



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:52 PM UTC

PDB ID : 4NF1 / pdb_00004nf1
Title : Structure of N-acetyltransferase domain of *X. fastidiosa* NAGS/K without his-tag
Authors : Zhao, G.; Jin, Z.; Allewell, N.M.; Tuchman, M.; Shi, D.
Deposited on : 2013-10-30
Resolution : 1.40 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

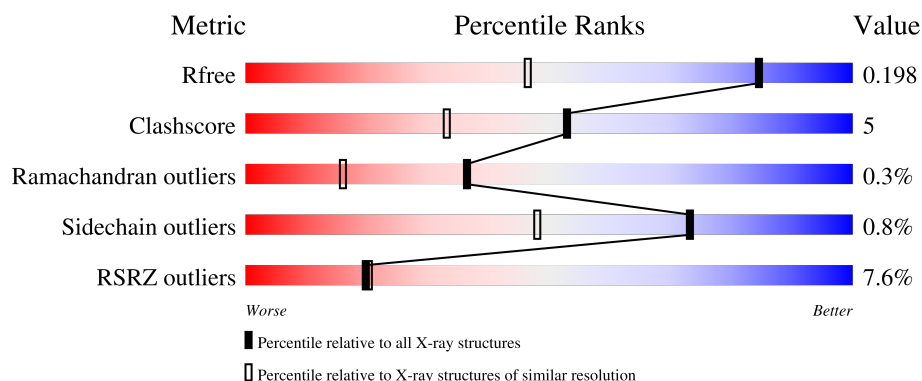
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	150	
1	B	150	
1	C	150	
1	D	150	
1	E	150	

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Mol	Chain	Length	Quality of chain
1	F	150	11% 87% 12%
1	G	150	3% 88% 9%
1	H	150	20% 81% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11687 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 Acetylglutamate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	0	2	0
			1232	794	219	216	3			
1	B	146	Total	C	N	O	S	0	3	0
			1235	794	220	218	3			
1	C	147	Total	C	N	O	S	0	4	0
			1248	804	220	220	4			
1	D	149	Total	C	N	O	S	0	0	0
			1248	801	224	219	4			
1	E	147	Total	C	N	O	S	0	1	0
			1235	794	220	217	4			
1	F	148	Total	C	N	O	S	0	1	0
			1250	803	226	217	4			
1	G	146	Total	C	N	O	S	0	2	0
			1232	794	219	216	3			
1	H	147	Total	C	N	O	S	0	1	0
			1236	796	222	214	4			

There are 32 discrepancies between the modelled and reference sequences:

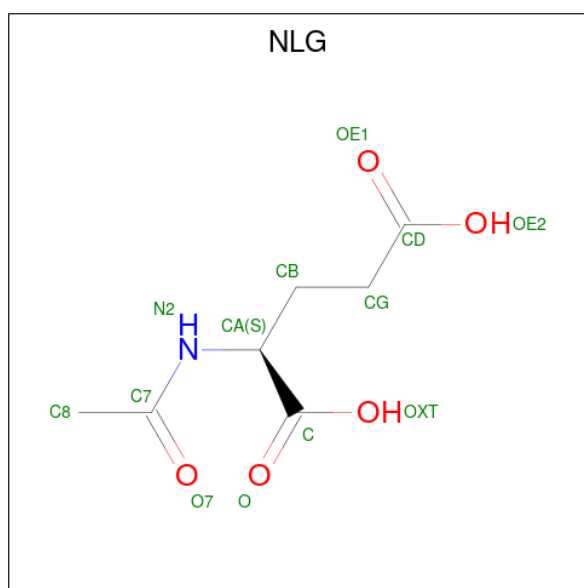
Chain	Residue	Modelled	Actual	Comment	Reference
A	289	GLY	-	expression tag	UNP Q87EL2
A	290	SER	-	expression tag	UNP Q87EL2
A	291	HIS	-	expression tag	UNP Q87EL2
A	292	MET	-	expression tag	UNP Q87EL2
B	289	GLY	-	expression tag	UNP Q87EL2
B	290	SER	-	expression tag	UNP Q87EL2
B	291	HIS	-	expression tag	UNP Q87EL2
B	292	MET	-	expression tag	UNP Q87EL2
C	289	GLY	-	expression tag	UNP Q87EL2
C	290	SER	-	expression tag	UNP Q87EL2
C	291	HIS	-	expression tag	UNP Q87EL2
C	292	MET	-	expression tag	UNP Q87EL2
D	289	GLY	-	expression tag	UNP Q87EL2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	290	SER	-	expression tag	UNP Q87EL2
D	291	HIS	-	expression tag	UNP Q87EL2
D	292	MET	-	expression tag	UNP Q87EL2
E	289	GLY	-	expression tag	UNP Q87EL2
E	290	SER	-	expression tag	UNP Q87EL2
E	291	HIS	-	expression tag	UNP Q87EL2
E	292	MET	-	expression tag	UNP Q87EL2
F	289	GLY	-	expression tag	UNP Q87EL2
F	290	SER	-	expression tag	UNP Q87EL2
F	291	HIS	-	expression tag	UNP Q87EL2
F	292	MET	-	expression tag	UNP Q87EL2
G	289	GLY	-	expression tag	UNP Q87EL2
G	290	SER	-	expression tag	UNP Q87EL2
G	291	HIS	-	expression tag	UNP Q87EL2
G	292	MET	-	expression tag	UNP Q87EL2
H	289	GLY	-	expression tag	UNP Q87EL2
H	290	SER	-	expression tag	UNP Q87EL2
H	291	HIS	-	expression tag	UNP Q87EL2
H	292	MET	-	expression tag	UNP Q87EL2

