



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:03 AM UTC

PDB ID : 3FG3 / pdb_00003fg3
Title : Crystal structure of Delta413-417:GS I805W LOX
Authors : Neau, D.B.; Newcomer, M.E.
Deposited on : 2008-12-04
Resolution : 1.90 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

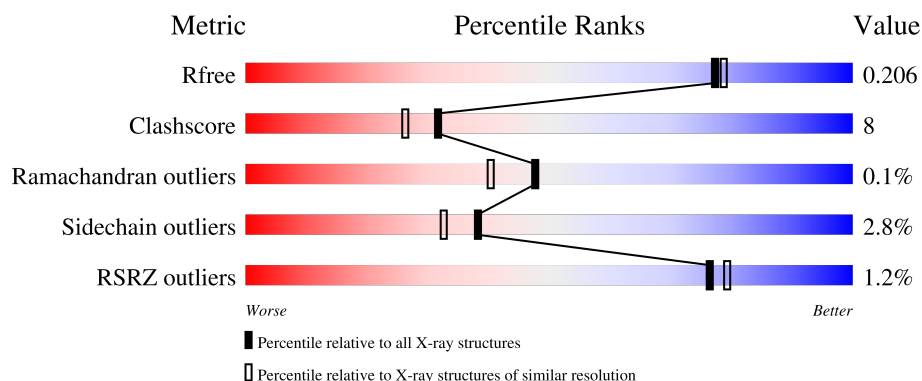
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	696	% 83% 14% ..
1	B	696	2% 82% 15% ..
1	C	696	% 83% 14% ..
1	D	696	% 84% 13% ..

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
4	ACY	A	2200[B]	-	-	X	-
4	ACY	A	2201	-	-	X	-
4	ACY	A	2204	-	-	X	-
4	ACY	A	2222	-	-	X	-
4	ACY	C	2209[A]	-	-	X	-
4	ACY	C	2210	-	-	X	-
4	ACY	C	2213	-	-	X	-
4	ACY	D	2219	-	-	X	-
5	GOL	A	2306	-	-	X	-
5	GOL	B	2310	-	X	X	-
5	GOL	C	2315	-	-	X	-
5	GOL	C	2321	-	-	X	-
5	GOL	C	2322	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25025 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 Allene oxide synthase-lipoxygenase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	25	0
			5624	3596	943	1071	14			
1	B	682	Total	C	N	O	S	0	23	0
			5552	3554	928	1056	14			
1	C	686	Total	C	N	O	S	3	21	0
			5576	3565	938	1060	13			
1	D	681	Total	C	N	O	S	0	22	0
			5538	3549	926	1049	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	MET	-	expression tag	UNP O16025
A	369	HIS	-	expression tag	UNP O16025
A	370	HIS	-	expression tag	UNP O16025
A	371	HIS	-	expression tag	UNP O16025
A	372	HIS	-	expression tag	UNP O16025
A	373	HIS	-	expression tag	UNP O16025
A	?	-	TRP	deletion	UNP O16025
A	?	-	PHE	deletion	UNP O16025
A	?	-	HIS	deletion	UNP O16025
A	413	GLY	ASN	engineered mutation	UNP O16025
A	414	SER	ASP	engineered mutation	UNP O16025
A	782	ILE	VAL	SEE REMARK 999	UNP O16025
A	805	TRP	ILE	engineered mutation	UNP O16025
A	963	ILE	VAL	SEE REMARK 999	UNP O16025
B	368	MET	-	expression tag	UNP O16025
B	369	HIS	-	expression tag	UNP O16025
B	370	HIS	-	expression tag	UNP O16025
B	371	HIS	-	expression tag	UNP O16025
B	372	HIS	-	expression tag	UNP O16025
B	373	HIS	-	expression tag	UNP O16025
B	?	-	TRP	deletion	UNP O16025

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP O16025
B	?	-	HIS	deletion	UNP O16025
B	413	GLY	ASN	engineered mutation	UNP O16025
B	414	SER	ASP	engineered mutation	UNP O16025
B	782	ILE	VAL	SEE REMARK 999	UNP O16025
B	805	TRP	ILE	engineered mutation	UNP O16025
B	963	ILE	VAL	SEE REMARK 999	UNP O16025
C	368	MET	-	expression tag	UNP O16025
C	369	HIS	-	expression tag	UNP O16025
C	370	HIS	-	expression tag	UNP O16025
C	371	HIS	-	expression tag	UNP O16025
C	372	HIS	-	expression tag	UNP O16025
C	373	HIS	-	expression tag	UNP O16025
C	?	-	TRP	deletion	UNP O16025
C	?	-	PHE	deletion	UNP O16025
C	?	-	HIS	deletion	UNP O16025
C	413	GLY	ASN	engineered mutation	UNP O16025
C	414	SER	ASP	engineered mutation	UNP O16025
C	782	ILE	VAL	SEE REMARK 999	UNP O16025
C	805	TRP	ILE	engineered mutation	UNP O16025
C	963	ILE	VAL	SEE REMARK 999	UNP O16025
D	368	MET	-	expression tag	UNP O16025
D	369	HIS	-	expression tag	UNP O16025
D	370	HIS	-	expression tag	UNP O16025
D	371	HIS	-	expression tag	UNP O16025
D	372	HIS	-	expression tag	UNP O16025
D	373	HIS	-	expression tag	UNP O16025
D	?	-	TRP	deletion	UNP O16025
D	?	-	PHE	deletion	UNP O16025
D	?	-	HIS	deletion	UNP O16025
D	413	GLY	ASN	engineered mutation	UNP O16025
D	414	SER	ASP	engineered mutation	UNP O16025
D	782	ILE	VAL	SEE REMARK 999	UNP O16025
D	805	TRP	ILE	engineered mutation	UNP O16025
D	963	ILE	VAL	SEE REMARK 999	UNP O16025

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

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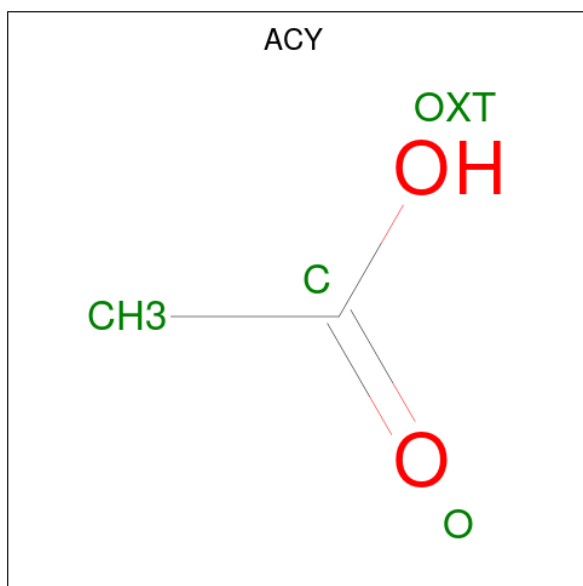
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	1	Total	Ca	0	0
			1	1		
3	C	3	Total	Ca	0	0
			3	3		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 8	C 4	O 4	0	1
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	1
			12	6	6		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0
6	B	1	Total Cl 1 1	0	0
6	C	2	Total Cl 2 2	0	0
6	D	1	Total Cl 1 1	0	0

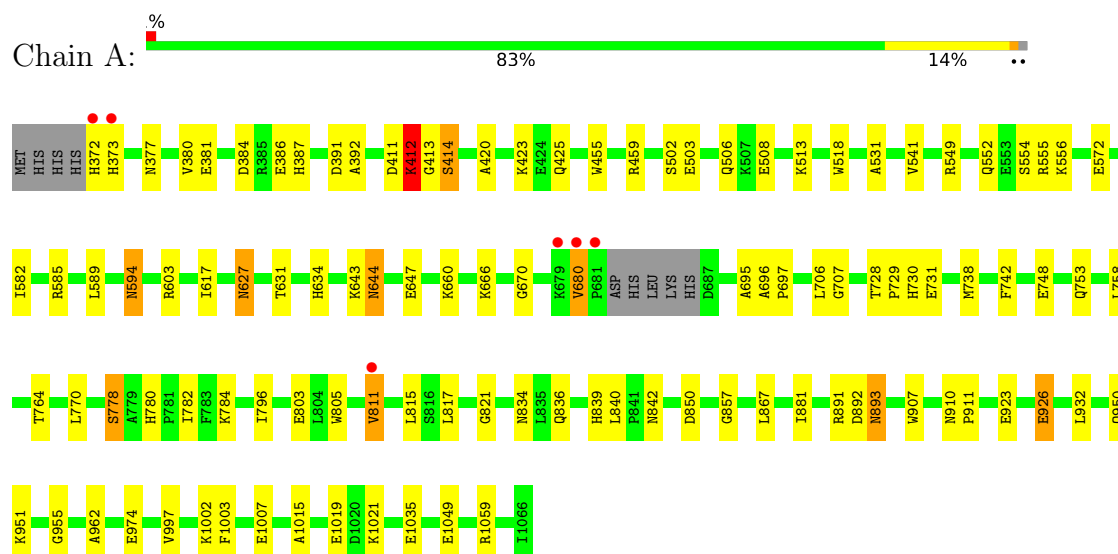
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	748	Total O 748 748	0	0
7	B	526	Total O 526 526	0	0
7	C	672	Total O 672 672	0	0
7	D	539	Total O 539 539	0	0

