HG23	1:C:199:LYS:HD2	1.59	0.85
1:A:136:PHE:HZ	2:A:302:ACT:H2	1.44	0.83
1:A:97:ASN:CB	2:A:302:ACT:O	2.29	0.78
1:D:126:LYS:HB2	1:D:169:THR:HG22	1.66	0.75
1:D:160:LEU:HD21	1:D:203:ASN:ND2	2.02	0.75
1:C:162:ILE:HG12	1:C:199:LYS:HD3	1.70	0.74
1:C:113:LYS:HG2	4:C:305:HOH:O	1.88	0.74
1:B:229:GLY:O	1:B:230:LYS:NZ	2.18	0.74
1:B:125:ASP:N	1:B:125:ASP:OD1	2.19	0.73
1:C:27:LEU:O	1:C:27:LEU:HD23	1.91	0.71
1:A:39:GLN:HB3	1:C:27:LEU:HD13	1.74	0.69
1:C:72:ILE:HD13	4:C:302:HOH:O	1.92	0.69
1:D:126:LYS:CB	1:D:169:THR:HG22	2.21	0.69
1:A:136:PHE:CZ	2:A:302:ACT:H2	2.29	0.68
1:C:30:LYS:HD3	1:C:72:ILE:HD11	1.74	0.68
1:B:125:ASP:O	1:B:170:THR:HG23	1.96	0.66
1:A:40:TYR:C	1:C:27:LEU:HD11	2.21	0.65
1:A:183:VAL:HG12	1:A:183:VAL:O	1.97	0.64
1:B:142:LEU:HD23	1:B:149:SER:HA	1.78	0.64
1:A:64:LEU:HD21	1:A:212:LEU:HD13	1.81	0.63
1:D:127:MET:HE3	1:D:127:MET:C	2.22	0.63
1:A:35:ARG:NH2	1:A:75:ASP:OD1	2.31	0.63
1:A:40:TYR:O	1:C:27:LEU:HD21	2.00	0.61
1:B:40:TYR:HB3	1:B:44:ILE:HD12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:TYR:O	1:C:27:LEU:HD11	2.00	0.60
1:B:137:VAL:HB	1:B:204:ILE:HD11	1.83	0.60
1:C:162:ILE:HG23	1:C:199:LYS:CD	2.29	0.60
1:C:64:LEU:HD21	1:C:212:LEU:HD13	1.83	0.59
1:D:160:LEU:CD2	1:D:203:ASN:ND2	2.66	0.59
1:B:164:GLU:CD	1:B:199:LYS:HZ1	2.04	0.58
1:C:162:ILE:CG2	1:C:199:LYS:HD2	2.33	0.58
1:C:119:LEU:H	1:C:119:LEU:HD23	1.71	0.56
1:D:121:SER:O	1:D:123:GLY:HA3	2.06	0.56
1:A:96:MET:HG2	1:A:139:VAL:HG22	1.88	0.56
1:C:130:VAL:HG22	1:C:165:LYS:HG2	1.88	0.56
1:B:34:LEU:HD12	1:B:74:VAL:HG21	1.87	0.55
1:C:31:ILE:HD11	1:C:69:TYR:CG	2.41	0.55
1:C:168:LYS:HB3	1:C:187:ASP:HB2	1.87	0.55
1:C:137:VAL:HG11	1:C:204:ILE:HD11	1.87	0.55
1:C:216:ASN:ND2	4:C:304:HOH:O	2.41	0.54
1:D:142:LEU:HD23	1:D:149:SER:HA	1.88	0.53
1:B:28:ASP:OD1	1:B:28:ASP:N	2.41	0.53
1:B:91:TYR:OH	1:B:217:LEU:O	2.26	0.53
1:D:69:TYR:CE2	1:D:217:LEU:HD12	2.44	0.53
1:B:162:ILE:HG23	1:B:199:LYS:HD2	1.90	0.53
1:D:160:LEU:CD2	1:D:203:ASN:CG	2.82	0.53
1:B:64:LEU:HD21	1:B:212:LEU:HD13	1.91	0.52
1:B:27:LEU:HD23	1:B:27:LEU:N	2.25	0.51
1:B:164:GLU:OE2	1:B:199:LYS:CE	2.59	0.51
1:C:150:LEU:HD21	1:C:227:LEU:CD1	2.40	0.51
1:A:188:ASN:HA	4:A:413:HOH:O	2.13	0.49
1:A:178:LEU:HD12	1:A:182:MET:HB3	1.94	0.49
1:C:119:LEU:H	1:C:119:LEU:CD2	2.25	0.48
1:D:124:LEU:HD22	1:D:171:HIS:N	2.27	0.48
1:A:142:LEU:HD23	1:A:149:SER:HA	1.95	0.48
1:B:34:LEU:HD12	1:B:74:VAL:CG2	2.44	0.48
1:D:205:MET:HE2	1:D:208:ILE:HD12	1.96	0.48
1:A:108:ARG:NH2	1:A:163:GLN:OE1	2.47	0.48
