



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:24 PM UTC

PDB ID : 6D8W / pdb_00006d8w
Title : Crystal structure of InvbI.18715.a.KN11: Influenza hemagglutinin from strain A/Jiangsu/ALSI/2011
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2018-04-27
Resolution : 2.35 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

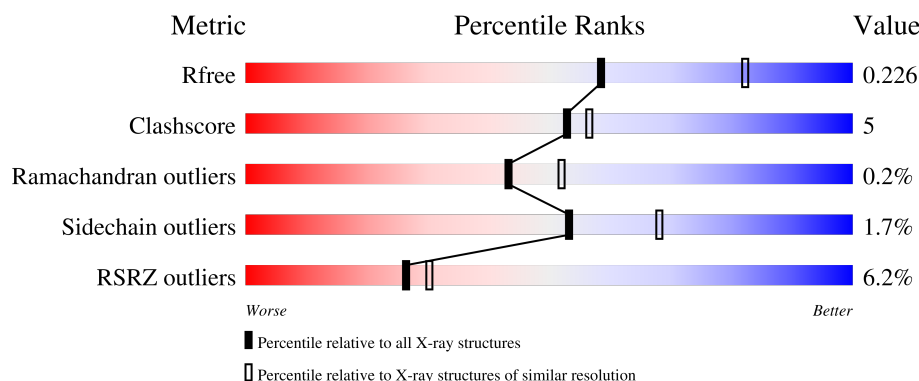
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	499	6% 80% 13% 7%
1	B	499	7% 87% 10% 7%
1	C	499	5% 85% 10% 5%
1	D	499	9% 79% 10% 11%
1	E	499	4% 84% 12% 7%

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Mol	Chain	Length	Quality of chain
1	F	499	

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
3	OXM	A	502	-	X	-	-
3	OXM	B	502	-	X	-	-
3	OXM	D	700	-	X	-	-
3	OXM	E	502	-	X	-	-
3	OXM	F	503	-	X	-	-
3	OXM	F	504	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22584 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	4	0
			3577	2250	625	683	19			
1	B	491	Total	C	N	O	S	0	5	0
			3729	2352	650	708	19			
1	C	476	Total	C	N	O	S	0	7	0
			3630	2292	632	687	19			
1	D	443	Total	C	N	O	S	0	3	0
			3344	2108	582	639	15			
1	E	477	Total	C	N	O	S	0	4	0
			3631	2292	625	695	19			
1	F	476	Total	C	N	O	S	0	3	0
			3636	2286	637	694	19			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP G0Z9B7
A	2	SER	-	expression tag	UNP G0Z9B7
A	493	PHE	-	expression tag	UNP G0Z9B7
A	494	LEU	-	expression tag	UNP G0Z9B7
A	495	VAL	-	expression tag	UNP G0Z9B7
A	496	PRO	-	expression tag	UNP G0Z9B7
A	497	ARG	-	expression tag	UNP G0Z9B7
B	1	GLY	-	expression tag	UNP G0Z9B7
B	2	SER	-	expression tag	UNP G0Z9B7
B	495	PHE	-	expression tag	UNP G0Z9B7
B	496	LEU	-	expression tag	UNP G0Z9B7
B	497	VAL	-	expression tag	UNP G0Z9B7
B	498	PRO	-	expression tag	UNP G0Z9B7
B	499	ARG	-	expression tag	UNP G0Z9B7
C	1	GLY	-	expression tag	UNP G0Z9B7
C	2	SER	-	expression tag	UNP G0Z9B7
C	495	PHE	-	expression tag	UNP G0Z9B7

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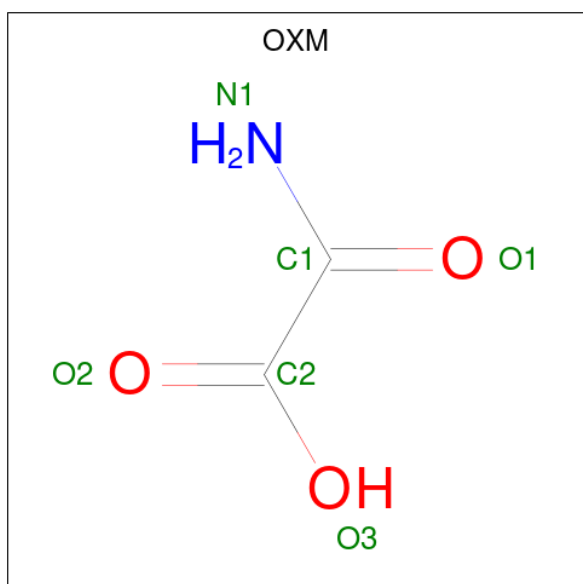
Chain	Residue	Modelled	Actual	Comment	Reference
C	496	LEU	-	expression tag	UNP G0Z9B7
C	497	VAL	-	expression tag	UNP G0Z9B7
C	498	PRO	-	expression tag	UNP G0Z9B7
C	499	ARG	-	expression tag	UNP G0Z9B7
D	1	GLY	-	expression tag	UNP G0Z9B7
D	2	SER	-	expression tag	UNP G0Z9B7
D	495	PHE	-	expression tag	UNP G0Z9B7
D	496	LEU	-	expression tag	UNP G0Z9B7
D	497	VAL	-	expression tag	UNP G0Z9B7
D	498	PRO	-	expression tag	UNP G0Z9B7
D	499	ARG	-	expression tag	UNP G0Z9B7
E	1	GLY	-	expression tag	UNP G0Z9B7
E	2	SER	-	expression tag	UNP G0Z9B7
E	495	PHE	-	expression tag	UNP G0Z9B7
E	496	LEU	-	expression tag	UNP G0Z9B7
E	497	VAL	-	expression tag	UNP G0Z9B7
E	498	PRO	-	expression tag	UNP G0Z9B7
E	499	ARG	-	expression tag	UNP G0Z9B7
F	1	GLY	-	expression tag	UNP G0Z9B7
F	2	SER	-	expression tag	UNP G0Z9B7
F	495	PHE	-	expression tag	UNP G0Z9B7
F	496	LEU	-	expression tag	UNP G0Z9B7
F	497	VAL	-	expression tag	UNP G0Z9B7
F	498	PRO	-	expression tag	UNP G0Z9B7
F	499	ARG	-	expression tag	UNP G0Z9B7