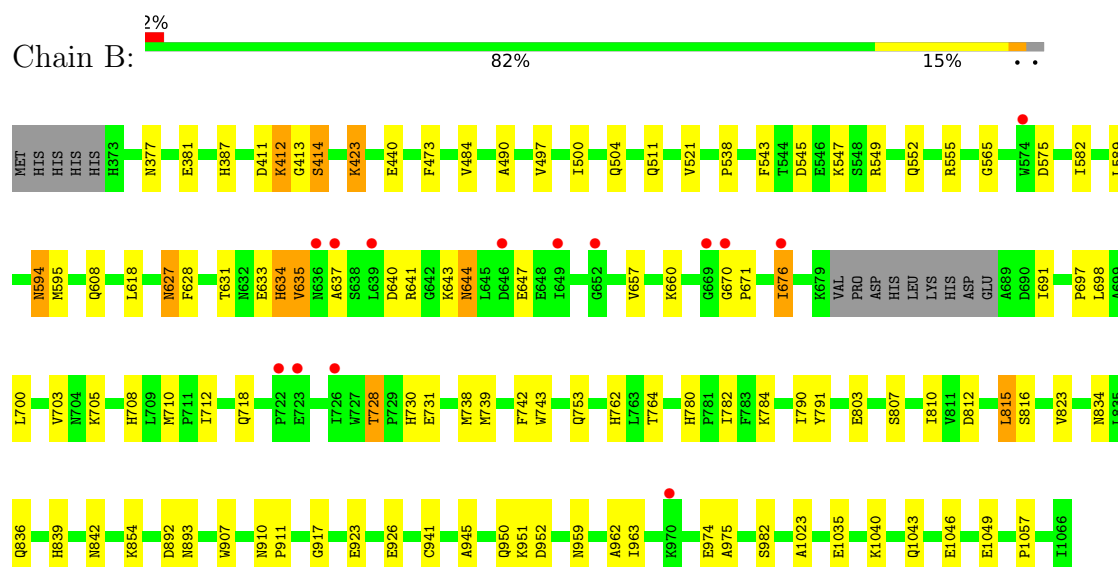
3 Residue-property plots [i](#)

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.

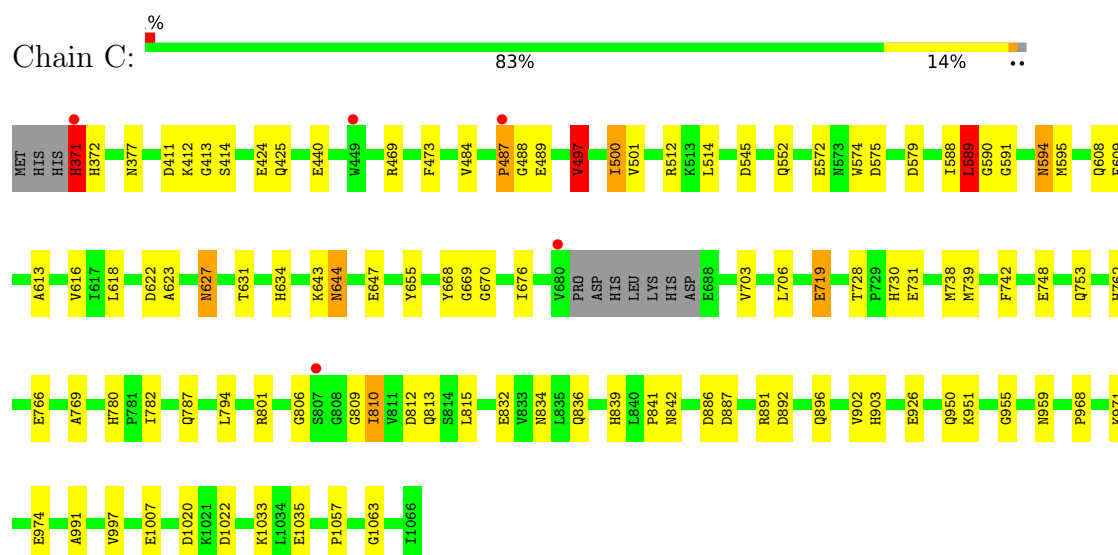
- Molecule 1: Allene oxide synthase-lipoxygenase protein



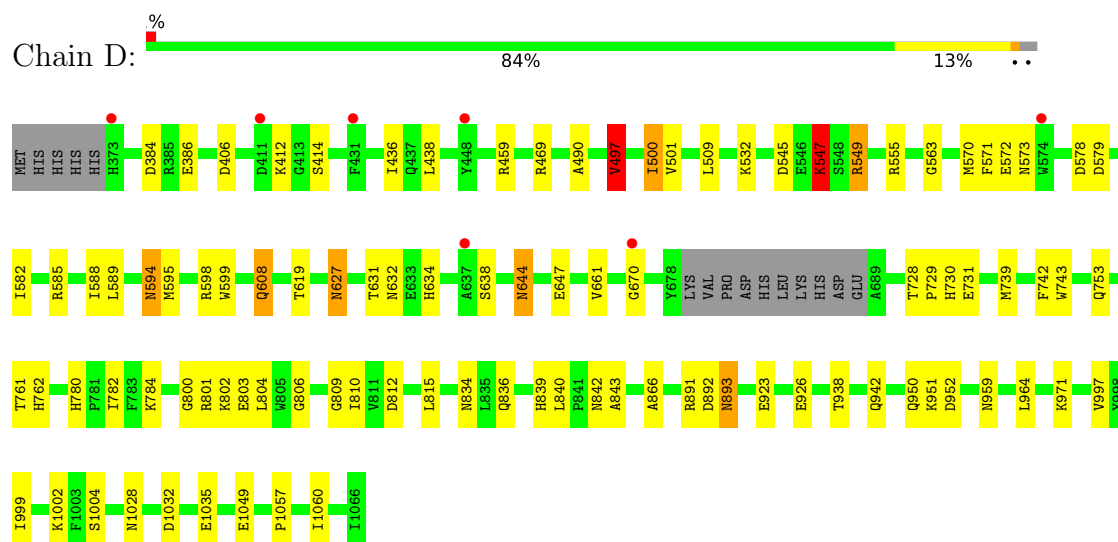
- Molecule 1: Allene oxide synthase-lipoxygenase protein



- Molecule 1: Allene oxide synthase-lipoxygenase protein



• Molecule 1: Allene oxide synthase-lipoxygenase protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.70Å 170.21Å 104.20Å 90.00° 96.13° 90.00°	Depositor
Resolution (Å)	34.54 – 1.90 34.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.54-1.90) 98.6 (34.54-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.89Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.206 0.162 , 0.206	Depositor DCC
R_{free} test set	14029 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.098 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25025	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: ACY, CA, GOL, CL, FE2

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	1.38	11/5851 (0.2%)	1.15	12/7955 (0.2%)
1	B	1.28	9/5773 (0.2%)	1.10	11/7856 (0.1%)
1	C	1.43	12/5791 (0.2%)	1.17	21/7878 (0.3%)
1	D	1.32	11/5754 (0.2%)	1.10	9/7827 (0.1%)
All	All	1.35	43/23169 (0.2%)	1.13	53/31516 (0.2%)

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
1	B	0	1
1	C	0	3
All	All	0	6

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	414	SER	C-N	14.97	1.52	1.33
1	B	414	SER	C-N	8.65	1.50	1.34
1	C	623	ALA	CA-CB	7.61	1.66	1.53
1	D	843	ALA	CA-CB	7.14	1.64	1.53
1	D	414	SER	C-N	7.03	1.47	1.34
1	A	420	ALA	N-CA	6.09	1.53	1.46
1	C	991	ALA	CA-CB	6.04	1.62	1.53
1	D	563	GLY	CA-C	5.84	1.58	1.52
1	D	547	LYS	CG-CD	5.78	1.69	1.52
1	B	676	ILE	CA-CB	5.72	1.62	1.54
1	C	968	PRO	CA-C	5.69	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	436	ILE	CA-CB	5.63	1.61	1.54
1	B	473	PHE	N-CA	-5.61	1.40	1.46
1	A	932	LEU	N-CA	5.61	1.53	1.46
1	A	796	ILE	CA-CB	5.61	1.62	1.54
1	D	661	VAL	CA-CB	5.53	1.61	1.54
1	B	945	ALA	CA-CB	5.50	1.61	1.53
1	A	881	ILE	CA-CB	5.43	1.61	1.54
1	D	1028	ASN	N-CA	5.42	1.52	1.46
1	C	903	HIS	N-CA	5.37	1.52	1.46
1	C	616	VAL	N-CA	5.36	1.52	1.46
1	A	541	VAL	CA-CB	5.35	1.60	1.54
1	A	617	ILE	CA-C	5.33	1.59	1.53
1	C	613	ALA	CA-CB	5.28	1.62	1.53
1	B	538	PRO	C-O	5.26	1.30	1.23
1	C	955	GLY	C-O	5.24	1.30	1.23
1	A	680	VAL	CA-CB	5.22	1.60	1.54
1	A	696	ALA	CA-CB	5.20	1.59	1.53
1	D	964	LEU	N-CA	5.19	1.52	1.45
1	C	769	ALA	CA-CB	5.16	1.61	1.53
1	A	955	GLY	N-CA	5.13	1.52	1.45
1	B	790	ILE	CA-CB	5.13	1.61	1.54
1	B	565	GLY	C-O	5.13	1.29	1.23
1	B	1023	ALA	CA-CB	5.12	1.61	1.53
1	C	512	ARG	N-CA	5.12	1.52	1.46
1	A	531	ALA	CA-CB	5.12	1.62	1.53
1	D	866	ALA	CA-CB	5.12	1.61	1.53
1	D	608	GLN	N-CA	5.11	1.52	1.46
1	C	902	VAL	C-O	-5.09	1.18	1.24
1	C	669	GLY	N-CA	-5.07	1.38	1.45
1	B	497	VAL	CA-CB	5.06	1.60	1.54
1	D	840	LEU	CA-C	5.02	1.58	1.52
1	A	867	LEU	N-CA	5.01	1.52	1.46