1:D:127:MET:HE2	1:D:168:LYS:HG2	1.95	0.47
1:B:79:LYS:HE2	2:B:302:ACT:O	2.14	0.47
1:A:150:LEU:O	1:B:83:SER:HB2	2.15	0.47
1:A:92:LEU:HD22	1:A:150:LEU:HD12	1.98	0.46
1:A:130:VAL:HG11	1:A:163:GLN:HB3	1.98	0.46
1:B:204:ILE:CG2	1:B:205:MET:HE2	2.46	0.46
1:D:160:LEU:HD22	1:D:203:ASN:CG	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:THR:OG1	1:C:216:ASN:HB2	2.16	0.45
1:D:34:LEU:HA	1:D:74:VAL:HG23	1.98	0.45
1:A:178:LEU:HD12	1:A:182:MET:CB	2.46	0.45
1:B:87:LYS:O	1:B:228:LYS:NZ	2.49	0.45
1:A:228:LYS:O	1:A:232:ASN:N	2.47	0.45
1:D:118:LEU:C	1:D:118:LEU:HD13	2.40	0.45
1:B:124:LEU:HD23	1:B:124:LEU:O	2.17	0.45
1:D:171:HIS:CG	1:D:172:SER:H	2.35	0.45
1:A:118:LEU:O	1:A:119:LEU:HB3	2.16	0.45
1:A:205:MET:HE2	1:A:208:ILE:HD12	1.97	0.45
1:A:97:ASN:HD22	2:A:302:ACT:CH3	2.29	0.44
1:A:30:LYS:HD2	1:A:89:GLU:HB3	1.99	0.44
1:C:223:ASP:O	1:C:227:LEU:HD12	2.17	0.44
1:D:121:SER:OG	1:D:122:THR:N	2.50	0.44
1:A:111:GLN:HG2	1:A:113:LYS:HE3	1.99	0.44
1:B:137:VAL:CB	1:B:204:ILE:HD11	2.46	0.44
1:D:120:PHE:O	1:D:122:THR:N	2.50	0.44
1:B:137:VAL:HG21	1:B:204:ILE:CD1	2.48	0.44
1:C:225:LYS:O	1:C:225:LYS:HD3	2.17	0.44
1:D:46:LYS:HE3	1:D:46:LYS:HA	1.99	0.44
1:D:170:THR:O	1:D:171:HIS:HB2	2.18	0.43
1:C:121:SER:O	1:C:122:THR:C	2.61	0.43
1:C:204:ILE:HG23	1:C:205:MET:HE2	2.00	0.43
1:C:133:PRO:HD3	1:C:162:ILE:HB	2.00	0.43
1:D:122:THR:O	1:D:122:THR:OG1	2.35	0.43
1:A:122:THR:O	1:A:122:THR:HG22	2.18	0.43
1:A:165:LYS:HB3	4:A:418:HOH:O	2.18	0.43
1:C:67:GLN:OE1	1:C:213:THR:HA	2.19	0.42
1:D:31:ILE:HD11	1:D:69:TYR:CG	2.55	0.42
1:C:41:SER:HB3	1:C:101:VAL:HG13	2.02	0.42
1:C:105:ASP:OD2	1:C:108:ARG:NE	2.51	0.42
1:B:204:ILE:HG22	1:B:205:MET:HE2	2.00	0.42
1:C:151:ASP:OD2	1:C:220:TYR:OH	2.38	0.42
1:B:54:ASN:O	1:B:58:LEU:HG	2.20	0.42
1:B:133:PRO:HG3	1:B:162:ILE:HB	2.02	0.42
1:A:30:LYS:CD	1:A:89:GLU:HB3	2.50	0.41
1:D:46:LYS:NZ	1:D:49:GLU:OE1	2.33	0.41
1:C:162:ILE:HG23	1:C:199:LYS:HZ2	1.84	0.41
1:B:69:TYR:CE2	1:B:217:LEU:HD12	2.56	0.41
1:B:169:THR:OG1	1:B:186:THR:HA	2.19	0.41
1:D:59:LYS:HD2	1:D:205:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG22	1:A:165:LYS:HG2	2.03	0.41
1:B:137:VAL:CG2	1:B:204:ILE:HD11	2.51	0.41
1:C:150:LEU:HD21	1:C:227:LEU:HD13	2.03	0.41
1:C:171:HIS:NE2	1:C:177:GLY:HA2	2.36	0.41
1:A:218:GLU:HA	1:A:218:GLU:OE1	2.20	0.40
1:A:109:THR:HA	1:A:128:GLU:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LYS:NZ	1:D:226:GLU:O[2_546]	2.16	0.04
1:C:61:GLU:OE1	1:D:215:LYS:NZ[1_545]	2.19	0.01
1:C:87:LYS:HZ2	1:D:226:GLU:O[2_546]	1.59	0.01