- Molecule 2 is N-ACETYL-L-GLUTAMATE (CCD ID: NLG) (formula: $C_7H_{11}NO_5$).



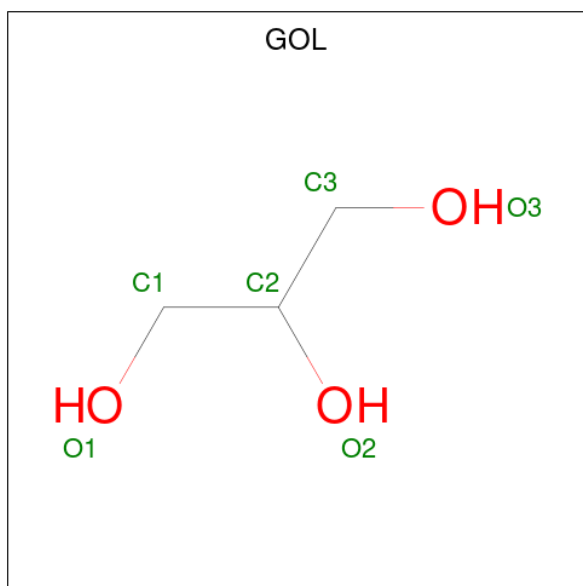
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	7	1	5		
2	B	1	Total	C	N	O	0	0
			13	7	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			13	7	1	5		
2	D	1	Total	C	N	O	0	0
			13	7	1	5		
2	E	1	Total	C	N	O	0	0
			13	7	1	5		
2	F	1	Total	C	N	O	0	0
			13	7	1	5		
2	G	1	Total	C	N	O	0	0
			13	7	1	5		
2	H	1	Total	C	N	O	0	0
			13	7	1	5		

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Cl 2	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	2	Total 2	Cl 2	0	0
4	G	2	Total 2	Cl 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	249	Total 249	O 249	0	0
5	B	165	Total 165	O 165	0	0
5	C	278	Total 278	O 278	0	0
5	D	202	Total 202	O 202	0	0
5	E	217	Total 217	O 217	0	0
5	F	174	Total 174	O 174	0	0
5	G	215	Total 215	O 215	0	0
5	H	147	Total 147	O 147	0	0

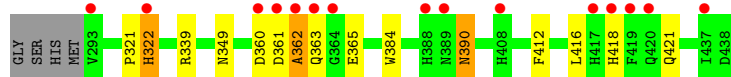
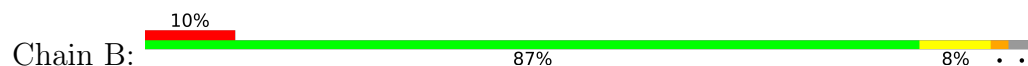
3 Residue-property plots [i](#)