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	372	HIS	N-CA-C	10.99	126.79	113.16
1	C	589	LEU	N-CA-C	9.42	124.97	113.38
1	D	549	ARG	NE-CZ-NH2	-7.83	112.15	119.20
1	C	886	ASP	N-CA-C	7.45	119.40	111.28
1	B	414	SER	O-C-N	-7.43	112.99	122.20
1	A	414[A]	SER	O-C-N	-7.18	114.91	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414[B]	SER	O-C-N	-7.18	114.91	123.03
1	C	414	SER	CA-C-N	-7.11	111.71	123.37
1	C	414	SER	C-N-CA	-7.11	111.71	123.37
1	D	497	VAL	N-CA-CB	-6.82	101.67	111.21
1	C	497	VAL	N-CA-CB	-6.61	101.96	111.21
1	C	371	HIS	CA-C-N	6.40	133.96	122.38
1	C	371	HIS	C-N-CA	6.40	133.96	122.38
1	D	585	ARG	NE-CZ-NH1	-6.34	115.16	121.50
1	C	414	SER	O-C-N	6.31	130.16	122.84
1	C	813	GLN	N-CA-C	6.14	120.24	112.87
1	A	670	GLY	N-CA-C	6.03	124.63	112.34
1	C	589	LEU	CA-C-N	5.84	132.22	121.70
1	C	589	LEU	C-N-CA	5.84	132.22	121.70
1	B	521	VAL	N-CA-C	-5.83	104.64	111.00
1	B	633	GLU	N-CA-C	-5.78	104.67	110.97
1	D	585	ARG	NE-CZ-NH2	5.77	124.39	119.20
1	A	811	VAL	N-CA-C	5.73	116.47	110.62
1	C	769	ALA	N-CA-C	-5.72	104.95	111.07
1	D	497	VAL	CG1-CB-CG2	5.67	123.28	110.80
1	A	414[A]	SER	CA-C-N	5.62	131.67	123.12
1	A	414[A]	SER	C-N-CA	5.62	131.67	123.12
1	A	414[B]	SER	CA-C-N	5.62	131.67	123.12
1	A	414[B]	SER	C-N-CA	5.62	131.67	123.12
1	B	975	ALA	N-CA-C	5.58	118.32	109.96
1	C	787	GLN	CA-C-N	-5.53	114.12	119.87
1	C	787	GLN	C-N-CA	-5.53	114.12	119.87
1	C	703	VAL	CB-CA-C	-5.44	105.35	111.23
1	B	974	GLU	N-CA-C	5.42	117.27	111.36
1	D	384	ASP	N-CA-C	5.40	119.71	113.18
1	B	697	PRO	N-CA-C	5.35	119.10	111.13
1	A	412	LYS	CB-CA-C	-5.28	103.44	110.79
1	B	917	GLY	CA-C-N	-5.28	118.79	122.59
1	B	917	GLY	C-N-CA	-5.28	118.79	122.59
1	C	1063	GLY	N-CA-C	5.26	118.89	111.42
1	A	840	LEU	CA-C-N	-5.24	113.23	119.05
1	A	840	LEU	C-N-CA	-5.24	113.23	119.05
1	C	670	GLY	CA-C-N	-5.24	114.36	119.76
1	C	670	GLY	C-N-CA	-5.24	114.36	119.76
1	B	812	ASP	CB-CA-C	-5.21	99.42	110.31
1	B	549	ARG	NE-CZ-NH2	-5.21	114.52	119.20
1	C	591	GLY	N-CA-C	-5.16	100.95	113.18
1	D	670	GLY	N-CA-C	5.11	122.77	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	532	LYS	CB-CA-C	5.11	118.97	110.90
1	C	589	LEU	O-C-N	-5.07	115.78	122.42
1	D	1060	ILE	CB-CA-C	-5.04	105.39	111.18
1	B	941	CYS	N-CA-C	5.02	116.44	111.07
1	A	412	LYS	N-CA-C	-5.02	98.88	107.61

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	414[A]	SER	Mainchain
1	A	680	VAL	Peptide
1	B	414	SER	Mainchain
1	C	371	HIS	Peptide
1	C	589	LEU	Peptide
1	C	668	TYR	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	5624	0	5393	107	0
1	B	5552	0	5281	84	0
1	C	5576	0	5311	85	1
1	D	5538	0	5281	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	36	0	27	11	0
4	B	16	0	12	2	0
4	C	28	0	21	9	0
4	D	20	0	15	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	60	0	78	17	0
5	B	24	0	32	10	0
5	C	36	0	48	20	0
5	D	12	0	16	3	0
6	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	1	0
6	D	1	0	0	0	0
7	A	748	0	0	30	0
7	B	526	0	0	16	1
7	C	672	0	0	26	0
7	D	539	0	0	9	0
All	All	25025	0	21515	358	1

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 8.