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



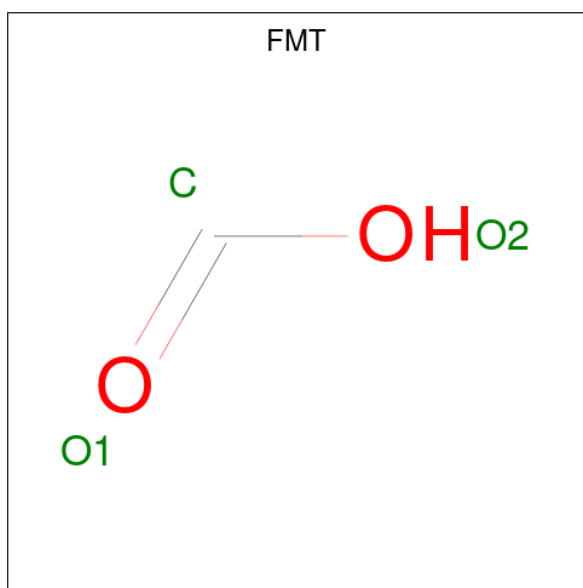
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is OXAMIC ACID (CCD ID: OXM) (formula: $C_2H_3NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	A	1	Total	C	N	O	0	0
			6	2	1	3		
3	B	1	Total	C	N	O	0	0
			6	2	1	3		
3	C	1	Total	C	N	O	0	0
			6	2	1	3		
3	D	1	Total	C	N	O	0	0
			6	2	1	3		
3	E	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		
3	F	1	Total	C	N	O	0	0
			6	2	1	3		

- Molecule 4 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	215	Total	O	0	2
			216	216		

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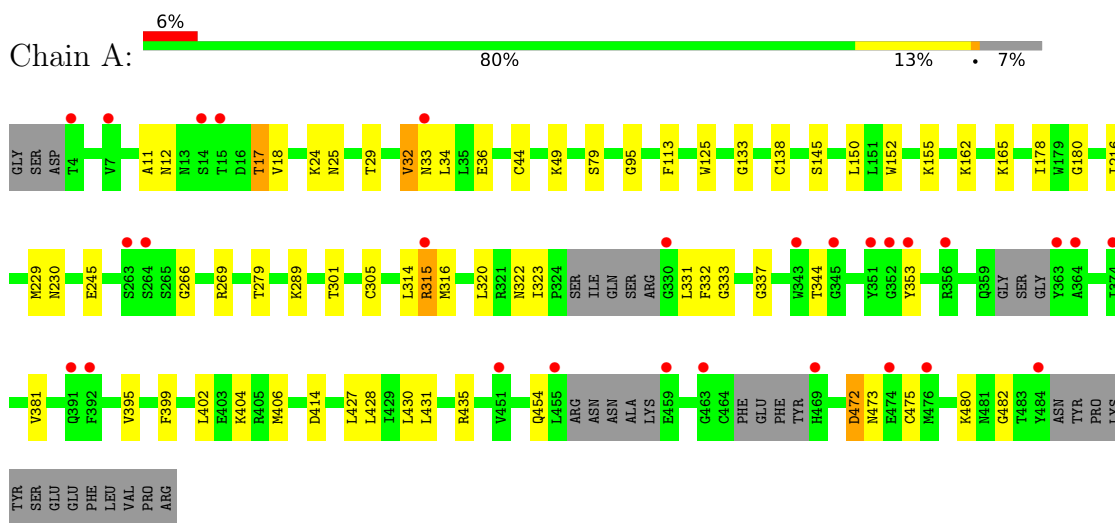
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	96	Total 96	O 96	0	0
5	C	156	Total 156	O 156	0	0
5	D	118	Total 120	O 120	0	2
5	E	152	Total 155	O 155	0	3
5	F	172	Total 173	O 173	0	1

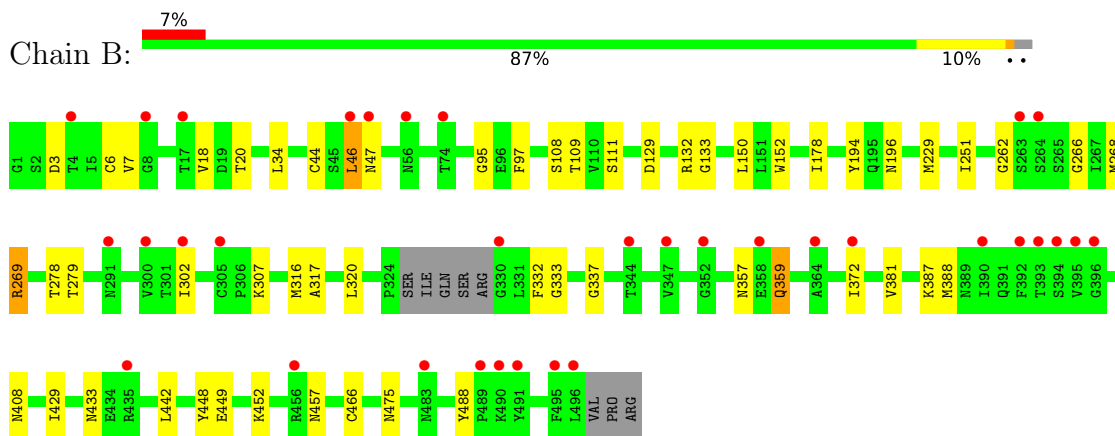
3 Residue-property plots [i](#)

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.