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: Acetylglutamate kinase



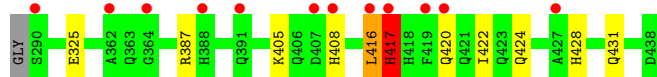
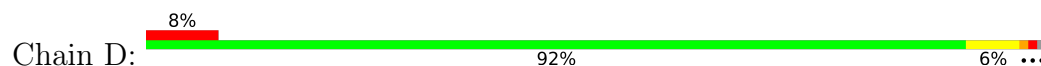
- Molecule 1: Acetylglutamate kinase



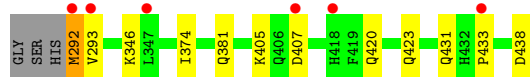
- Molecule 1: Acetylglutamate kinase



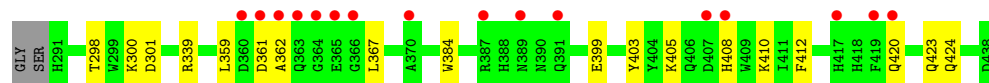
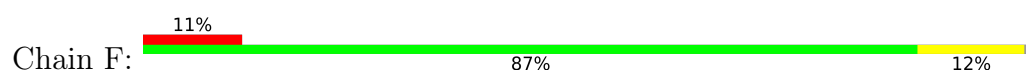
- Molecule 1: Acetylglutamate kinase



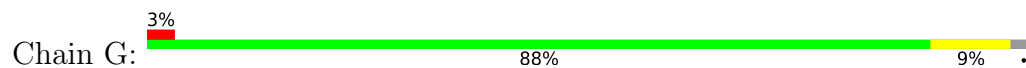
- Molecule 1: Acetylglutamate kinase



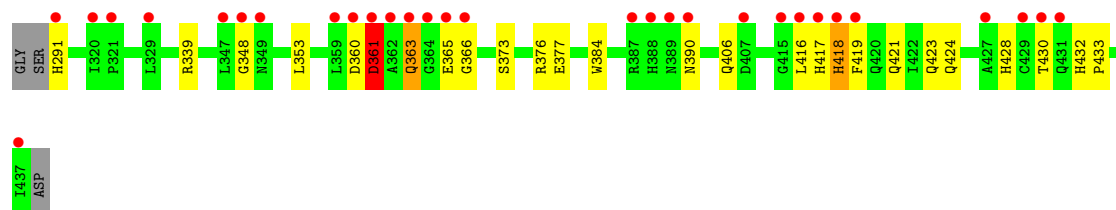
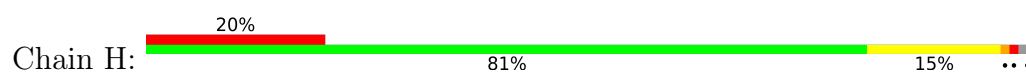
- Molecule 1: Acetylglutamate kinase



- Molecule 1: Acetylglutamate kinase



- Molecule 1: Acetylglutamate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.87Å 123.35Å 76.66Å 90.00° 107.62° 90.00°	Depositor
Resolution (Å)	34.07 – 1.40 34.07 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.07-1.40) 90.5 (34.07-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 1.40Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.179 , 0.199 0.180 , 0.198	Depositor DCC
R_{free} test set	2000 reflections (0.58%)	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11687	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.35 % 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 1.1236e-03. 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

5.1 Standard geometry

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

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	0.52	1/1277 (0.1%)	0.68	1/1738 (0.1%)
1	B	0.41	0/1283	0.74	2/1746 (0.1%)
1	C	0.45	0/1299	0.64	0/1767
1	D	0.40	0/1288	0.70	0/1752
1	E	0.45	0/1277	0.67	0/1737
1	F	0.40	0/1293	0.66	0/1758
1	G	0.44	0/1277	0.65	0/1738
1	H	0.38	0/1279	0.75	2/1741 (0.1%)
All	All	0.43	1/10273 (0.0%)	0.69	5/13977 (0.0%)