All (358) 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:1035:GLU:OE2	5:B:2310:GOL:H31	1.25	1.25
1:A:459:ARG:NH2	7:A:2081:HOH:O	1.69	1.25
1:D:1002:LYS:HE2	7:D:1225:HOH:O	1.31	1.23
1:C:832:GLU:HG3	7:C:2400:HOH:O	1.40	1.21
1:C:489:GLU:CB	1:C:1020[B]:ASP:OD2	1.89	1.19
1:B:547:LYS:HD2	1:B:791[B]:TYR:OH	1.43	1.16
1:C:572[B]:GLU:OE2	5:C:2322:GOL:H31	1.45	1.16
1:C:1035:GLU:OE2	5:C:2321:GOL:H31	1.43	1.13
1:B:547:LYS:HE3	1:B:791[B]:TYR:HE2	1.14	1.10
1:C:1020[B]:ASP:OD1	6:C:2402:CL:CL	2.06	1.10
5:C:2315:GOL:H12	7:C:1254:HOH:O	1.51	1.09
1:D:579:ASP:OD2	5:D:2319:GOL:H2	1.51	1.08
1:B:644[A]:ASN:HD22	1:B:647:GLU:HG3	1.18	1.06
1:A:552[A]:GLN:HE21	4:A:2201:ACY:H1	1.13	1.06
1:C:572[B]:GLU:OE2	5:C:2322:GOL:C3	2.03	1.05
1:B:644[A]:ASN:ND2	1:B:647:GLU:HG3	1.75	1.02
5:A:2320[A]:GOL:H31	1:B:413:GLY:O	1.57	1.02
1:D:608:GLN:HE22	1:D:959:ASN:HD21	1.07	1.00
1:C:413:GLY:O	5:C:2315:GOL:H11	1.61	1.00
1:B:728:THR:HG23	1:B:730:HIS:H	1.27	0.97
1:B:1035:GLU:OE2	5:B:2310:GOL:C3	2.13	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:THR:H	1:C:634:HIS:HD2	1.10	0.97
1:C:608:GLN:HE22	1:C:959:ASN:HD21	1.14	0.95
1:B:780:HIS:HD2	1:B:782:ILE:H	1.17	0.93
1:B:387:HIS:ND1	7:B:2320:HOH:O	1.79	0.93
1:C:810:ILE:HD13	7:C:2170:HOH:O	1.66	0.93
1:B:547:LYS:HE3	1:B:791[B]:TYR:CE2	2.04	0.92
1:C:579:ASP:OD2	5:C:2322:GOL:H11	1.68	0.92
1:A:413:GLY:O	5:B:2310:GOL:H12	1.70	0.92
1:A:603[B]:ARG:HG2	1:A:603[B]:ARG:HH11	1.32	0.91
1:C:572[B]:GLU:HG2	1:C:574:TRP:NE1	1.85	0.91
1:A:1049:GLU:OE1	7:A:2059:HOH:O	1.87	0.91
1:A:631:THR:H	1:A:634:HIS:HD2	1.18	0.91
1:A:834:ASN:HD22	1:A:836[A]:GLN:H	1.20	0.90
1:C:572[B]:GLU:HG2	1:C:574:TRP:HE1	1.35	0.90
1:D:834:ASN:HD22	1:D:836:GLN:H	1.15	0.90
1:C:834:ASN:HD22	1:C:836:GLN:H	1.19	0.90
1:C:780:HIS:HD2	1:C:782:ILE:H	1.15	0.90
1:A:1049:GLU:OE2	7:A:2098:HOH:O	1.88	0.90
1:B:893[B]:ASN:OD1	7:B:2342:HOH:O	1.90	0.89
4:C:2210:ACY:H2	7:C:2407:HOH:O	1.68	0.89
5:C:2321:GOL:H2	7:C:1145:HOH:O	1.70	0.89
1:D:780:HIS:HD2	1:D:782:ILE:H	1.13	0.89
1:A:834:ASN:HD22	1:A:836[B]:GLN:H	1.21	0.89
1:A:780:HIS:HD2	1:A:782:ILE:H	1.22	0.87
1:D:608:GLN:HB2	4:D:2214:ACY:H3	1.56	0.86
1:A:387:HIS:ND1	7:A:2318:HOH:O	1.91	0.86
1:C:489:GLU:CB	7:C:1238:HOH:O	2.23	0.85
1:B:511[B]:GLN:OE1	7:B:1933:HOH:O	1.95	0.85
1:A:730:HIS:ND1	7:A:2193:HOH:O	2.08	0.85
1:B:640:ASP:OD2	1:B:705:LYS:HG2	1.77	0.85
1:B:412:LYS:NZ	7:B:2404:HOH:O	2.10	0.83
1:A:748:GLU:OE1	4:A:2200[B]:ACY:CH3	2.26	0.83
1:D:627:ASN:H	1:D:627:ASN:HD22	1.26	0.83
1:A:384:ASP:H	5:A:2306:GOL:H31	1.44	0.82
1:C:579:ASP:CG	5:C:2322:GOL:H11	2.04	0.82
1:B:834:ASN:HD22	1:B:836:GLN:H	1.26	0.82
1:C:627:ASN:HD22	1:C:627:ASN:H	1.27	0.82
1:A:552[A]:GLN:HE21	4:A:2201:ACY:CH3	1.91	0.81
1:A:748:GLU:OE1	4:A:2200[B]:ACY:H1	1.79	0.81
1:B:839:HIS:HD2	1:B:842:ASN:H	1.29	0.81
1:A:603[B]:ARG:NH1	7:A:2378:HOH:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552[A]:GLN:NE2	4:A:2201:ACY:H1	1.95	0.80
5:A:2320[B]:GOL:H12	1:B:411:ASP:OD1	1.81	0.80
1:A:603[B]:ARG:HD3	7:A:1219:HOH:O	1.81	0.80
1:A:627:ASN:HD22	1:A:627:ASN:H	1.29	0.80
1:B:381[B]:GLU:HG2	1:B:423:LYS:HG2	1.64	0.79
1:B:893[A]:ASN:ND2	7:B:2341:HOH:O	1.80	0.79
1:A:582:ILE:HD11	1:D:582:ILE:HD11	1.64	0.79
1:C:572[B]:GLU:HG2	1:C:574:TRP:CD1	2.17	0.79
1:A:384:ASP:OD1	7:A:2239:HOH:O	2.01	0.79
1:D:753[A]:GLN:HE22	1:D:950:GLN:NE2	1.80	0.79
1:A:413:GLY:O	5:B:2310:GOL:C1	2.30	0.78
1:A:753[A]:GLN:HE22	1:A:950:GLN:HE22	1.33	0.77
1:A:582:ILE:CD1	1:D:582:ILE:HD11	2.14	0.77
1:A:381[B]:GLU:HG2	1:A:423:LYS:HG2	1.66	0.76
1:C:488:GLY:O	7:C:2462:HOH:O	2.02	0.76
1:C:753[A]:GLN:HE22	1:C:950:GLN:NE2	1.84	0.76
1:B:547:LYS:HD2	1:B:791[B]:TYR:HH	1.46	0.76
1:D:632[B]:ASN:HD22	1:D:632[B]:ASN:H	1.32	0.75
1:D:753[A]:GLN:HE22	1:D:950:GLN:HE22	1.33	0.75
1:B:608:GLN:HE22	1:B:959:ASN:HD21	1.34	0.75
5:A:2306:GOL:H31	7:A:1109:HOH:O	1.87	0.75
1:C:971:LYS:HE2	1:C:974:GLU:OE2	1.87	0.75
1:B:547:LYS:CD	1:B:791[B]:TYR:OH	2.31	0.74
1:D:632[B]:ASN:H	1:D:632[B]:ASN:ND2	1.85	0.74
1:A:572:GLU:HG3	5:A:2305:GOL:O3	1.89	0.73
1:B:631:THR:H	1:B:634:HIS:HD2	1.35	0.73
1:C:1007:GLU:OE2	7:C:2176:HOH:O	2.05	0.73
1:D:839:HIS:HE1	7:D:1168:HOH:O	1.72	0.73
1:A:753[A]:GLN:HE22	1:A:950:GLN:NE2	1.87	0.72
1:C:497:VAL:HG13	1:C:501:VAL:HB	1.71	0.72
1:D:459:ARG:NH2	7:D:1952:HOH:O	2.11	0.72
1:A:589:LEU:HB3	1:A:951:LYS:HG3	1.72	0.72
1:A:1003:PHE:CE1	4:A:2204:ACY:H2	2.26	0.71
5:A:2303:GOL:O1	5:B:2310:GOL:H2	1.92	0.70
1:B:643:LYS:HD3	1:B:647:GLU:HB3	1.74	0.70
1:B:644[A]:ASN:HD22	1:B:647:GLU:CG	2.00	0.70
1:A:603[B]:ARG:HH11	1:A:603[B]:ARG:CG	2.04	0.69
1:B:641:ARG:NH2	1:B:703:VAL:O	2.26	0.69
1:C:676:ILE:HG22	1:C:719:GLU:HG2	1.74	0.69
1:C:631:THR:H	1:C:634:HIS:CD2	2.01	0.69
1:B:627:ASN:H	1:B:627:ASN:HD22	1.39	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:753[A]:GLN:HE22	1:C:950:GLN:HE22	1.39	0.68
1:C:839:HIS:HD2	1:C:842:ASN:H	1.41	0.68
1:C:377:ASN:ND2	7:C:1219:HOH:O	2.27	0.68
1:A:412:LYS:HE2	7:B:1105:HOH:O	1.93	0.67
1:B:552:GLN:NE2	4:B:2208:ACY:OXT	2.26	0.67
1:B:728:THR:CG2	1:B:730:HIS:H	2.05	0.67
1:D:547:LYS:HD3	1:D:1004:SER:HB3	1.77	0.67
1:D:839:HIS:HD2	1:D:842:ASN:H	1.43	0.67
1:C:780:HIS:CD2	1:C:782:ILE:H	2.06	0.66
1:C:887[A]:ASP:OD2	1:C:891:ARG:HD2	1.96	0.66
1:A:784:LYS:HE3	7:A:1352:HOH:O	1.95	0.65
1:C:839:HIS:HE1	7:C:1121:HOH:O	1.80	0.65
1:A:391:ASP:OD1	7:A:1096:HOH:O	2.14	0.65
1:C:579:ASP:OD1	5:C:2322:GOL:H11	1.96	0.65
1:C:589:LEU:HB3	1:C:951:LYS:HG3	1.79	0.65
4:C:2210:ACY:CH3	7:C:2407:HOH:O	2.37	0.65
1:C:1035:GLU:CD	5:C:2321:GOL:H31	2.21	0.64
4:C:2210:ACY:C	7:C:2407:HOH:O	2.45	0.64
1:D:780:HIS:CD2	1:D:782:ILE:H	2.06	0.64
1:A:780:HIS:CD2	1:A:782:ILE:H	2.10	0.64
1:C:425[A]:GLN:HG2	7:C:1813:HOH:O	1.97	0.64
1:C:1035:GLU:OE2	5:C:2321:GOL:C3	2.35	0.64
4:C:2210:ACY:H1	7:C:2395:HOH:O	1.96	0.64
1:A:839:HIS:HD2	1:A:842:ASN:H	1.44	0.63
1:C:997:VAL:HG23	4:C:2213:ACY:H1	1.81	0.63
1:A:627:ASN:H	1:A:627:ASN:ND2	1.97	0.62
1:C:572[B]:GLU:CG	1:C:574:TRP:CD1	2.82	0.62
1:D:644:ASN:C	1:D:644:ASN:HD22	2.07	0.62
1:D:579:ASP:CG	5:D:2319:GOL:H2	2.23	0.62
1:D:739:MET:HE3	1:D:742:PHE:HB2	1.80	0.62
5:A:2320[A]:GOL:C3	1:B:413:GLY:O	2.43	0.61
1:C:609:PHE:CE1	4:C:2209[A]:ACY:H2	2.35	0.61
1:B:589:LEU:HB3	1:B:951:LYS:HG3	1.82	0.61
1:D:570[A]:MET:HG2	1:D:571:PHE:CE2	2.35	0.61
1:A:384:ASP:H	5:A:2306:GOL:C3	2.12	0.61
1:C:473:PHE:CE2	1:C:487:PRO:HB3	2.36	0.60
1:A:631:THR:H	1:A:634:HIS:CD2	2.09	0.60
1:A:1035:GLU:OE2	5:A:2320[B]:GOL:H32	2.00	0.60
1:C:590:GLY:HA2	7:C:249:HOH:O	2.00	0.60
1:D:555:ARG:HH21	1:D:803:GLU:HB3	1.66	0.60
1:D:627:ASN:H	1:D:627:ASN:ND2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:839:HIS:HE1	7:B:1471:HOH:O	1.84	0.60
1:B:547:LYS:CE	1:B:791[B]:TYR:HE2	2.04	0.59
1:B:839:HIS:CD2	1:B:842:ASN:H	2.14	0.59
1:D:589:LEU:HB3	1:D:951:LYS:HG3	1.85	0.59
5:A:2303:GOL:O2	5:B:2310:GOL:H11	2.02	0.59
1:C:411:ASP:OD1	5:C:2315:GOL:H32	2.02	0.59
1:A:582:ILE:CD1	1:D:582:ILE:CD1	2.79	0.59
1:B:412:LYS:HD3	7:B:157:HOH:O	2.02	0.59
1:D:728:THR:HB	1:D:729:PRO:HD2	1.85	0.59
1:A:585:ARG:HE	1:D:572:GLU:CD	2.12	0.58
1:D:497:VAL:HG13	1:D:501:VAL:HB	1.85	0.58
1:D:555:ARG:HD3	1:D:999:ILE:HD13	1.84	0.58
1:B:1049[B]:GLU:HG3	7:B:1189:HOH:O	2.04	0.57
1:A:413:GLY:C	5:B:2310:GOL:H12	2.29	0.57
1:C:834:ASN:ND2	1:C:836:GLN:H	1.97	0.57
1:A:603[B]:ARG:CD	7:A:1219:HOH:O	2.45	0.57
1:A:572:GLU:OE2	5:A:2305:GOL:O3	2.22	0.56
1:D:386[A]:GLU:CD	1:D:549:ARG:HH22	2.14	0.56
1:A:857:GLY:HA3	4:A:2222:ACY:H2	1.86	0.56
1:C:809:GLY:O	1:C:812:ASP:HB3	2.06	0.56
1:D:631:THR:H	1:D:634:HIS:HD2	1.53	0.56
1:C:706:LEU:HG	7:C:1157:HOH:O	2.06	0.55
1:C:631:THR:N	1:C:634:HIS:HD2	1.93	0.55
1:A:891:ARG:HD3	7:A:1326:HOH:O	2.07	0.55
1:C:839:HIS:CD2	1:C:842:ASN:H	2.22	0.55
1:D:893[A]:ASN:ND2	1:D:893[A]:ASN:H	2.03	0.55
1:C:411:ASP:OD1	5:C:2315:GOL:C3	2.55	0.55
1:D:573:ASN:O	5:D:2319:GOL:O2	2.25	0.54
1:A:644[A]:ASN:ND2	1:A:647:GLU:H	2.06	0.54
1:A:780:HIS:HE1	1:A:892:ASP:OD2	1.90	0.54
1:A:780:HIS:HD2	1:A:782:ILE:N	2.00	0.54