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	211/215 (98%)	201 (95%)	9 (4%)	1 (0%)	24	54
1	B	186/215 (86%)	178 (96%)	8 (4%)	0	100	100
1	C	203/215 (94%)	198 (98%)	5 (2%)	0	100	100
1	D	182/215 (85%)	175 (96%)	6 (3%)	1 (0%)	24	54
All	All	782/860 (91%)	752 (96%)	28 (4%)	2 (0%)	36	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	171	HIS
1	A	117	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	190/192 (99%)	176 (93%)	14 (7%)	13	38
1	B	171/192 (89%)	154 (90%)	17 (10%)	7	24
1	C	182/192 (95%)	166 (91%)	16 (9%)	9	29
1	D	169/192 (88%)	156 (92%)	13 (8%)	12	35
All	All	712/768 (93%)	652 (92%)	60 (8%)	10	31

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	75	ASP
1	A	110	ILE
1	A	112	LYS
1	A	113	LYS
1	A	118	LEU
1	A	119	LEU
1	A	122	THR
1	A	167	LEU
1	A	170	THR
1	A	180	SER
1	A	182	MET
1	A	184	LYS
1	A	204	ILE
1	B	27	LEU
1	B	28	ASP
1	B	35	ARG
1	B	43	ASN
1	B	109	THR
1	B	110	ILE
1	B	113	LYS
1	B	124	LEU
1	B	125	ASP
1	B	127	MET

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Mol	Chain	Res	Type
1	B	167	LEU
1	B	170	THR
1	B	204	ILE
1	B	221	GLN
1	B	225	LYS
1	B	228	LYS
1	B	230	LYS
1	C	28	ASP
1	C	29	GLU
1	C	46	LYS
1	C	107	LYS
1	C	118	LEU
1	C	119	LEU
1	C	124	LEU
1	C	126	LYS
1	C	127	MET
1	C	131	LEU
1	C	167	LEU
1	C	170	THR
1	C	172	SER
1	C	183	VAL
1	C	204	ILE
1	C	230	LYS
1	D	34	LEU
1	D	46	LYS
1	D	59	LYS
1	D	110	ILE
1	D	112	LYS
1	D	119	LEU
1	D	122	THR
1	D	126	LYS
1	D	127	MET
1	D	167	LEU
1	D	203	ASN
1	D	204	ILE
1	D	225	LYS

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	39	GLN
1	B	221	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	D	301	-	5,5,5	0.32	0	5,5,5	0.31	0
2	ACT	B	302	-	3,3,3	0.85	0	3,3,3	0.70	0
2	ACT	B	301	-	3,3,3	0.89	0	3,3,3	0.85	0
2	ACT	A	301	-	3,3,3	0.81	0	3,3,3	0.74	0
2	ACT	A	302	-	3,3,3	0.79	0	3,3,3	0.86	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	GOL	D	301	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	301	GOL	C1-C2-C3-O3
3	D	301	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	302	ACT	1	0
2	A	302	ACT	5	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	213/215 (99%)	0.12	3 (1%) 73 65	40, 69, 115, 137	0
1	B	189/215 (87%)	0.53	5 (2%) 57 48	51, 93, 141, 174	1 (0%)
1	C	205/215 (95%)	0.59	9 (4%) 39 30	48, 91, 125, 139	0
1	D	188/215 (87%)	0.75	8 (4%) 40 31	56, 102, 154, 173	0
All	All	795/860 (92%)	0.49	25 (3%) 51 42	40, 88, 139, 174	1 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	LEU	4.0
1	B	59	LYS	3.3
1	C	26	ALA	3.0
1	B	27	LEU	3.0
1	C	199	LYS	2.9
1	A	238	HIS	2.9
1	D	106	PRO	2.7
1	C	149	SER	2.7
1	C	81	ASP	2.6
1	C	162	ILE	2.6
1	C	203	ASN	2.6
1	A	170	THR	2.5
1	C	208	ILE	2.5
1	D	121	SER	2.4
1	D	84	PHE	2.2
1	D	186	THR	2.2
1	C	175	SER	2.2
1	D	170	THR	2.2
1	C	75	ASP	2.2
1	B	117	GLY	2.1
1	A	111	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	150	LEU	2.1
1	D	150	LEU	2.1
1	D	149	SER	2.0
1	D	68	GLY	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
3	GOL	D	301	6/6	0.41	0.32	195,243,280,292	0
2	ACT	A	302	4/4	0.55	0.28	97,122,147,147	0
2	ACT	B	302	4/4	0.61	0.26	114,137,179,225	0
2	ACT	B	301	4/4	0.79	0.19	36,43,63,68	0
2	ACT	A	301	4/4	0.89	0.49	50,60,126,222	0

6.5 Other polymers [i](#)

There are no such residues in this entry.