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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	LEU	C-O	-6.43	1.16	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PRO	CA-C-N	7.52	133.07	122.46
1	B	321	PRO	C-N-CA	7.52	133.07	122.46
1	H	361	ASP	N-CA-C	-5.59	106.50	113.38
1	A	408	HIS	CB-CA-C	-5.22	101.15	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	363	GLN	N-CA-C	-5.11	105.80	112.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	416	LEU	Peptide
1	D	417	HIS	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	1232	0	1193	16	0
1	B	1235	0	1193	9	0
1	C	1248	0	1211	10	0
1	D	1248	0	1198	11	1
1	E	1235	0	1191	9	1
1	F	1250	0	1206	15	0
1	G	1232	0	1193	13	0
1	H	1236	0	1194	21	1
2	A	13	0	9	0	0
2	B	13	0	9	0	0
2	C	13	0	9	1	0
2	D	13	0	9	0	0
2	E	13	0	9	0	0
2	F	13	0	9	0	0
2	G	13	0	9	1	0
2	H	13	0	9	0	0
3	A	6	0	8	2	0
3	G	6	0	8	0	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	1	0
4	E	2	0	0	0	0
4	G	2	0	0	0	0
5	A	249	0	0	9	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	165	0	0	5	3
5	C	278	0	0	7	0
5	D	202	0	0	4	1
5	E	217	0	0	5	0
5	F	174	0	0	7	1
5	G	215	0	0	3	0
5	H	147	0	0	10	0
All	All	11687	0	9667	98	5

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 5.