1:D:438:LEU:HD21	1:D:500:ILE:HD13	1.89	0.54
1:B:959:ASN:O	4:B:2205:ACY:H1	2.08	0.54
1:D:780:HIS:HE1	1:D:892:ASP:OD2	1.91	0.54
1:B:780:HIS:CD2	1:B:782:ILE:H	2.09	0.54
1:B:670:GLY:N	1:B:671:PRO:HD2	2.23	0.54
1:B:764:THR:HB	1:B:907:TRP:CZ2	2.43	0.54
1:D:834:ASN:ND2	1:D:836:GLN:H	1.96	0.54
1:D:631:THR:H	1:D:634:HIS:CD2	2.26	0.53
1:B:547:LYS:CE	1:B:791[B]:TYR:CE2	2.85	0.53
1:C:575:ASP:OD1	5:C:2322:GOL:H12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:891:ARG:HD3	7:D:2372:HOH:O	2.08	0.53
1:A:377:ASN:ND2	7:A:1183:HOH:O	2.40	0.53
1:B:589:LEU:HB3	1:B:951:LYS:CG	2.39	0.53
1:C:489:GLU:CB	1:C:1020[B]:ASP:CG	2.78	0.53
1:C:738:MET:HG3	1:C:742:PHE:CE1	2.44	0.53
1:B:1035:GLU:CD	5:B:2310:GOL:H31	2.24	0.52
1:B:753[A]:GLN:HE22	1:B:950:GLN:HE22	1.58	0.52
1:B:555:ARG:HH21	1:B:803:GLU:HB3	1.75	0.52
1:D:997:VAL:HG23	4:D:2215:ACY:H1	1.92	0.52
1:B:387:HIS:CE1	7:B:2320:HOH:O	2.42	0.52
1:B:710:MET:HE3	7:B:1220:HOH:O	2.08	0.52
1:B:547:LYS:HD2	1:B:791[B]:TYR:CZ	2.43	0.52
1:A:589:LEU:HB3	1:A:951:LYS:CG	2.40	0.52
1:B:753[A]:GLN:HE22	1:B:950:GLN:NE2	2.07	0.51
1:B:708:HIS:ND1	7:B:1701:HOH:O	2.34	0.51
1:A:997:VAL:HG23	4:A:2202:ACY:H1	1.93	0.51
1:C:730:HIS:ND1	7:C:1671:HOH:O	1.76	0.51
1:B:377:ASN:ND2	7:B:1444:HOH:O	2.44	0.51
1:B:739:MET:HE2	1:B:743:TRP:NE1	2.26	0.51
1:C:371:HIS:N	7:C:1944:HOH:O	2.42	0.51
1:C:579:ASP:OD2	5:C:2322:GOL:C1	2.49	0.51
1:D:644:ASN:ND2	1:D:647:GLU:H	2.07	0.51
1:A:1003:PHE:CE1	4:A:2204:ACY:CH3	2.93	0.51
1:C:739:MET:HE3	1:C:742:PHE:HB2	1.93	0.51
1:D:599:TRP:HE1	4:D:2219:ACY:H3	1.75	0.51
1:A:834:ASN:ND2	1:A:836[B]:GLN:H	2.00	0.50
1:B:893[A]:ASN:OD1	7:B:1216:HOH:O	2.19	0.50
1:C:780:HIS:HE1	1:C:892:ASP:OD2	1.95	0.50
1:B:780:HIS:HE1	1:B:892:ASP:OD2	1.94	0.50
1:B:575:ASP:OD2	5:B:2311:GOL:O3	2.25	0.50
1:D:386[A]:GLU:OE2	1:D:549:ARG:NH2	2.42	0.50
1:C:608:GLN:HB2	4:C:2209[A]:ACY:H3	1.93	0.50
5:C:2315:GOL:O2	1:D:1035:GLU:OE2	2.28	0.50
1:D:570[A]:MET:HG2	1:D:571:PHE:CZ	2.47	0.50
1:D:578:ASP:OD1	4:D:2219:ACY:H2	2.12	0.50
1:A:503:GLU:OE2	7:A:1182:HOH:O	2.18	0.50
1:B:728:THR:O	1:B:731:GLU:HG2	2.12	0.50
1:A:839:HIS:CD2	1:A:842:ASN:H	2.28	0.49
1:C:594:ASN:C	1:C:594:ASN:HD22	2.19	0.49
1:A:513:LYS:CE	7:A:1375:HOH:O	2.60	0.49
1:A:784:LYS:CE	7:A:1352:HOH:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:ASN:H	1:C:627:ASN:ND2	2.00	0.49
1:A:695:ALA:C	1:A:697:PRO:HD3	2.38	0.49
1:A:834:ASN:ND2	1:A:836[A]:GLN:H	1.99	0.49
1:A:1059:ARG:HA	4:A:2204:ACY:H1	1.94	0.49
1:D:490:ALA:HB2	1:D:784:LYS:HE3	1.95	0.48
1:C:801:ARG:O	1:C:806:GLY:HA3	2.13	0.48
1:B:631:THR:H	1:B:634:HIS:CD2	2.24	0.48
1:D:547:LYS:HD2	1:D:547:LYS:O	2.14	0.48
1:A:815:LEU:HD23	1:A:962:ALA:HB1	1.94	0.48
1:A:926[A]:GLU:CD	1:A:926[A]:GLU:H	2.22	0.48
1:A:502:SER:O	1:A:506[B]:GLN:HG3	2.14	0.48
1:B:739:MET:HE3	1:B:742:PHE:HB2	1.96	0.48
1:A:372:HIS:O	1:A:373[B]:HIS:CD2	2.66	0.47
1:D:469[A]:ARG:NH2	7:D:1529:HOH:O	2.46	0.47
1:A:594:ASN:C	1:A:594:ASN:HD22	2.22	0.47
1:C:552:GLN:NE2	7:C:2395:HOH:O	2.26	0.47
1:C:1033:LYS:CG	7:C:1948:HOH:O	2.61	0.47
1:D:638:SER:OG	1:D:730:HIS:HE1	1.97	0.47
5:A:2304:GOL:O2	7:A:1549:HOH:O	2.20	0.47
1:A:392:ALA:O	5:A:2303:GOL:H2	2.15	0.47
1:A:811:VAL:HG13	1:A:815:LEU:HD12	1.96	0.47
1:C:425[A]:GLN:CG	7:C:1813:HOH:O	2.59	0.47
1:C:579:ASP:OD2	5:C:2322:GOL:H32	2.15	0.47
1:C:748:GLU:OE1	4:C:2209[A]:ACY:O	2.33	0.47
1:D:594:ASN:C	1:D:594:ASN:HD22	2.22	0.47
1:B:628:PHE:HB2	1:B:698:LEU:HD22	1.97	0.47
1:A:603[B]:ARG:NH1	1:A:603[B]:ARG:CG	2.73	0.47
1:A:413:GLY:O	5:B:2310:GOL:H11	2.14	0.47
1:A:758[A]:LEU:HD21	1:A:805:TRP:CG	2.49	0.46
1:A:839:HIS:HE1	7:A:1132:HOH:O	1.99	0.46
1:B:594:ASN:ND2	1:B:952:ASP:HB3	2.30	0.46
1:A:728:THR:HB	1:A:729:PRO:HD2	1.97	0.46
1:C:728:THR:O	1:C:731:GLU:HG2	2.16	0.46
1:A:412:LYS:CD	7:A:1340:HOH:O	2.63	0.46
1:B:670:GLY:N	1:B:671:PRO:CD	2.79	0.46
1:B:1043:GLN:O	1:B:1046:GLU:HG2	2.16	0.46
5:A:2304:GOL:H31	7:A:1549:HOH:O	2.15	0.46
1:D:627:ASN:HD22	1:D:627:ASN:N	2.05	0.46
1:B:504:GLN:NE2	7:B:1192:HOH:O	2.41	0.46
1:A:738:MET:HG3	1:A:742:PHE:CE1	2.52	0.45
1:B:594:ASN:HD22	1:B:595:MET:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:938:THR:HA	1:D:942:GLN:HB3	1.97	0.45
1:B:637:ALA:HB3	1:B:730:HIS:CE1	2.51	0.45
1:B:815:LEU:HD12	1:B:962:ALA:HB1	1.99	0.45
1:B:834:ASN:ND2	1:B:836:GLN:H	2.04	0.45
1:C:892:ASP:O	1:C:896:GLN:HG2	2.17	0.45
1:B:440:GLU:HG2	1:B:484:VAL:HG22	1.97	0.45
1:A:386:GLU:CD	1:A:549:ARG:HH22	2.23	0.45
1:A:412:LYS:HD3	7:A:1340:HOH:O	2.17	0.45
1:C:424:GLU:OE2	1:C:424:GLU:HA	2.17	0.45
1:A:603[B]:ARG:HG2	1:A:603[B]:ARG:NH1	2.13	0.45
1:A:707:GLY:O	4:A:2222:ACY:H3	2.17	0.45
1:C:618:LEU:HD11	1:C:655:TYR:HB3	1.99	0.45
1:D:728:THR:O	1:D:731:GLU:HG2	2.16	0.45
1:A:380:VAL:HG11	1:A:455:TRP:CZ2	2.52	0.45
1:B:910:ASN:HB3	1:B:911:PRO:HD2	1.98	0.45
5:C:2315:GOL:C1	7:C:1254:HOH:O	2.32	0.45
1:D:1002:LYS:CE	7:D:1225:HOH:O	2.17	0.45
1:A:508:GLU:OE2	1:A:778[A]:SER:OG	2.28	0.44
1:B:635:VAL:O	1:B:635:VAL:HG13	2.16	0.44
1:B:784:LYS:HE3	7:B:2387:HOH:O	2.17	0.44
5:A:2306:GOL:C3	7:A:1109:HOH:O	2.54	0.44
1:B:738:MET:HG3	1:B:742:PHE:CE1	2.51	0.44
1:C:469:ARG:HE	1:C:469:ARG:HB3	1.67	0.44
1:C:997:VAL:CG2	4:C:2213:ACY:H1	2.45	0.44
1:D:644:ASN:HD22	1:D:647:GLU:H	1.64	0.44
1:A:1007:GLU:HB2	7:A:1234:HOH:O	2.18	0.44
1:B:618:LEU:HA	1:B:657:VAL:HG12	2.00	0.43
1:B:635:VAL:O	1:B:635:VAL:CG1	2.66	0.43
1:B:753[B]:GLN:CD	1:B:815:LEU:HD11	2.43	0.43
1:B:594:ASN:HD22	1:B:594:ASN:C	2.26	0.43
1:B:1040:LYS:HA	1:B:1043:GLN:HE21	1.83	0.43
1:C:1020[A]:ASP:OD1	1:C:1022:ASP:HB2	2.18	0.43
1:B:700:LEU:HD23	1:B:712:ILE:HD11	1.99	0.43
1:D:804:LEU:HD22	1:D:810:ILE:HD11	1.99	0.43
1:D:598:ARG:NH1	1:D:1049[B]:GLU:OE1	2.51	0.43
1:A:513:LYS:HE2	7:A:1375:HOH:O	2.18	0.43
1:D:893[A]:ASN:H	1:D:893[A]:ASN:HD22	1.66	0.43
1:A:910:ASN:HB3	1:A:911:PRO:HD2	2.01	0.43
1:C:412:LYS:HE2	7:C:1158:HOH:O	2.19	0.43
1:A:1015:ALA:HB2	5:A:2306:GOL:H12	2.01	0.42
1:C:766:GLU:HG3	1:C:794:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:LEU:HD23	1:D:509:LEU:HA	1.91	0.42
1:D:809:GLY:O	1:D:812:ASP:HB3	2.19	0.42
1:A:556:LYS:HB3	1:A:556:LYS:HE2	1.87	0.42
1:A:643:LYS:HB3	1:A:647:GLU:HB2	2.01	0.42
1:A:554:SER:HB3	1:A:1002:LYS:HD3	2.01	0.42
1:C:839:HIS:CD2	1:C:841:PRO:HD2	2.55	0.42
1:D:810:ILE:CG2	7:D:2148:HOH:O	2.67	0.42
1:A:459:ARG:NH1	1:A:1019:GLU:OE2	2.52	0.42
1:A:1035:GLU:HG3	7:A:1123:HOH:O	2.20	0.42
1:B:490:ALA:HB2	1:B:784:LYS:HD2	2.01	0.42
5:C:2315:GOL:H12	1:D:1032:ASP:OD1	2.20	0.42
1:A:764:THR:HB	1:A:907:TRP:CZ2	2.55	0.42
1:A:518:TRP:CE3	1:A:770:LEU:HD23	2.55	0.41
1:B:660:LYS:HB3	1:B:718:GLN:CD	2.46	0.41
1:A:706:LEU:HG	7:A:1677:HOH:O	2.20	0.41
1:A:893:ASN:ND2	1:A:893:ASN:H	2.18	0.41
1:C:412:LYS:CE	7:C:1158:HOH:O	2.67	0.41
1:D:594:ASN:ND2	1:D:952:ASP:HB3	2.35	0.41
1:A:384:ASP:N	5:A:2306:GOL:H31	2.24	0.41
1:A:910:ASN:HB3	1:A:911:PRO:CD	2.50	0.41
1:D:594:ASN:HD22	1:D:595:MET:N	2.19	0.41
1:D:780:HIS:CE1	1:D:892:ASP:OD2	2.73	0.41
1:A:555:ARG:HH21	1:A:803:GLU:HB3	1.86	0.41
1:A:728:THR:O	1:A:731:GLU:HG2	2.20	0.41
1:C:412:LYS:NZ	7:C:1507:HOH:O	2.52	0.41
1:D:800:GLY:HA2	1:D:804:LEU:HB2	2.02	0.41
1:C:500:ILE:O	1:C:500:ILE:HG13	2.20	0.41
1:C:780:HIS:HD2	1:C:782:ILE:N	1.97	0.41
5:C:2321:GOL:C2	7:C:1145:HOH:O	2.47	0.41
1:D:739:MET:HE2	1:D:743:TRP:NE1	2.36	0.41
1:D:761:THR:O	1:D:762:HIS:C	2.62	0.41
1:A:850:ASP:OD1	7:A:1821:HOH:O	2.22	0.41
1:B:660:LYS:HE3	1:B:660:LYS:HB2	1.85	0.41
1:A:666:LYS:O	1:A:821:GLY:HA3	2.21	0.40
1:A:974[A]:GLU:HB2	7:A:1121:HOH:O	2.20	0.40
1:B:670:GLY:H	1:B:671:PRO:HD2	1.86	0.40
1:C:594:ASN:HD22	1:C:595:MET:N	2.20	0.40
1:C:643:LYS:HB3	1:C:647:GLU:HB2	2.03	0.40
1:C:440:GLU:HG2	1:C:484:VAL:HG22	2.02	0.40
1:C:572[B]:GLU:HG3	1:C:574:TRP:HD1	1.87	0.40
1:A:377:ASN:HB3	1:A:425[A]:GLN:HE22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:780:HIS:CE1	1:A:892:ASP:OD2	2.74	0.40
1:D:555:ARG:HD2	7:D:1162:HOH:O	2.20	0.40
1:D:801:ARG:O	1:D:806:GLY:HA3	2.21	0.40
1:A:1021:LYS:NZ	7:A:1543:HOH:O	2.27	0.40
1:B:816:SER:OG	1:B:963:ILE:HA	2.21	0.40