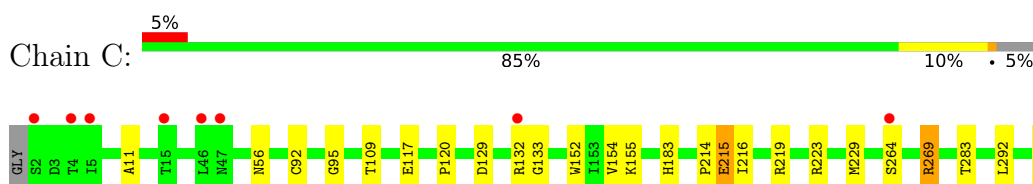
• Molecule 1: Hemagglutinin

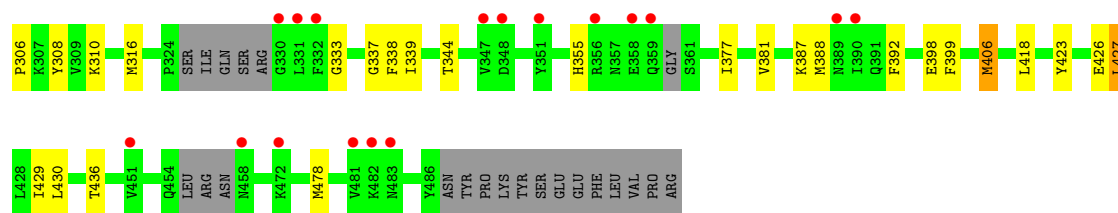


• Molecule 1: Hemagglutinin

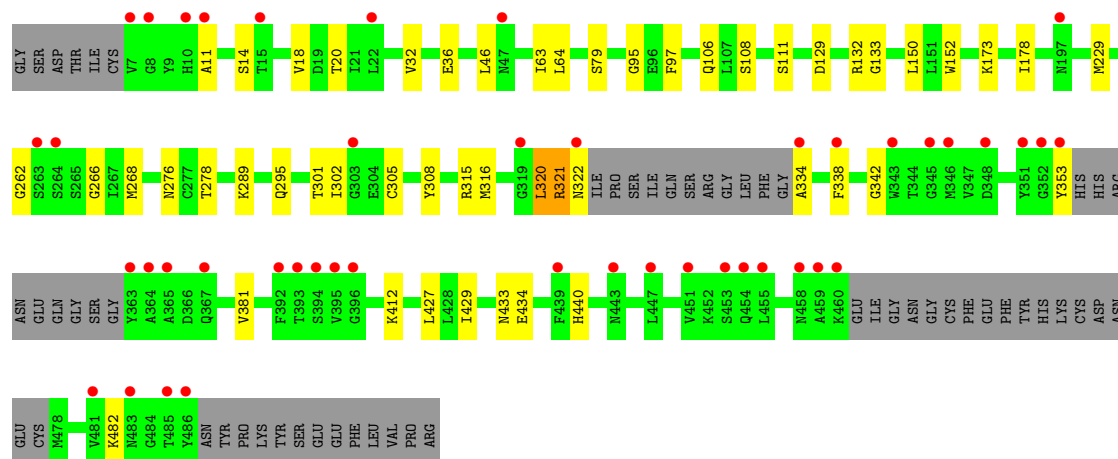
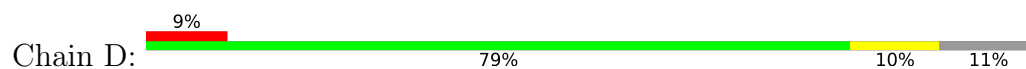


• Molecule 1: Hemagglutinin

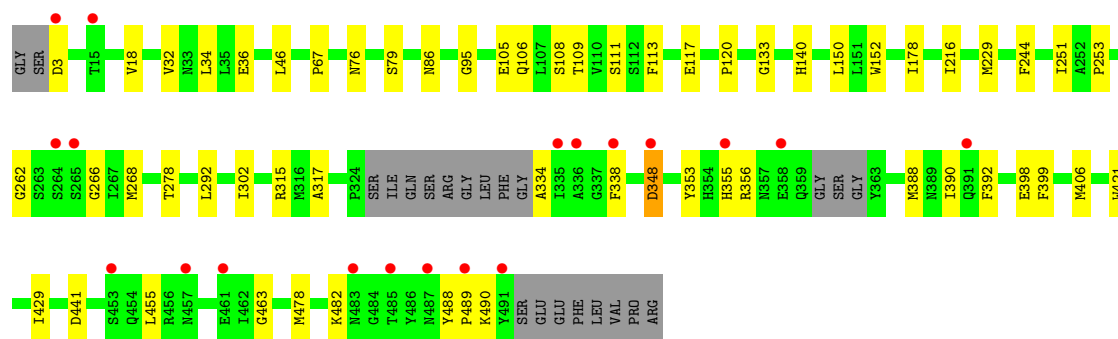
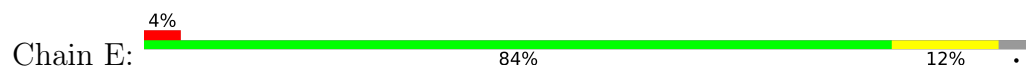




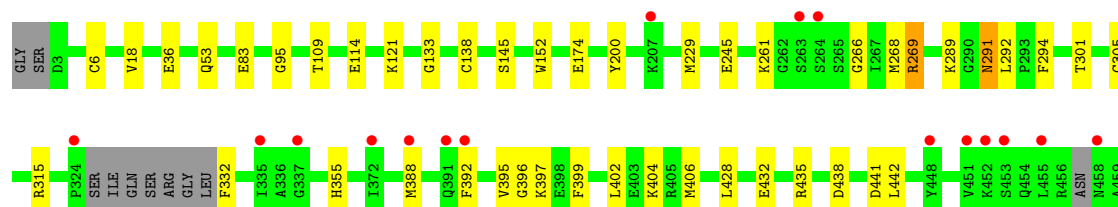
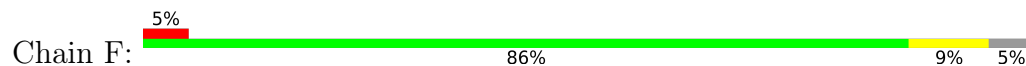
• Molecule 1: Hemagglutinin

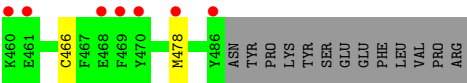


• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.30Å 113.33Å 130.12Å 110.16° 90.85° 90.28°	Depositor
Resolution (Å)	43.29 – 2.35 43.29 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.5 (43.29-2.35) 97.5 (43.29-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.179 , 0.225 0.181 , 0.226	Depositor DCC
R_{free} test set	2044 reflections (1.36%)	wwPDB-VP
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22584	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3547e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, NAG, OXM

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	0.36	0/3668	0.56	0/4985
1	B	0.31	0/3830	0.51	0/5216
1	C	0.33	0/3736	0.53	0/5086
1	D	0.33	0/3429	0.53	0/4672
1	E	0.33	0/3730	0.54	0/5086
1	F	0.36	0/3725	0.55	0/5066
All	All	0.34	0/22118	0.54	0/30111

There are no bond length outliers.

There are no bond angle outliers.

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	3577	0	3354	52	0
1	B	3729	0	3430	32	0
1	C	3630	0	3349	33	0
1	D	3344	0	3075	32	0
1	E	3631	0	3340	31	0
1	F	3636	0	3383	32	0
2	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	14	0	13	0	0
2	E	14	0	13	0	0
2	F	28	0	26	1	0
3	A	12	0	4	2	0
3	B	6	0	2	0	0
3	C	6	0	2	1	0
3	D	6	0	2	1	0
3	E	6	0	2	0	0
3	F	12	0	4	2	0
4	B	3	0	1	0	0
5	A	216	0	0	4	0
5	B	96	0	0	0	0
5	C	156	0	0	6	0
5	D	120	0	0	5	0
5	E	155	0	0	3	0
5	F	173	0	0	6	0
All	All	22584	0	20013	208	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 5.