All (98) 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:390:ASN:ND2	5:B:797:HOH:O	1.90	1.04
1:A:408:HIS:CD2	1:G:378:GLU:HB3	1.99	0.98
1:D:416:LEU:O	5:D:773:HOH:O	1.82	0.95
1:E:433:PRO:HG2	1:G:431:GLN:HB3	1.48	0.95
1:G:293:VAL:N	5:G:689:HOH:O	2.08	0.86
1:D:405:LYS:NZ	5:D:767:HOH:O	2.02	0.84
1:F:298:THR:OG1	5:F:863:HOH:O	1.95	0.84
1:F:405:LYS:NZ	5:F:782:HOH:O	2.12	0.82
1:C:405:LYS:NZ	5:C:732:HOH:O	2.13	0.82
1:A:408:HIS:HD2	1:G:378:GLU:HB3	1.41	0.82
1:H:339:ARG:HH21	1:H:361:ASP:HB2	1.48	0.79
1:D:428:HIS:ND1	5:D:755:HOH:O	2.16	0.78
1:F:300:LYS:HG2	5:F:863:HOH:O	1.83	0.78
1:C:391:GLN:NE2	5:C:867:HOH:O	2.16	0.77
1:G:405:LYS:NZ	5:G:792:HOH:O	2.19	0.75
1:A:421:GLN:NE2	5:A:779:HOH:O	2.23	0.71
1:A:421:GLN:NE2	5:A:836:HOH:O	2.23	0.71
1:H:390:ASN:ND2	5:H:840:HOH:O	2.25	0.68
1:G:336:GLU:OE1	5:G:760:HOH:O	2.11	0.68
1:C:436:LEU:HD12	2:C:501:NLG:HGC1	1.75	0.67
1:F:420:GLN:NE2	1:F:424:GLN:OE1	2.27	0.67
1:D:417:HIS:HD2	1:D:422:ILE:HD11	1.60	0.66
1:B:349:ASN:OD1	5:B:703:HOH:O	2.13	0.66
1:A:293:VAL:N	5:A:690:HOH:O	2.29	0.65
1:A:408:HIS:ND1	1:A:409:TRP:CE2	2.59	0.62
1:H:376:ARG:NH1	5:H:785:HOH:O	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:348:GLY:HA2	1:H:428:HIS:CD2	2.34	0.62
1:F:423:GLN:NE2	5:F:874:HOH:O	2.34	0.61
1:G:353:LEU:HD12	1:G:382[A]:LEU:HD21	1.81	0.61
1:B:360:ASP:O	5:B:793:HOH:O	2.16	0.60
1:A:434:PRO:HG2	5:A:807:HOH:O	2.01	0.60
1:H:291:HIS:N	5:H:812:HOH:O	2.34	0.59
1:A:421:GLN:CD	5:A:836:HOH:O	2.46	0.58
1:D:417:HIS:CD2	1:D:422:ILE:HD11	2.36	0.58
1:D:387:ARG:NH1	1:D:408:HIS:ND1	2.52	0.57
1:F:403:TYR:CD1	1:F:405:LYS:HE3	2.40	0.57
1:C:399:GLU:O	5:C:857:HOH:O	2.17	0.57
1:D:420:GLN:HB3	5:D:745:HOH:O	2.05	0.56
1:B:339:ARG:HH21	1:B:361:ASP:HB3	1.71	0.56
1:B:362:ALA:O	5:B:780:HOH:O	2.18	0.55
1:C:376:ARG:NH2	5:C:785:HOH:O	2.39	0.55
1:E:293:VAL:HG21	1:E:374:ILE:HD12	1.89	0.54
1:H:366:GLY:N	5:H:835:HOH:O	2.35	0.54
1:G:436:LEU:HD12	2:G:501:NLG:HGC1	1.89	0.53
1:H:416:LEU:O	5:H:740:HOH:O	2.19	0.53
1:B:416:LEU:N	5:B:827:HOH:O	2.40	0.53
1:D:387:ARG:NH2	4:D:502:CL:CL	2.79	0.53
1:H:417:HIS:N	5:H:794:HOH:O	2.42	0.52
1:H:416:LEU:N	5:H:783:HOH:O	2.42	0.50
1:E:405:LYS:NZ	5:E:803:HOH:O	2.44	0.50
1:G:318:THR:HB	1:G:437:ILE:HD12	1.94	0.50
1:H:360:ASP:HA	1:H:363:GLN:HG2	1.94	0.50
1:E:407:ASP:OD1	5:E:778:HOH:O	2.20	0.49
1:H:424:GLN:HB2	5:H:839:HOH:O	2.12	0.49
1:C:433:PRO:HG3	5:C:792:HOH:O	2.12	0.48
1:F:399:GLU:OE2	5:F:718:HOH:O	2.20	0.48
1:H:417:HIS:CG	1:H:417:HIS:O	2.67	0.47
1:F:339:ARG:NH2	1:F:361:ASP:OD1	2.37	0.47
1:E:292:MET:N	5:E:814:HOH:O	2.48	0.47
1:B:322:HIS:CD2	1:B:322:HIS:N	2.83	0.47
1:F:359:LEU:HB2	1:F:361:ASP:HB3	1.97	0.46
1:A:408:HIS:CE1	1:A:409:TRP:CZ2	3.04	0.46
1:F:405:LYS:HD2	1:F:410:LYS:HG2	1.97	0.46
1:A:314[B]:SER:HB2	3:A:502:GOL:H31	1.98	0.46
1:H:406:GLN:OE1	1:H:430:THR:HG21	2.16	0.45
1:A:421:GLN:OE1	5:A:836:HOH:O	2.21	0.45
1:C:402:GLY:HA3	1:C:413:TRP:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:ASP:HB3	5:F:865:HOH:O	2.16	0.45
1:F:359:LEU:CB	1:F:361:ASP:HB3	2.47	0.45
1:E:431:GLN:HA	5:E:744:HOH:O	2.17	0.45
1:A:408:HIS:CD2	1:G:378:GLU:CB	2.87	0.45
1:F:408:HIS:N	5:F:771:HOH:O	2.50	0.44
1:C:316:ARG:NH1	1:E:381:GLN:OE1	2.50	0.44
1:H:406:GLN:NE2	5:H:847:HOH:O	2.44	0.44
1:D:416:LEU:O	1:D:417:HIS:CG	2.71	0.43
1:H:418:HIS:HD2	1:H:421:GLN:OE1	2.01	0.43
1:D:387:ARG:NH1	1:D:408:HIS:CE1	2.87	0.43
1:G:419:PHE:CD1	1:H:423:GLN:HG2	2.54	0.43
1:A:293:VAL:HG21	1:A:374[A]:ILE:HD12	2.00	0.43
1:G:426:VAL:O	1:G:430:THR:HG23	2.19	0.43
1:F:362:ALA:HB1	1:F:367:LEU:HB3	2.02	0.42
3:A:502:GOL:H2	5:A:774:HOH:O	2.19	0.42
1:E:346:LYS:NZ	5:E:700:HOH:O	2.53	0.42
1:B:418:HIS:HB2	1:B:421:GLN:HG3	2.01	0.42
1:H:390:ASN:O	5:H:802:HOH:O	2.22	0.41
1:C:336:GLU:OE1	5:C:789:HOH:O	2.21	0.41
1:A:405:LYS:NZ	5:A:813:HOH:O	2.52	0.41
1:H:373:SER:O	1:H:377:GLU:HG3	2.21	0.41
1:B:384:TRP:CE2	1:B:412:PHE:HB2	2.56	0.41
1:E:423:GLN:NE2	1:G:325:GLU:O	2.53	0.41
1:F:384:TRP:CE2	1:F:412:PHE:HB2	2.56	0.41
1:H:419:PHE:O	1:H:423:GLN:HG3	2.20	0.41
1:C:421:GLN:OE1	5:C:808:HOH:O	2.22	0.40
1:A:391:GLN:HG2	5:A:772:HOH:O	2.20	0.40
1:H:432:HIS:HA	1:H:433:PRO:HD3	1.93	0.40
1:A:411:ILE:HD13	1:A:426:VAL:HG13	2.02	0.40
1:D:387:ARG:HH12	1:D:408:HIS:CE1	2.39	0.40
1:H:353:LEU:HB3	1:H:384:TRP:HB3	2.03	0.40