All (1) 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:622:ASP:OD2	7:B:1106:HOH:O[1_556]	1.91	0.29

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	708/696 (102%)	684 (97%)	24 (3%)	0	100	100
1	B	700/696 (101%)	676 (97%)	22 (3%)	2 (0%)	36	29
1	C	703/696 (101%)	675 (96%)	26 (4%)	2 (0%)	36	29
1	D	699/696 (100%)	676 (97%)	23 (3%)	0	100	100
All	All	2810/2784 (101%)	2711 (96%)	95 (3%)	4 (0%)	48	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	634	HIS
1	B	762	HIS
1	C	762	HIS
1	C	487	PRO

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	605/602 (100%)	592 (98%)	13 (2%)	47	44
1	B	590/602 (98%)	566 (96%)	24 (4%)	27	19
1	C	593/602 (98%)	578 (98%)	15 (2%)	42	37
1	D	585/602 (97%)	565 (97%)	20 (3%)	32	25
All	All	2373/2408 (98%)	2301 (97%)	72 (3%)	38	30

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	412	LYS
1	A	594	ASN
1	A	627	ASN
1	A	644[A]	ASN
1	A	644[B]	ASN
1	A	660	LYS
1	A	778[A]	SER
1	A	778[B]	SER
1	A	817	LEU
1	A	893	ASN
1	A	923	GLU
1	A	926[A]	GLU
1	A	926[B]	GLU
1	B	412	LYS
1	B	423	LYS
1	B	500	ILE
1	B	543	PHE
1	B	545	ASP
1	B	582	ILE
1	B	594	ASN
1	B	627	ASN
1	B	635	VAL
1	B	644[A]	ASN
1	B	644[B]	ASN

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Mol	Chain	Res	Type
1	B	676	ILE
1	B	691	ILE
1	B	728	THR
1	B	807	SER
1	B	810	ILE
1	B	815	LEU
1	B	823	VAL
1	B	854	LYS
1	B	923	GLU
1	B	926[A]	GLU
1	B	926[B]	GLU
1	B	982	SER
1	B	1057	PRO
1	C	371	HIS
1	C	497	VAL
1	C	500	ILE
1	C	514	LEU
1	C	545	ASP
1	C	588	ILE
1	C	594	ASN
1	C	627	ASN
1	C	644[A]	ASN
1	C	644[B]	ASN
1	C	719	GLU
1	C	810	ILE
1	C	815	LEU
1	C	926	GLU
1	C	1057	PRO
1	D	406	ASP
1	D	412	LYS
1	D	497	VAL
1	D	500	ILE
1	D	545	ASP
1	D	547	LYS
1	D	588	ILE
1	D	594	ASN
1	D	619	THR
1	D	627	ASN
1	D	644	ASN
1	D	802	LYS
1	D	815	LEU
1	D	893[A]	ASN