All (208) 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:315:ARG:HA	1:A:315:ARG:CZ	1.90	1.00
1:A:33:ASN:HA	1:A:315:ARG:NH2	1.82	0.94
1:D:64:LEU:HD23	1:D:178[B]:ILE:HD11	1.51	0.91
1:A:32:VAL:O	1:A:315:ARG:NH1	2.12	0.82
1:F:266:GLY:HA3	1:F:395:VAL:HG11	1.61	0.79
1:A:33:ASN:HA	1:A:315:ARG:CZ	2.15	0.77
3:A:502:OXM:N1	5:A:601:HOH:O	2.16	0.75
1:C:316:MET:HE3	1:C:381:VAL:HG22	1.68	0.74
1:E:34:LEU:HD12	1:E:429:ILE:HD11	1.70	0.73
3:C:700:OXM:N1	5:C:801:HOH:O	2.14	0.72
1:C:219[A]:ARG:NH2	5:C:804:HOH:O	2.23	0.70
1:D:133:GLY:HA3	1:D:152:TRP:HB3	1.73	0.70
1:F:133:GLY:HA3	1:F:152:TRP:HB3	1.74	0.70
1:A:315:ARG:NH1	1:A:316:MET:H	1.92	0.68
1:C:355:HIS:HB2	1:C:478:MET:HE3	1.75	0.67
1:B:316:MET:HE3	1:B:381:VAL:HG22	1.77	0.66
1:E:399:PHE:HE1	1:E:406:MET:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:ARG:HA	1:A:315:ARG:NH2	2.11	0.66
1:D:111:SER:HB3	1:D:262:GLY:HA3	1.77	0.65
1:B:457:ASN:OD1	1:B:488:TYR:OH	2.14	0.64
1:C:132:ARG:NH2	1:C:155:LYS:O	2.31	0.64
1:E:399:PHE:CE1	1:E:406:MET:HE2	2.33	0.62
1:F:355:HIS:HB2	1:F:478:MET:HE3	1.81	0.62
1:B:46:LEU:HD21	1:B:302:ILE:HG22	1.81	0.61
1:E:86:ASN:ND2	5:E:602:HOH:O	2.33	0.61
1:A:314:LEU:O	1:A:315:ARG:NH2	2.34	0.61
1:A:95:GLY:HA3	1:A:229:MET:O	2.01	0.60
1:F:399:PHE:CD1	1:F:406:MET:HE3	2.36	0.60
1:F:332:PHE:HE2	1:F:438:ASP:HB3	1.65	0.60
1:F:95:GLY:HA3	1:F:229:MET:O	2.01	0.59
1:F:83:GLU:OE1	3:F:504:OXM:N1	2.35	0.59
1:C:283:THR:HG22	1:C:301:THR:HG22	1.83	0.59
1:F:269:ARG:NH1	5:F:601:HOH:O	2.29	0.59
1:D:129:ASP:OD2	1:D:132:ARG:NH1	2.36	0.58
2:F:502:NAG:H3	2:F:502:NAG:H83	1.86	0.58
1:B:95:GLY:HA3	1:B:229:MET:O	2.05	0.57
1:C:133:GLY:HA3	1:C:152:TRP:HB3	1.86	0.57
1:A:399:PHE:CE1	1:A:406:MET:HE2	2.39	0.57
1:E:67:PRO:HB2	1:E:140:HIS:HB2	1.87	0.56
1:C:95:GLY:HA3	1:C:229:MET:O	2.06	0.56
1:D:95:GLY:HA3	1:D:229:MET:O	2.06	0.55
1:D:322:ASN:OD1	5:D:801:HOH:O	2.18	0.55
1:B:129:ASP:OD2	1:B:132:ARG:NH1	2.40	0.55
1:A:315:ARG:HA	1:A:315:ARG:NE	2.22	0.55
1:A:34:LEU:H	1:A:315:ARG:NH2	2.05	0.55
1:E:133:GLY:HA3	1:E:152:TRP:HB3	1.88	0.55
1:D:64:LEU:CD2	1:D:178[B]:ILE:HD11	2.30	0.55
1:E:348:ASP:OD1	1:E:348:ASP:N	2.32	0.55
1:B:34:LEU:HD12	1:B:429:ILE:HD11	1.89	0.54
1:A:427:LEU:HD21	1:F:428:LEU:HD13	1.90	0.54
1:F:294:PHE:HZ	1:F:388:MET:HE3	1.73	0.54
1:D:276:ASN:ND2	5:D:804:HOH:O	2.35	0.53
1:C:56:ASN:HB2	5:C:911:HOH:O	2.08	0.53
1:F:397[A]:LYS:HB3	5:F:746:HOH:O	2.09	0.53
1:B:108:SER:HB3	1:B:266:GLY:HA2	1.91	0.53
1:D:320:LEU:HD12	1:D:321:ARG:O	2.09	0.52
1:B:133:GLY:HA3	1:B:152:TRP:HB3	1.91	0.52
1:E:18:VAL:HG21	1:E:317:ALA:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:GLU:OE1	5:E:601:HOH:O	2.19	0.52
1:A:353:TYR:CD1	1:A:480:LYS:HG2	2.45	0.52
1:F:432:GLU:OE2	1:F:435:ARG:NH1	2.43	0.52
1:A:454:GLN:HE22	1:A:482:GLY:HA2	1.76	0.51
1:A:12:ASN:HD21	1:A:29:THR:HB	1.74	0.51
1:B:268:MET:HE3	1:B:302:ILE:HD12	1.92	0.51
1:E:95:GLY:HA3	1:E:229:MET:O	2.10	0.51
1:F:399:PHE:HD1	1:F:406:MET:HE3	1.74	0.51
1:A:431:LEU:O	1:A:435:ARG:HG3	2.11	0.51
1:D:353:TYR:CD1	1:D:482:LYS:HG2	2.45	0.51
1:D:108:SER:HB2	1:D:266:GLY:HA2	1.92	0.50
1:F:397[B]:LYS:HB3	5:F:746:HOH:O	2.10	0.50
1:C:303:GLY:HA2	1:C:392:PHE:CE2	2.45	0.50
1:B:387:LYS:HD2	1:C:426:GLU:HB3	1.92	0.50
1:F:18:VAL:HG12	1:F:315:ARG:HG2	1.94	0.50
1:D:150:LEU:HD21	1:D:178[A]:ILE:HG13	1.93	0.50
1:F:53[B]:GLN:NE2	5:F:604:HOH:O	2.44	0.50
1:F:269:ARG:HG2	3:F:504:OXM:N1	2.27	0.50
1:E:488:TYR:O	1:E:490:LYS:N	2.38	0.49
3:D:700:OXM:N1	5:D:802:HOH:O	2.24	0.49
1:E:3:ASP:HA	1:E:356:ARG:O	2.11	0.49
1:D:268:MET:HE3	1:D:302:ILE:HD12	1.93	0.49
1:A:316:MET:HE1	1:A:381:VAL:HA	1.94	0.49
1:C:215[B]:GLU:OE1	5:C:802:HOH:O	2.19	0.49
1:D:18:VAL:HG12	1:D:315:ARG:HG2	1.94	0.49
1:D:301:THR:HB	1:D:305:CYS:SG	2.53	0.49
1:D:334:ALA:HA	1:D:338:PHE:CE1	2.47	0.48
1:F:6:CYS:HA	1:F:466:CYS:HA	1.95	0.48
1:A:133:GLY:HA3	1:A:152:TRP:HB3	1.95	0.48
1:D:63:ILE:HG22	1:D:178[B]:ILE:HD12	1.95	0.48
1:F:200:TYR:OH	1:F:245:GLU:OE2	2.28	0.48
1:F:395:VAL:HG23	1:F:396:GLY:O	2.13	0.48
1:E:111:SER:HB3	1:E:262:GLY:HA3	1.96	0.48
1:E:46:LEU:HB2	1:E:79:SER:HB2	1.95	0.48
1:A:12:ASN:ND2	1:A:29:THR:HB	2.28	0.48
1:B:150:LEU:HD21	1:B:178[A]:ILE:HG23	1.95	0.48
1:A:17:THR:OG1	1:A:25:ASN:HA	2.13	0.48
1:B:316:MET:HE1	1:B:381:VAL:HA	1.95	0.48
1:C:308:TYR:CD2	1:C:418:LEU:HD13	2.49	0.48
1:B:20:THR:HG22	1:B:433:ASN:HB3	1.96	0.47
1:A:49:LYS:HB3	1:A:79:SER:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:ALA:O	1:C:344:THR:HA	2.15	0.47
1:C:338:PHE:CD1	1:C:339:ILE:HG13	2.50	0.47
1:E:106:GLN:O	1:E:109:THR:HG22	2.14	0.47
1:A:125:TRP:CZ3	1:A:165[B]:LYS:HG3	2.50	0.47
1:C:129:ASP:OD2	1:C:132:ARG:NH1	2.48	0.47
1:F:289:LYS:HB3	1:F:291:ASN:ND2	2.30	0.47
1:E:108:SER:HB3	1:E:266:GLY:HA2	1.96	0.46
1:A:472:ASP:CG	1:A:473:ASN:H	2.23	0.46
1:B:269:ARG:HH21	1:B:269:ARG:HG3	1.81	0.46