All (5) 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:H:365:GLU:OE1	5:A:646:HOH:O[2_855]	1.90	0.30
1:D:424:GLN:NE2	5:B:855:HOH:O[1_454]	2.03	0.17
5:B:836:HOH:O	5:D:737:HOH:O[1_656]	2.07	0.13
5:B:816:HOH:O	5:F:762:HOH:O[2_746]	2.18	0.02
1:E:438:ASP:OD2	5:A:682:HOH:O[2_755]	2.19	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	146/150 (97%)	143 (98%)	3 (2%)	0	100	100
1	B	147/150 (98%)	139 (95%)	5 (3%)	3 (2%)	6	0
1	C	149/150 (99%)	146 (98%)	3 (2%)	0	100	100
1	D	147/150 (98%)	142 (97%)	4 (3%)	1 (1%)	18	4
1	E	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
1	F	147/150 (98%)	144 (98%)	3 (2%)	0	100	100
1	G	146/150 (97%)	144 (99%)	2 (1%)	0	100	100
1	H	146/150 (97%)	140 (96%)	6 (4%)	0	100	100
All	All	1174/1200 (98%)	1142 (97%)	28 (2%)	4 (0%)	36	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ALA
1	B	363	GLN
1	D	417	HIS
1	B	390	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/132 (99%)	131 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	132/132 (100%)	130 (98%)	2 (2%)	57	26
1	C	134/132 (102%)	134 (100%)	0	100	100
1	D	132/132 (100%)	130 (98%)	2 (2%)	57	26
1	E	131/132 (99%)	129 (98%)	2 (2%)	57	26
1	F	132/132 (100%)	132 (100%)	0	100	100
1	G	131/132 (99%)	131 (100%)	0	100	100
1	H	131/132 (99%)	129 (98%)	2 (2%)	57	26
All	All	1054/1056 (100%)	1046 (99%)	8 (1%)	73	48

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	322	HIS
1	B	365	GLU
1	D	325	GLU
1	D	431	GLN
1	E	292	MET
1	E	420	GLN
1	H	361	ASP
1	H	418	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	414	ASN
1	A	417	HIS
1	A	421	GLN
1	B	322	HIS
1	B	363	GLN
1	B	418	HIS
1	B	421	GLN
1	C	431	GLN
1	D	322	HIS
1	D	406	GLN
1	E	349	ASN
1	F	337	ASN
1	F	418	HIS
1	G	417	HIS

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Mol	Chain	Res	Type
1	G	418	HIS
1	G	420	GLN
1	H	291	HIS
1	H	309	HIS
1	H	418	HIS
1	H	428	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	$\# Z > 2$
2	NLG	A	501	-	12,12,12	1.33	1 (8%)	15,15,15	1.48	4 (26%)
2	NLG	D	501	-	12,12,12	1.52	1 (8%)	15,15,15	1.21	1 (6%)
3	GOL	G	502	-	5,5,5	0.34	0	5,5,5	0.33	0
2	NLG	G	501	-	12,12,12	1.36	1 (8%)	15,15,15	1.37	2 (13%)
2	NLG	H	600	-	12,12,12	1.52	1 (8%)	15,15,15	1.28	1 (6%)
2	NLG	E	501	-	12,12,12	1.46	1 (8%)	15,15,15	1.22	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NLG	F	600	-	12,12,12	1.47	1 (8%)	15,15,15	1.34	1 (6%)
2	NLG	C	501	-	12,12,12	1.36	1 (8%)	15,15,15	1.38	2 (13%)
3	GOL	A	502	-	5,5,5	0.27	0	5,5,5	0.31	0
2	NLG	B	600	-	12,12,12	1.53	1 (8%)	15,15,15	1.13	1 (6%)