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Mol	Chain	Res	Type
1	D	893[B]	ASN
1	D	923	GLU
1	D	926[A]	GLU
1	D	926[B]	GLU
1	D	971	LYS
1	D	1057	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	429	GLN
1	A	467	GLN
1	A	511	GLN
1	A	594	ASN
1	A	627	ASN
1	A	634	HIS
1	A	718	GLN
1	A	730	HIS
1	A	750	ASN
1	A	775	ASN
1	A	780	HIS
1	A	834	ASN
1	A	839	HIS
1	A	842	ASN
1	A	893	ASN
1	A	947	ASN
1	A	950	GLN
1	B	377	ASN
1	B	504	GLN
1	B	594	ASN
1	B	614	ASN
1	B	627	ASN
1	B	634	HIS
1	B	708	HIS
1	B	730	HIS
1	B	735	HIS
1	B	750	ASN
1	B	780	HIS
1	B	834	ASN
1	B	839	HIS
1	B	842	ASN

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Mol	Chain	Res	Type
1	B	947	ASN
1	B	950	GLN
1	B	959	ASN
1	B	1043	GLN
1	C	371	HIS
1	C	377	ASN
1	C	467	GLN
1	C	511	GLN
1	C	594	ASN
1	C	627	ASN
1	C	634	HIS
1	C	750	ASN
1	C	780	HIS
1	C	834	ASN
1	C	839	HIS
1	C	842	ASN
1	C	893	ASN
1	C	947	ASN
1	C	950	GLN
1	C	959	ASN
1	D	517	GLN
1	D	594	ASN
1	D	627	ASN
1	D	634	HIS
1	D	644	ASN
1	D	730	HIS
1	D	750	ASN
1	D	780	HIS
1	D	834	ASN
1	D	839	HIS
1	D	842	ASN
1	D	947	ASN
1	D	950	GLN
1	D	959	ASN
1	D	1043	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 ⓘ

Of 65 ligands modelled in this entry, 18 are monoatomic - leaving 47 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	$\# Z > 2$
4	ACY	A	2202	-	3,3,3	1.06	0	3,3,3	2.89	2 (66%)
5	GOL	B	2309	-	5,5,5	0.54	0	5,5,5	0.27	0
4	ACY	A	2200[B]	-	3,3,3	0.97	0	3,3,3	0.97	0
5	GOL	B	2311	-	5,5,5	0.54	0	5,5,5	1.54	1 (20%)
5	GOL	A	2302	-	5,5,5	0.56	0	5,5,5	0.67	0
4	ACY	A	2222	-	3,3,3	0.70	0	3,3,3	1.19	0
4	ACY	D	2216	-	3,3,3	0.88	0	3,3,3	1.01	0
4	ACY	D	2215	-	3,3,3	0.63	0	3,3,3	2.32	1 (33%)
5	GOL	C	2322	-	5,5,5	0.95	0	5,5,5	3.26	2 (40%)
4	ACY	C	2211	-	3,3,3	0.68	0	3,3,3	1.47	0
4	ACY	D	2217	-	3,3,3	0.93	0	3,3,3	0.81	0
4	ACY	D	2214	-	3,3,3	1.02	0	3,3,3	0.50	0
5	GOL	D	2319	-	5,5,5	1.08	0	5,5,5	1.24	0
4	ACY	A	2203	-	3,3,3	0.55	0	3,3,3	1.36	0
5	GOL	C	2313	-	5,5,5	0.88	0	5,5,5	1.43	1 (20%)
4	ACY	A	2200[A]	-	3,3,3	0.71	0	3,3,3	1.41	0
4	ACY	B	2207	-	3,3,3	0.78	0	3,3,3	1.02	0
4	ACY	D	2219	-	3,3,3	0.92	0	3,3,3	0.24	0
4	ACY	A	2220	-	3,3,3	1.06	0	3,3,3	1.03	0
4	ACY	A	2201	-	3,3,3	0.77	0	3,3,3	1.23	0
5	GOL	B	2310	-	5,5,5	0.76	0	5,5,5	3.07	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ACY	B	2206	-	3,3,3	0.70	0	3,3,3	1.73	1 (33%)
5	GOL	A	2320[B]	-	5,5,5	0.60	0	5,5,5	1.18	0
4	ACY	C	2221	-	3,3,3	0.81	0	3,3,3	0.89	0
4	ACY	C	2209[B]	-	3,3,3	1.19	0	3,3,3	0.53	0
5	GOL	A	2305	-	5,5,5	0.36	0	5,5,5	2.12	1 (20%)
5	GOL	C	2314	-	5,5,5	0.39	0	5,5,5	0.71	0
4	ACY	B	2208	-	3,3,3	0.91	0	3,3,3	0.48	0
5	GOL	A	2307	-	5,5,5	0.89	0	5,5,5	1.32	0
5	GOL	C	2317	-	5,5,5	0.43	0	5,5,5	1.24	1 (20%)
4	ACY	B	2205	-	3,3,3	0.77	0	3,3,3	1.16	0
5	GOL	A	2308	-	5,5,5	0.42	0	5,5,5	0.48	0
4	ACY	C	2210	-	3,3,3	0.96	0	3,3,3	0.36	0
4	ACY	A	2218	-	3,3,3	0.98	0	3,3,3	0.47	0
5	GOL	B	2312	-	5,5,5	0.47	0	5,5,5	0.95	0
4	ACY	C	2212	-	3,3,3	0.60	0	3,3,3	1.52	1 (33%)
5	GOL	A	2306	-	5,5,5	0.35	0	5,5,5	2.01	2 (40%)
5	GOL	A	2304	-	5,5,5	0.99	1 (20%)	5,5,5	1.57	2 (40%)
4	ACY	A	2204	-	3,3,3	0.64	0	3,3,3	1.62	1 (33%)
5	GOL	A	2303	-	5,5,5	0.81	0	5,5,5	0.87	0
5	GOL	A	2320[A]	-	5,5,5	0.54	0	5,5,5	1.07	0
4	ACY	C	2213	-	3,3,3	0.74	0	3,3,3	1.88	1 (33%)
5	GOL	D	2318	-	5,5,5	0.45	0	5,5,5	0.56	0
5	GOL	C	2315	-	5,5,5	0.80	0	5,5,5	0.60	0
4	ACY	C	2209[A]	-	3,3,3	0.66	0	3,3,3	2.25	2 (66%)
5	GOL	C	2321	-	5,5,5	0.94	0	5,5,5	1.43	1 (20%)
5	GOL	A	2301	-	5,5,5	0.72	0	5,5,5	0.93	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
5	GOL	B	2309	-	-	0/4/4/4	-
5	GOL	B	2311	-	-	3/4/4/4	-
5	GOL	A	2302	-	-	0/4/4/4	-
5	GOL	C	2322	-	-	3/4/4/4	-
5	GOL	D	2319	-	-	4/4/4/4	-
5	GOL	C	2313	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	2310	-	-	4/4/4/4	-
5	GOL	A	2320[B]	-	-	4/4/4/4	-
5	GOL	A	2305	-	-	3/4/4/4	-
5	GOL	C	2314	-	-	0/4/4/4	-
5	GOL	A	2307	-	-	2/4/4/4	-
5	GOL	C	2317	-	-	2/4/4/4	-
5	GOL	A	2308	-	-	0/4/4/4	-
5	GOL	B	2312	-	-	4/4/4/4	-
5	GOL	A	2306	-	-	2/4/4/4	-
5	GOL	A	2304	-	-	2/4/4/4	-
5	GOL	A	2303	-	-	0/4/4/4	-
5	GOL	A	2320[A]	-	-	3/4/4/4	-
5	GOL	D	2318	-	-	2/4/4/4	-
5	GOL	C	2315	-	-	2/4/4/4	-
5	GOL	C	2321	-	-	2/4/4/4	-
5	GOL	A	2301	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2304	GOL	O3-C3	-2.01	1.34	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2322	GOL	C3-C2-C1	-6.02	89.71	111.80
5	B	2310	GOL	O3-C3-C2	-4.76	88.94	110.38
5	B	2310	GOL	O2-C2-C1	4.19	126.53	109.18
5	A	2305	GOL	O1-C1-C2	-4.11	91.85	110.38
4	A	2202	ACY	O-C-CH3	-3.79	106.98	122.53
5	C	2322	GOL	O2-C2-C3	3.40	123.25	109.18
5	A	2306	GOL	O2-C2-C1	3.23	122.55	109.18
4	D	2215	ACY	O-C-CH3	-3.20	109.41	122.53
4	A	2202	ACY	OXT-C-O	3.08	133.45	122.03
4	C	2209[A]	ACY	O-C-CH3	-2.93	110.52	122.53
5	C	2321	GOL	O2-C2-C1	2.65	120.17	109.18
5	A	2306	GOL	O2-C2-C3	2.64	120.09	109.18
4	C	2213	ACY	O-C-CH3	-2.59	111.92	122.53
5	C	2317	GOL	O2-C2-C1	2.50	119.51	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2304	GOL	O3-C3-C2	-2.45	99.33	110.38
4	C	2209[A]	ACY	OXT-C-O	2.44	131.07	122.03
4	B	2206	ACY	O-C-CH3	-2.27	113.22	122.53
5	C	2313	GOL	O1-C1-C2	-2.22	100.37	110.38
5	A	2304	GOL	O1-C1-C2	2.16	120.12	110.38
5	B	2311	GOL	O2-C2-C1	2.15	118.09	109.18
4	A	2204	ACY	O-C-CH3	-2.15	113.73	122.53
5	B	2310	GOL	C3-C2-C1	-2.06	104.22	111.80
4	C	2212	ACY	O-C-CH3	-2.02	114.25	122.53