1:F:174:GLU:HG2	5:F:681:HOH:O	2.15	0.46
1:A:162:LYS:HZ1	1:A:245:GLU:CD	2.17	0.46
1:B:3:ASP:OD1	1:B:357:ASN:HA	2.15	0.46
1:A:331:LEU:HG	1:F:442:LEU:HD23	1.97	0.46
1:A:301:THR:HB	1:A:305:CYS:SG	2.54	0.46
1:B:359:GLN:NE2	1:B:475:ASN:H	2.14	0.46
1:E:338:PHE:HB2	1:E:463:GLY:O	2.16	0.46
1:E:36:GLU:HG3	1:E:292:LEU:HB2	1.98	0.46
1:F:332:PHE:N	1:F:441:ASP:OD2	2.49	0.46
1:A:428:LEU:HD13	1:D:427:LEU:HD21	1.98	0.46
1:F:301:THR:HB	1:F:305:CYS:SG	2.55	0.46
1:A:32:VAL:C	1:A:315:ARG:NH1	2.73	0.46
1:A:333:GLY:O	1:A:337:GLY:HA3	2.16	0.46
1:A:266:GLY:HA3	1:A:395:VAL:HG11	1.99	0.45
1:C:398:GLU:OE1	5:C:803:HOH:O	2.21	0.45
1:C:377:ILE:HD12	1:C:436:THR:HG23	1.98	0.45
1:F:109:THR:OG1	1:F:261:LYS:HD2	2.16	0.45
1:C:183:HIS:CE1	1:C:214:PRO:HA	2.52	0.45
1:C:388:MET:HE2	1:C:388:MET:HB2	1.66	0.45
1:E:76:ASN:HA	1:E:113:PHE:HB3	1.97	0.45
1:C:377:ILE:O	1:C:381:VAL:HG23	2.17	0.45
1:A:315:ARG:CZ	1:A:315:ARG:CA	2.81	0.45
1:A:404:LYS:NZ	5:A:614:HOH:O	2.47	0.44
1:C:269:ARG:NH1	5:C:817:HOH:O	2.49	0.44
1:A:36:GLU:OE2	1:A:289:LYS:N	2.49	0.44
1:D:268:MET:HE3	1:D:268:MET:HB2	1.78	0.44
1:D:295:GLN:O	1:D:308:TYR:HA	2.17	0.44
1:A:18:VAL:HG12	1:A:315:ARG:HG3	1.98	0.44
1:D:20:THR:HB	1:D:434:GLU:HB2	1.98	0.44
1:D:36:GLU:OE2	1:D:289:LYS:N	2.51	0.44
1:A:399:PHE:HE1	1:A:406:MET:HE2	1.80	0.44
1:A:399:PHE:CD1	1:A:406:MET:HE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLY:O	1:B:337:GLY:HA3	2.18	0.43
1:C:423:TYR:CE2	1:C:427:LEU:HD22	2.52	0.43
1:C:117:GLU:HG2	1:C:120:PRO:HA	1.99	0.43
1:E:18:VAL:HG12	1:E:315:ARG:HG2	2.01	0.43
1:B:150:LEU:HB3	1:B:251:ILE:HG22	2.01	0.43
1:D:20:THR:HG22	1:D:433:ASN:HB3	2.00	0.43
1:D:106:GLN:NE2	1:F:404:LYS:HG3	2.33	0.43
1:B:388:MET:HG2	1:C:423:TYR:CE1	2.53	0.43
1:A:138:CYS:O	1:A:145:SER:HB3	2.18	0.43
1:A:162:LYS:NZ	1:A:245:GLU:OE2	2.28	0.43
1:C:399:PHE:CE1	1:C:406:MET:HE3	2.54	0.43
1:D:353:TYR:CE1	1:D:482:LYS:HG2	2.54	0.43
1:A:155:LYS:NZ	5:A:619:HOH:O	2.51	0.43
1:A:414:ASP:OD1	1:D:412:LYS:NZ	2.52	0.43
1:B:97:PHE:CZ	1:B:178[A]:ILE:HD11	2.54	0.43
1:B:332:PHE:CD1	1:B:442:LEU:HD13	2.54	0.43
1:C:292:LEU:O	1:C:306:PRO:HB3	2.19	0.43
1:A:11:ALA:O	1:A:344:THR:HA	2.19	0.42
1:A:331:LEU:HD23	1:A:332:PHE:CE1	2.54	0.42
1:E:46:LEU:HD23	1:E:46:LEU:HA	1.93	0.42
1:E:334:ALA:HB3	1:E:441:ASP:OD1	2.19	0.42
1:F:399:PHE:CE1	1:F:406:MET:HE3	2.53	0.42
1:C:109:THR:HG22	1:C:264:SER:HA	2.00	0.42
1:C:338:PHE:CE1	1:C:339:ILE:HG13	2.55	0.42
1:B:18:VAL:HG21	1:B:317:ALA:HB2	2.01	0.42
1:D:14:SER:N	5:D:801:HOH:O	2.52	0.42
1:B:449:GLU:HA	1:B:452:LYS:HB3	2.01	0.42
1:C:333:GLY:O	1:C:337:GLY:HA3	2.19	0.42
1:A:315:ARG:NH1	1:A:316:MET:N	2.65	0.42
1:C:387:LYS:HD3	1:C:387:LYS:HA	1.88	0.42
1:E:150:LEU:HB3	1:E:251:ILE:HG22	2.02	0.42
1:C:310:LYS:HG3	1:C:418:LEU:HD11	2.00	0.42
1:E:268:MET:HE3	1:E:302:ILE:HD12	2.02	0.42
1:B:44:CYS:HB2	1:B:279:THR:HG22	2.00	0.42
1:B:408:ASN:ND2	1:E:105:GLU:OE2	2.32	0.42
1:F:121:LYS:NZ	5:F:602:HOH:O	2.40	0.42
1:B:111:SER:HB3	1:B:262:GLY:HA3	2.01	0.41
1:D:46:LEU:HB3	1:D:79:SER:HB2	2.01	0.41
1:C:92:CYS:O	1:C:223:ARG:NE	2.34	0.41
1:F:36:GLU:HG3	1:F:292:LEU:HB2	2.02	0.41
1:E:390:ILE:HA	5:E:727:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:C	1:A:323:ILE:HG13	2.46	0.41
1:B:6:CYS:HA	1:B:466:CYS:HA	2.03	0.41
1:A:18:VAL:HG12	1:A:315:ARG:CG	2.50	0.41
1:A:269:ARG:NH2	3:A:503:OXM:O1	2.54	0.41
1:A:402:LEU:HD23	1:A:402:LEU:HA	1.94	0.41
1:E:117:GLU:HG2	1:E:120:PRO:HA	2.02	0.41
1:E:388:MET:HE1	1:E:421:TRP:CZ3	2.55	0.41
1:A:150:LEU:HD21	1:A:178[A]:ILE:HG13	2.03	0.41
1:A:180:GLY:HA2	1:A:230:ASN:O	2.21	0.41
1:B:307:LYS:HG3	1:B:388:MET:HE1	2.02	0.41
1:B:320:LEU:H	1:B:320:LEU:HG	1.72	0.41
1:D:97:PHE:HB2	5:D:873:HOH:O	2.21	0.41
1:D:320:LEU:HB3	1:D:440:HIS:CG	2.55	0.41
1:E:353:TYR:CD1	1:E:482:LYS:HG2	2.56	0.41
1:F:138:CYS:O	1:F:145:SER:HB3	2.21	0.41
1:A:44:CYS:HB2	1:A:279:THR:HG22	2.03	0.41
1:D:11:ALA:HB2	1:D:342:GLY:HA3	2.03	0.41
1:D:316:MET:HE1	1:D:381:VAL:HA	2.02	0.41
1:E:355:HIS:HB2	1:E:478:MET:HE3	2.03	0.41
1:F:402:LEU:HD23	1:F:402:LEU:HA	1.91	0.41
1:A:395:VAL:HG22	5:A:690:HOH:O	2.20	0.40
1:B:194:TYR:O	1:B:196:ASN:N	2.51	0.40
1:C:132:ARG:HH21	1:C:154:VAL:HG23	1.86	0.40
1:A:32:VAL:O	1:A:315:ARG:CZ	2.67	0.40
1:B:7:VAL:HG21	1:B:448:TYR:HA	2.03	0.40
1:E:244:PHE:CZ	1:E:253:PRO:HG2	2.56	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	460/499 (92%)	443 (96%)	16 (4%)	1 (0%)	43	52
1	B	492/499 (99%)	474 (96%)	17 (4%)	1 (0%)	43	52
1	C	475/499 (95%)	463 (98%)	12 (2%)	0	100	100
1	D	438/499 (88%)	425 (97%)	13 (3%)	0	100	100
1	E	475/499 (95%)	457 (96%)	16 (3%)	2 (0%)	30	34
1	F	473/499 (95%)	458 (97%)	14 (3%)	1 (0%)	43	52
All	All	2813/2994 (94%)	2720 (97%)	88 (3%)	5 (0%)	43	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	392	PHE
1	B	47	ASN
1	A	472	ASP
1	E	489	PRO
1	E	392	PHE