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	NLG	A	501	-	-	0/13/13/13	-
2	NLG	D	501	-	-	2/13/13/13	-
3	GOL	G	502	-	-	2/4/4/4	-
2	NLG	G	501	-	-	0/13/13/13	-
2	NLG	H	600	-	-	2/13/13/13	-
2	NLG	E	501	-	-	2/13/13/13	-
2	NLG	F	600	-	-	2/13/13/13	-
2	NLG	C	501	-	-	0/13/13/13	-
3	GOL	A	502	-	-	0/4/4/4	-
2	NLG	B	600	-	-	2/13/13/13	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	600	NLG	C7-N2	3.80	1.46	1.34
2	D	501	NLG	C7-N2	3.60	1.46	1.34
2	B	600	NLG	C7-N2	3.51	1.45	1.34
2	F	600	NLG	C7-N2	3.50	1.45	1.34
2	C	501	NLG	C7-N2	3.44	1.45	1.34
2	G	501	NLG	C7-N2	3.40	1.45	1.34
2	E	501	NLG	C7-N2	3.40	1.45	1.34
2	A	501	NLG	C7-N2	3.29	1.45	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	NLG	CG-CB-CA	3.81	120.18	113.16
2	A	501	NLG	OXT-C-O	-2.84	117.65	124.08
2	E	501	NLG	CG-CB-CA	2.82	118.37	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	600	NLG	CG-CB-CA	2.80	118.32	113.16
2	A	501	NLG	CB-CG-CD	2.71	119.71	112.49
2	D	501	NLG	CG-CB-CA	2.56	117.88	113.16
2	C	501	NLG	CB-CG-CD	2.56	119.32	112.49
2	G	501	NLG	CB-CG-CD	2.50	119.16	112.49
2	A	501	NLG	OXT-C-CA	2.31	121.34	113.51
2	A	501	NLG	OE2-CD-CG	2.28	121.22	114.00
2	B	600	NLG	CG-CB-CA	2.14	117.10	113.16
2	E	501	NLG	OXT-C-CA	2.12	120.69	113.51
2	C	501	NLG	OXT-C-CA	2.11	120.64	113.51
2	G	501	NLG	OXT-C-CA	2.03	120.39	113.51

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	502	GOL	O1-C1-C2-C3
3	G	502	GOL	O1-C1-C2-O2
2	D	501	NLG	OE2-CD-CG-CB
2	E	501	NLG	OE2-CD-CG-CB
2	D	501	NLG	OE1-CD-CG-CB
2	F	600	NLG	OE2-CD-CG-CB
2	B	600	NLG	OE2-CD-CG-CB
2	E	501	NLG	OE1-CD-CG-CB
2	F	600	NLG	OE1-CD-CG-CB
2	B	600	NLG	OE1-CD-CG-CB
2	H	600	NLG	OE2-CD-CG-CB
2	H	600	NLG	OE1-CD-CG-CB

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	501	NLG	1	0
2	C	501	NLG	1	0
3	A	502	GOL	2	0