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2305	GOL	O1-C1-C2-C3
5	A	2306	GOL	O1-C1-C2-C3
5	A	2306	GOL	O2-C2-C3-O3
5	A	2307	GOL	C1-C2-C3-O3
5	A	2320[A]	GOL	O1-C1-C2-O2
5	A	2320[A]	GOL	O1-C1-C2-C3
5	A	2320[B]	GOL	O1-C1-C2-C3
5	A	2320[B]	GOL	C1-C2-C3-O3
5	A	2320[B]	GOL	O2-C2-C3-O3
5	B	2310	GOL	O1-C1-C2-C3
5	B	2311	GOL	C1-C2-C3-O3
5	B	2312	GOL	O1-C1-C2-C3
5	B	2312	GOL	C1-C2-C3-O3
5	C	2317	GOL	O1-C1-C2-C3
5	C	2321	GOL	C1-C2-C3-O3
5	C	2315	GOL	C1-C2-C3-O3
5	D	2319	GOL	O1-C1-C2-C3
5	D	2319	GOL	C1-C2-C3-O3
5	C	2315	GOL	O2-C2-C3-O3
5	A	2304	GOL	C1-C2-C3-O3
5	D	2318	GOL	C1-C2-C3-O3
5	A	2305	GOL	O1-C1-C2-O2
5	A	2307	GOL	O2-C2-C3-O3
5	A	2320[B]	GOL	O1-C1-C2-O2
5	B	2310	GOL	O1-C1-C2-O2
5	B	2310	GOL	O2-C2-C3-O3
5	B	2311	GOL	O2-C2-C3-O3
5	B	2312	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	C	2317	GOL	O1-C1-C2-O2
5	C	2321	GOL	O2-C2-C3-O3
5	C	2322	GOL	O2-C2-C3-O3
5	D	2319	GOL	O2-C2-C3-O3
5	B	2311	GOL	O1-C1-C2-O2
5	C	2322	GOL	O1-C1-C2-O2
5	D	2319	GOL	O1-C1-C2-O2
5	A	2305	GOL	O2-C2-C3-O3
5	B	2310	GOL	C1-C2-C3-O3
5	C	2322	GOL	C1-C2-C3-O3
5	A	2304	GOL	O2-C2-C3-O3
5	D	2318	GOL	O2-C2-C3-O3
5	A	2320[A]	GOL	O2-C2-C3-O3
5	B	2312	GOL	O1-C1-C2-O2

There are no ring outliers.

25 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2202	ACY	1	0
4	A	2200[B]	ACY	2	0
5	B	2311	GOL	1	0
4	A	2222	ACY	2	0
4	D	2215	ACY	1	0
5	C	2322	GOL	8	0
4	D	2214	ACY	1	0
5	D	2319	GOL	3	0
4	D	2219	ACY	2	0
4	A	2201	ACY	3	0
5	B	2310	GOL	9	0
5	A	2320[B]	GOL	2	0
5	A	2305	GOL	2	0
4	B	2208	ACY	1	0
4	B	2205	ACY	1	0
4	C	2210	ACY	4	0
5	A	2306	GOL	6	0
5	A	2304	GOL	2	0
4	A	2204	ACY	3	0
5	A	2303	GOL	3	0
5	A	2320[A]	GOL	2	0
4	C	2213	ACY	2	0
5	C	2315	GOL	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2209[A]	ACY	3	0
5	C	2321	GOL	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	687/696 (98%)	-0.59	6 (0%) 81 83	10, 21, 35, 71	30 (4%)
1	B	682/696 (97%)	-0.06	14 (2%) 63 67	12, 29, 52, 67	30 (4%)
1	C	686/696 (98%)	-0.50	5 (0%) 84 86	11, 23, 36, 58	33 (4%)
1	D	681/696 (97%)	-0.21	7 (1%) 79 82	12, 27, 44, 52	28 (4%)
All	All	2736/2784 (98%)	-0.34	32 (1%) 76 79	10, 24, 44, 71	121 (4%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	680	VAL	3.9
1	A	680	VAL	3.9
1	D	574	TRP	3.6
1	C	487	PRO	3.5
1	B	676	ILE	3.4
1	B	574	TRP	3.1
1	B	726	ILE	2.8
1	D	670	GLY	2.8
1	D	637	ALA	2.8
1	A	372	HIS	2.8
1	D	373	HIS	2.7
1	A	681	PRO	2.7
1	C	807	SER	2.6
1	C	371	HIS	2.6
1	B	639	LEU	2.6
1	A	811	VAL	2.5
1	B	970	LYS	2.4
1	B	646	ASP	2.4
1	B	649	ILE	2.2
1	A	373[A]	HIS	2.2
1	B	722	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	449	TRP	2.1
1	D	411	ASP	2.1
1	B	669	GLY	2.1
1	D	431	PHE	2.1
1	B	670	GLY	2.1
1	B	723	GLU	2.1
1	B	652	GLY	2.1
1	B	637	ALA	2.1
1	A	679	LYS	2.0
1	B	636	ASN	2.0
1	D	448	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(Å ²)	Q<0.9
4	ACY	C	2210	4/4	0.74	0.18	45,46,46,46	0
4	ACY	D	2219	4/4	0.76	0.18	43,44,46,48	0
4	ACY	A	2218	4/4	0.78	0.19	40,41,41,42	0
4	ACY	B	2208	4/4	0.81	0.19	53,53,54,54	0
4	ACY	D	2215	4/4	0.82	0.19	40,42,44,44	0
4	ACY	A	2220	4/4	0.82	0.13	37,40,41,43	0
5	GOL	C	2321	6/6	0.83	0.14	24,40,43,50	0
4	ACY	C	2212	4/4	0.85	0.14	38,39,40,40	0
4	ACY	D	2216	4/4	0.86	0.15	44,46,46,46	0
4	ACY	D	2217	4/4	0.86	0.16	50,51,51,52	0
4	ACY	A	2201	4/4	0.86	0.18	47,47,48,50	0
5	GOL	A	2303	6/6	0.86	0.11	28,41,41,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ACY	A	2203	4/4	0.86	0.14	44,44,45,45	0
5	GOL	C	2315	6/6	0.86	0.12	24,34,37,43	0
4	ACY	B	2207	4/4	0.87	0.14	40,43,43,43	0
5	GOL	B	2311	6/6	0.87	0.14	28,46,50,53	0
4	ACY	A	2202	4/4	0.88	0.15	36,38,41,41	0
4	ACY	C	2211	4/4	0.88	0.15	45,47,48,48	0
5	GOL	C	2322	6/6	0.88	0.11	12,36,37,38	0
5	GOL	A	2307	6/6	0.88	0.16	39,49,49,51	0
4	ACY	C	2221	4/4	0.89	0.12	41,43,44,44	0
5	GOL	A	2308	6/6	0.89	0.10	47,51,52,53	0
4	ACY	C	2213	4/4	0.89	0.16	39,40,42,43	0
5	GOL	D	2319	6/6	0.89	0.14	30,38,41,41	0
5	GOL	A	2320[A]	6/6	0.90	0.12	15,23,27,30	6
5	GOL	A	2320[B]	6/6	0.90	0.12	25,30,31,34	6
5	GOL	B	2310	6/6	0.90	0.10	30,38,42,44	0
4	ACY	B	2206	4/4	0.90	0.15	45,49,49,50	0
5	GOL	A	2304	6/6	0.91	0.12	24,33,38,43	0
5	GOL	A	2305	6/6	0.91	0.11	20,36,40,41	0
4	ACY	B	2205	4/4	0.91	0.10	39,39,40,41	0
6	CL	A	2402	1/1	0.92	0.13	44,44,44,44	0
5	GOL	C	2317	6/6	0.93	0.10	31,37,38,41	0
4	ACY	A	2222	4/4	0.93	0.11	50,53,53,53	0
4	ACY	D	2214	4/4	0.93	0.12	34,36,37,39	0
5	GOL	A	2301	6/6	0.93	0.09	26,34,36,39	0
5	GOL	D	2318	6/6	0.93	0.09	29,30,31,34	0
5	GOL	B	2312	6/6	0.93	0.10	39,45,47,47	0
5	GOL	C	2313	6/6	0.93	0.09	26,30,37,39	0
4	ACY	A	2204	4/4	0.94	0.14	49,50,50,50	0
5	GOL	C	2314	6/6	0.95	0.06	27,29,30,32	0
5	GOL	A	2306	6/6	0.95	0.13	24,36,39,49	0
5	GOL	A	2302	6/6	0.96	0.07	25,30,35,35	0
4	ACY	C	2209[A]	4/4	0.97	0.07	16,16,16,18	4
4	ACY	C	2209[B]	4/4	0.97	0.07	18,20,20,21	4
5	GOL	B	2309	6/6	0.97	0.06	29,31,35,35	0
4	ACY	A	2200[A]	4/4	0.98	0.06	17,17,17,20	4
4	ACY	A	2200[B]	4/4	0.98	0.06	18,18,19,21	4
6	CL	C	2402	1/1	0.98	0.08	38,38,38,38	0
3	CA	D	1501	1/1	0.99	0.03	23,23,23,23	0
6	CL	B	2401	1/1	0.99	0.03	28,28,28,28	0
6	CL	C	2401	1/1	0.99	0.04	23,23,23,23	0
3	CA	B	1501	1/1	0.99	0.02	23,23,23,23	0
2	FE2	D	1500	1/1	1.00	0.02	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	A	1501	1/1	1.00	0.01	23,23,23,23	0
3	CA	A	1502	1/1	1.00	0.01	21,21,21,21	0
3	CA	A	1067	1/1	1.00	0.02	22,22,22,22	0
2	FE2	A	1500	1/1	1.00	0.01	17,17,17,17	0
3	CA	C	1501	1/1	1.00	0.03	24,24,24,24	0
6	CL	A	2401	1/1	1.00	0.04	26,26,26,26	0
3	CA	C	1502	1/1	1.00	0.01	21,21,21,21	0
3	CA	C	1067	1/1	1.00	0.01	23,23,23,23	0
2	FE2	B	1500	1/1	1.00	0.01	22,22,22,22	0
2	FE2	C	1500	1/1	1.00	0.01	18,18,18,18	0
6	CL	D	2401	1/1	1.00	0.03	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.