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	376/435 (86%)	367 (98%)	9 (2%)	43	57
1	B	378/435 (87%)	372 (98%)	6 (2%)	55	70
1	C	370/435 (85%)	362 (98%)	8 (2%)	45	59
1	D	337/435 (78%)	331 (98%)	6 (2%)	51	66
1	E	375/435 (86%)	368 (98%)	7 (2%)	50	65
1	F	377/435 (87%)	373 (99%)	4 (1%)	65	79
All	All	2213/2610 (85%)	2173 (98%)	40 (2%)	53	66

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	24	LYS
1	A	32	VAL
1	A	113	PHE
1	A	216	ILE
1	A	315	ARG
1	A	320	LEU
1	A	430	LEU
1	A	475	CYS
1	B	46	LEU
1	B	109	THR
1	B	269	ARG
1	B	278	THR
1	B	359	GLN
1	B	372	ILE
1	C	215[A]	GLU
1	C	215[B]	GLU
1	C	216	ILE
1	C	269	ARG
1	C	406	MET
1	C	427	LEU
1	C	429	ILE
1	C	430	LEU
1	D	32	VAL
1	D	173	LYS
1	D	278	THR
1	D	320	LEU
1	D	321	ARG
1	D	429	ILE
1	E	32	VAL
1	E	178[A]	ILE
1	E	178[B]	ILE
1	E	216	ILE
1	E	278	THR
1	E	348	ASP
1	E	455	LEU
1	F	114	GLU
1	F	268	MET
1	F	269	ARG
1	F	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	140	HIS
1	A	191	GLN
1	A	255	HIS
1	A	275	HIS
1	A	379	ASN
1	A	454	GLN
1	B	195	GLN
1	B	275	HIS
1	B	487	ASN
1	C	33	ASN
1	C	354	HIS
1	D	140	HIS
1	D	230	ASN
1	D	255	HIS
1	D	275	HIS
1	E	89	ASN
1	E	195	GLN
1	E	275	HIS
1	F	158	ASN
1	F	195	GLN
1	F	291	ASN
1	F	371	GLN