5.7 Other polymers ⓘ

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	146/150 (97%)	0.16	2 (1%) 73 76	8, 14, 32, 39	2 (1%)
1	B	146/150 (97%)	0.94	15 (10%) 12 11	11, 22, 51, 87	3 (2%)
1	C	147/150 (98%)	0.10	3 (2%) 65 68	6, 14, 28, 53	4 (2%)
1	D	149/150 (99%)	0.70	12 (8%) 18 18	12, 20, 44, 74	0
1	E	147/150 (98%)	0.37	6 (4%) 41 43	6, 18, 33, 54	1 (0%)
1	F	148/150 (98%)	0.80	16 (10%) 11 11	11, 21, 48, 74	1 (0%)
1	G	146/150 (97%)	0.34	5 (3%) 48 50	8, 17, 33, 56	2 (1%)
1	H	147/150 (98%)	1.26	30 (20%) 3 2	14, 27, 64, 94	1 (0%)
All	All	1176/1200 (98%)	0.58	89 (7%) 20 20	6, 19, 44, 94	14 (1%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	6.6
1	A	408	HIS	6.2
1	D	417	HIS	6.2
1	F	364	GLY	5.4
1	F	362	ALA	5.3
1	H	362	ALA	5.3
1	H	364	GLY	5.2
1	H	417	HIS	4.9
1	B	417	HIS	4.8
1	D	416	LEU	4.6
1	B	363	GLN	4.5
1	H	418	HIS	4.5
1	H	437	ILE	4.2
1	H	389	ASN	4.0
1	D	408	HIS	3.9
1	H	388	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	365	GLU	3.7
1	E	292	MET	3.7
1	H	416	LEU	3.7
1	B	388	HIS	3.6
1	H	347	LEU	3.6
1	D	407	ASP	3.6
1	B	360	ASP	3.5
1	B	389	ASN	3.5
1	B	364	GLY	3.4
1	E	407	ASP	3.3
1	G	437	ILE	3.3
1	D	290	SER	3.2
1	B	361	ASP	3.2
1	F	361	ASP	3.2
1	C	292	MET	3.2
1	B	322	HIS	3.2
1	F	417	HIS	3.0
1	C	438	ASP	3.0
1	B	419	PHE	3.0
1	H	363	GLN	2.9
1	B	293	VAL	2.9
1	F	408	HIS	2.9
1	H	349	ASN	2.9
1	F	420	GLN	2.8
1	F	365	GLU	2.8
1	F	363	GLN	2.8
1	H	361	ASP	2.8
1	H	427	ALA	2.8
1	G	438	ASP	2.7
1	D	419	PHE	2.7
1	H	419	PHE	2.7
1	H	407	ASP	2.6
1	F	360	ASP	2.6
1	F	407	ASP	2.6
1	G	347	LEU	2.6
1	H	360	ASP	2.6
1	D	364	GLY	2.5
1	H	366	GLY	2.5
1	B	420	GLN	2.4
1	H	320	ILE	2.4
1	H	430	THR	2.4
1	G	419	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	391	GLN	2.4
1	D	427	ALA	2.4
1	H	329	LEU	2.3
1	H	291	HIS	2.3
1	D	362	ALA	2.3
1	G	320	ILE	2.3
1	E	347	LEU	2.3
1	H	321	PRO	2.3
1	B	408	HIS	2.3
1	E	418	HIS	2.3
1	D	420	GLN	2.3
1	D	388	HIS	2.2
1	H	415	GLY	2.2
1	B	437	ILE	2.2
1	H	359	LEU	2.2
1	F	366	GLY	2.2
1	H	348	GLY	2.1
1	H	431	GLN	2.1
1	F	419	PHE	2.1
1	H	390	ASN	2.1
1	A	438	ASP	2.1
1	E	433	PRO	2.1
1	F	389	ASN	2.1
1	B	418	HIS	2.1
1	F	370	ALA	2.1
1	H	387	ARG	2.0
1	D	391	GLN	2.0
1	H	429	CYS	2.0
1	F	387	ARG	2.0
1	E	293	VAL	2.0
1	C	361[A]	ASP	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
3	GOL	G	502	6/6	0.78	0.18	27,44,47,48	0
3	GOL	A	502	6/6	0.85	0.15	23,31,37,46	0
2	NLG	G	501	13/13	0.95	0.08	12,16,18,20	0
2	NLG	H	600	13/13	0.95	0.08	17,22,31,32	0
2	NLG	A	501	13/13	0.96	0.06	10,12,17,22	0
2	NLG	B	600	13/13	0.96	0.07	14,17,26,27	0
2	NLG	C	501	13/13	0.96	0.07	10,14,22,24	0
2	NLG	E	501	13/13	0.96	0.07	10,14,19,22	0
2	NLG	D	501	13/13	0.97	0.06	12,16,23,23	0
2	NLG	F	600	13/13	0.97	0.06	14,17,27,34	0
4	CL	D	502	1/1	0.97	0.13	27,27,27,27	0
4	CL	G	503	1/1	0.98	0.05	16,16,16,16	0
4	CL	C	502	1/1	0.99	0.04	15,15,15,15	0
4	CL	E	502	1/1	0.99	0.04	17,17,17,17	0
4	CL	E	503	1/1	0.99	0.08	27,27,27,27	0
4	CL	C	503	1/1	0.99	0.04	21,21,21,21	0
4	CL	G	504	1/1	0.99	0.04	19,19,19,19	0
4	CL	A	503	1/1	1.00	0.02	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.