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 ⓘ

14 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	NAG	E	501	1	14,14,15	0.35	0	17,19,21	0.37	0
3	OXM	E	502	-	5,5,5	3.35	2 (40%)	2,6,6	1.12	0
3	OXM	C	700	-	5,5,5	4.10	1 (20%)	2,6,6	1.51	0
2	NAG	F	501	1	14,14,15	0.62	0	17,19,21	0.71	1 (5%)
3	OXM	B	502	-	5,5,5	3.81	2 (40%)	2,6,6	0.86	0
3	OXM	F	504	-	5,5,5	2.54	2 (40%)	2,6,6	1.26	0
2	NAG	B	501	1	14,14,15	0.66	1 (7%)	17,19,21	0.46	0
3	OXM	A	502	-	5,5,5	4.25	2 (40%)	2,6,6	1.16	0
4	FMT	B	503	-	2,2,2	0.68	0	1,1,1	0.24	0
3	OXM	D	700	-	5,5,5	3.53	2 (40%)	2,6,6	0.60	0
3	OXM	A	503	-	5,5,5	2.56	1 (20%)	2,6,6	1.36	0
3	OXM	F	503	-	5,5,5	3.43	2 (40%)	2,6,6	0.74	0
2	NAG	A	501	1	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	F	502	1	14,14,15	0.57	0	17,19,21	1.57	2 (11%)

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	NAG	E	501	1	-	2/6/23/26	0/1/1/1
3	OXM	E	502	-	-	4/4/4/4	-
3	OXM	C	700	-	-	3/4/4/4	-
2	NAG	F	501	1	-	2/6/23/26	0/1/1/1
3	OXM	B	502	-	-	4/4/4/4	-
3	OXM	F	504	-	-	4/4/4/4	-
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
3	OXM	A	502	-	-	4/4/4/4	-
3	OXM	D	700	-	-	4/4/4/4	-
3	OXM	A	503	-	-	4/4/4/4	-
3	OXM	F	503	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
2	NAG	F	502	1	-	6/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	OXM	C1-C2	-8.98	1.44	1.55
3	C	700	OXM	C1-C2	-8.85	1.45	1.55
3	B	502	OXM	C1-C2	-8.16	1.45	1.55
3	D	700	OXM	C1-C2	-7.47	1.46	1.55
3	F	503	OXM	C1-C2	-7.26	1.46	1.55
3	E	502	OXM	C1-C2	-6.88	1.47	1.55
3	A	503	OXM	C1-C2	-5.23	1.49	1.55
3	F	504	OXM	C1-C2	-5.11	1.49	1.55
3	A	502	OXM	O3-C2	-2.96	1.22	1.30
3	E	502	OXM	O3-C2	-2.87	1.22	1.30
3	B	502	OXM	O3-C2	-2.47	1.23	1.30
3	D	700	OXM	O3-C2	-2.45	1.23	1.30
3	F	503	OXM	O3-C2	-2.33	1.24	1.30
2	B	501	NAG	O5-C1	-2.17	1.40	1.43
3	F	504	OXM	O3-C2	-2.07	1.24	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	502	NAG	C2-N2-C7	4.71	129.21	122.90
2	F	502	NAG	C1-C2-N2	3.18	115.45	110.43
2	F	501	NAG	C1-O5-C5	2.10	115.00	112.19

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	OXM	N1-C1-C2-O2
3	A	502	OXM	N1-C1-C2-O3
3	A	502	OXM	O1-C1-C2-O3
3	A	503	OXM	N1-C1-C2-O2
3	A	503	OXM	N1-C1-C2-O3
3	A	503	OXM	O1-C1-C2-O3
3	B	502	OXM	N1-C1-C2-O3
3	B	502	OXM	O1-C1-C2-O3

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Mol	Chain	Res	Type	Atoms
3	C	700	OXM	N1-C1-C2-O2
3	C	700	OXM	N1-C1-C2-O3
3	D	700	OXM	N1-C1-C2-O2
3	D	700	OXM	N1-C1-C2-O3
3	D	700	OXM	O1-C1-C2-O2
3	D	700	OXM	O1-C1-C2-O3
3	E	502	OXM	N1-C1-C2-O2
3	E	502	OXM	N1-C1-C2-O3
3	E	502	OXM	O1-C1-C2-O3
3	F	503	OXM	N1-C1-C2-O2
3	F	503	OXM	N1-C1-C2-O3
3	F	503	OXM	O1-C1-C2-O3
3	F	504	OXM	N1-C1-C2-O2
3	F	504	OXM	N1-C1-C2-O3
3	F	504	OXM	O1-C1-C2-O3
2	E	501	NAG	C4-C5-C6-O6
2	F	502	NAG	O5-C5-C6-O6
2	E	501	NAG	O5-C5-C6-O6
2	F	502	NAG	C4-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	F	502	NAG	C8-C7-N2-C2
2	F	502	NAG	O7-C7-N2-C2
3	A	503	OXM	O1-C1-C2-O2
2	B	501	NAG	C4-C5-C6-O6
2	A	501	NAG	C4-C5-C6-O6
3	A	502	OXM	O1-C1-C2-O2
3	C	700	OXM	O1-C1-C2-O2
3	E	502	OXM	O1-C1-C2-O2
3	F	503	OXM	O1-C1-C2-O2
2	F	501	NAG	C1-C2-N2-C7
2	A	501	NAG	O5-C5-C6-O6
3	F	504	OXM	O1-C1-C2-O2
2	F	502	NAG	C3-C2-N2-C7
3	B	502	OXM	O1-C1-C2-O2
3	B	502	OXM	N1-C1-C2-O2
2	F	502	NAG	C1-C2-N2-C7
2	F	501	NAG	C3-C2-N2-C7

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	700	OXM	1	0
3	F	504	OXM	2	0
3	A	502	OXM	1	0
3	D	700	OXM	1	0
3	A	503	OXM	1	0
2	F	502	NAG	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

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	466/499 (93%)	0.15	28 (6%)	27	31	17, 50, 123, 145	4 (0%)
1	B	491/499 (98%)	0.40	34 (6%)	23	26	22, 65, 108, 125	5 (1%)
1	C	476/499 (95%)	0.26	26 (5%)	30	36	17, 58, 116, 150	7 (1%)
1	D	443/499 (88%)	0.42	45 (10%)	12	13	20, 61, 129, 151	3 (0%)
1	E	477/499 (95%)	0.16	19 (3%)	42	48	22, 55, 104, 132	4 (0%)
1	F	476/499 (95%)	0.10	23 (4%)	35	41	17, 51, 108, 133	3 (0%)
All	All	2829/2994 (94%)	0.25	175 (6%)	26	30	17, 57, 115, 151	26 (0%)

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	491	TYR	6.1
1	D	392	PHE	5.2
1	C	264	SER	5.2
1	F	264	SER	5.1
1	D	8	GLY	4.9
1	D	7	VAL	4.9
1	C	331	LEU	4.6
1	D	393	THR	4.6
1	D	264	SER	4.5
1	A	315	ARG	4.3
1	B	495	PHE	4.3
1	F	458	ASN	4.2
1	D	345	GLY	4.1
1	A	484	TYR	4.0
1	D	343	TRP	4.0
1	C	481	VAL	4.0
1	B	491	TYR	4.0
1	B	390	ILE	4.0
1	B	264	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	394	SER	3.8
1	D	364	ALA	3.8
1	A	474	GLU	3.8
1	E	3	ASP	3.7
1	C	332	PHE	3.7
1	F	335	ILE	3.7
1	F	460	LYS	3.7
1	B	263	SER	3.7
1	C	483	ASN	3.6
1	D	263	SER	3.6
1	C	389	ASN	3.6
1	A	330	GLY	3.6
1	D	454	GLN	3.5
1	D	395	VAL	3.5
1	C	2	SER	3.5
1	C	359	GLN	3.5
1	F	324	PRO	3.4
1	B	330	GLY	3.4
1	A	264	SER	3.3
1	A	33	ASN	3.3
1	E	457	ASN	3.3
1	A	455	LEU	3.3
1	E	15	THR	3.3
1	F	391	GLN	3.3
1	B	496	LEU	3.2
1	C	390	ILE	3.2
1	C	358	GLU	3.1
1	A	363	TYR	3.1
1	D	443	ASN	3.1
1	D	451	VAL	3.1
1	C	47	ASN	3.0
1	D	352	GLY	3.0
1	C	330	GLY	3.0
1	C	46	LEU	3.0
1	A	14	SER	3.0
1	D	453	SER	3.0
1	E	264	SER	3.0
1	A	476	MET	2.9
1	B	8	GLY	2.9
1	C	451	VAL	2.9
1	D	367	GLN	2.9
1	D	459	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	346	MET	2.8
1	A	263	SER	2.8
1	B	456	ARG	2.8
1	D	353	TYR	2.8
1	F	461	GLU	2.8
1	E	355	HIS	2.8
1	A	469	HIS	2.7
1	B	291	ASN	2.7
1	D	396	GLY	2.7
1	E	265	SER	2.7
1	B	395	VAL	2.7
1	A	345	GLY	2.7
1	F	263	SER	2.7
1	D	447	LEU	2.7
1	D	11	ALA	2.7
1	D	351	TYR	2.7
1	B	364	ALA	2.6
1	D	334	ALA	2.6
1	F	468	GLU	2.6
1	B	347	VAL	2.6
1	C	4	THR	2.6
1	C	458	ASN	2.6
1	D	322	ASN	2.6
1	A	15	THR	2.6
1	E	335	ILE	2.6
1	C	351	TYR	2.6
1	F	388	MET	2.6
1	F	451	VAL	2.6
1	F	392	PHE	2.6
1	B	352	GLY	2.5
1	B	393	THR	2.5
1	B	47	ASN	2.5
1	A	352	GLY	2.5
1	B	489	PRO	2.5
1	E	453	SER	2.5
1	F	478	MET	2.5
1	A	356	ARG	2.5
1	D	458	ASN	2.5
1	C	305	CYS	2.4
1	B	46	LEU	2.4
1	A	364	ALA	2.4
1	E	336	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	303	GLY	2.4
1	E	489	PRO	2.4
1	B	394	SER	2.4
1	B	435	ARG	2.4
1	A	392	PHE	2.4
1	D	460	LYS	2.4
1	D	486	TYR	2.4
1	E	391	GLN	2.4
1	F	337	GLY	2.4
1	B	396	GLY	2.3
1	C	472	LYS	2.3
1	D	365	ALA	2.3
1	B	4	THR	2.3
1	E	485	THR	2.3
1	B	302	ILE	2.3
1	D	483	ASN	2.3
1	B	74	THR	2.3
1	F	372	ILE	2.3
1	D	455	LEU	2.3
1	F	455	LEU	2.3
1	A	463	GLY	2.3
1	D	363	TYR	2.3
1	F	470	TYR	2.3
1	D	15	THR	2.3
1	E	358	GLU	2.3
1	B	300	VAL	2.3
1	D	439	PHE	2.3
1	C	348	ASP	2.3
1	B	344	THR	2.3
1	A	391	GLN	2.3
1	A	7	VAL	2.3
1	D	338	PHE	2.2
1	D	481	VAL	2.3
1	E	348	ASP	2.2
1	A	459	GLU	2.2
1	B	392	PHE	2.2
1	C	347	VAL	2.2
1	D	47	ASN	2.2
1	B	305	CYS	2.2
1	B	358	GLU	2.2
1	F	469	PHE	2.2
1	C	482	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	15	THR	2.2
1	E	461	GLU	2.2
1	B	17	THR	2.2
1	A	351	TYR	2.1
1	A	353	TYR	2.1
1	C	5	ILE	2.1
1	D	348	ASP	2.1
1	D	485	THR	2.1
1	A	374	ILE	2.1
1	E	483	ASN	2.1
1	E	487	ASN	2.1
1	F	448	TYR	2.1
1	F	486	TYR	2.1
1	A	451	VAL	2.1
1	A	343	TRP	2.1
1	D	319	GLY	2.1
1	F	453	SER	2.1
1	B	56[A]	ASN	2.1
1	B	372	ILE	2.1
1	D	197	ASN	2.1
1	E	338	PHE	2.1
1	B	490	LYS	2.0
1	F	207	LYS	2.0
1	D	22	LEU	2.0
1	F	452	LYS	2.0
1	A	4	THR	2.0
1	D	10	HIS	2.0
1	B	483	ASN	2.0
1	C	132	ARG	2.0
1	C	356	ARG	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

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	NAG	F	502	14/15	0.57	0.17	92,104,110,113	0
2	NAG	F	501	14/15	0.63	0.16	85,102,110,113	0
2	NAG	E	501	14/15	0.68	0.14	78,102,109,111	0
2	NAG	B	501	14/15	0.71	0.14	73,94,110,113	0
2	NAG	A	501	14/15	0.74	0.13	75,85,89,91	0
4	FMT	B	503	3/3	0.81	0.16	91,91,92,93	0
3	OXM	F	504	6/6	0.82	0.14	75,81,82,87	0
3	OXM	A	503	6/6	0.86	0.18	90,90,93,96	0
3	OXM	B	502	6/6	0.90	0.16	47,55,61,74	0
3	OXM	C	700	6/6	0.90	0.18	50,65,83,84	0
3	OXM	A	502	6/6	0.92	0.16	44,55,60,64	0
3	OXM	D	700	6/6	0.92	0.17	61,65,83,93	0
3	OXM	F	503	6/6	0.93	0.15	56,61,76,80	0
3	OXM	E	502	6/6	0.95	0.13	45,56,63,74	0

6.5 Other polymers

There are no such residues in this entry.