



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 10:46 PM EDT

PDB ID : 3FG3  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

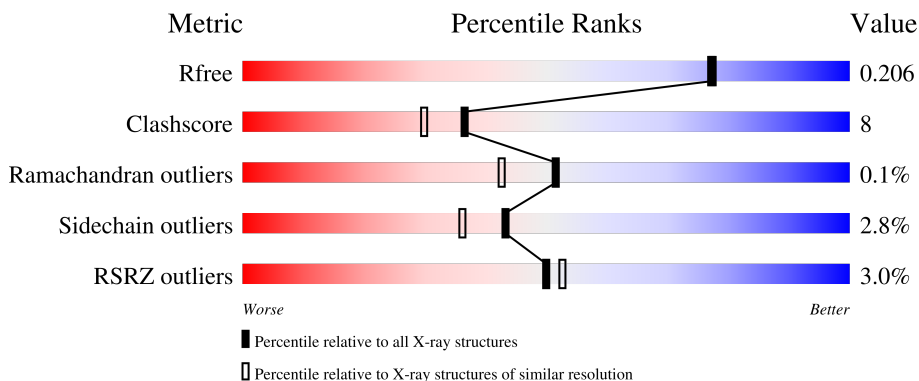
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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	6% 83% 14% ..
1	C	696	84% 12% ..
1	D	696	3% 85% 11% ..

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	2303	-	-	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	X	-

## 2 Entry composition [i](#)

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

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 (three-letter code: 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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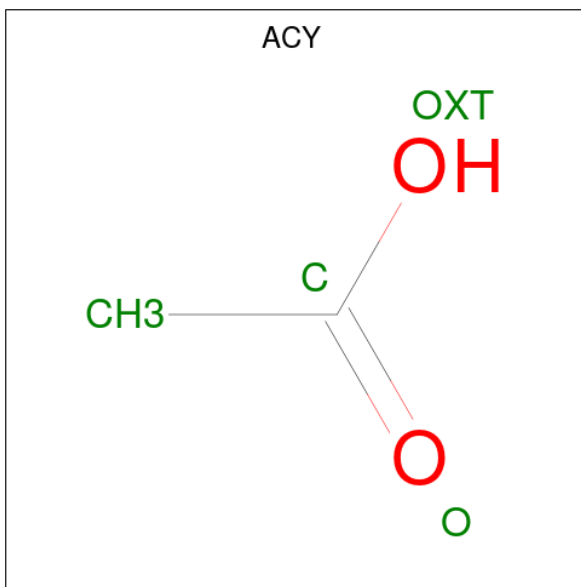
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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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 (three-letter code: 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

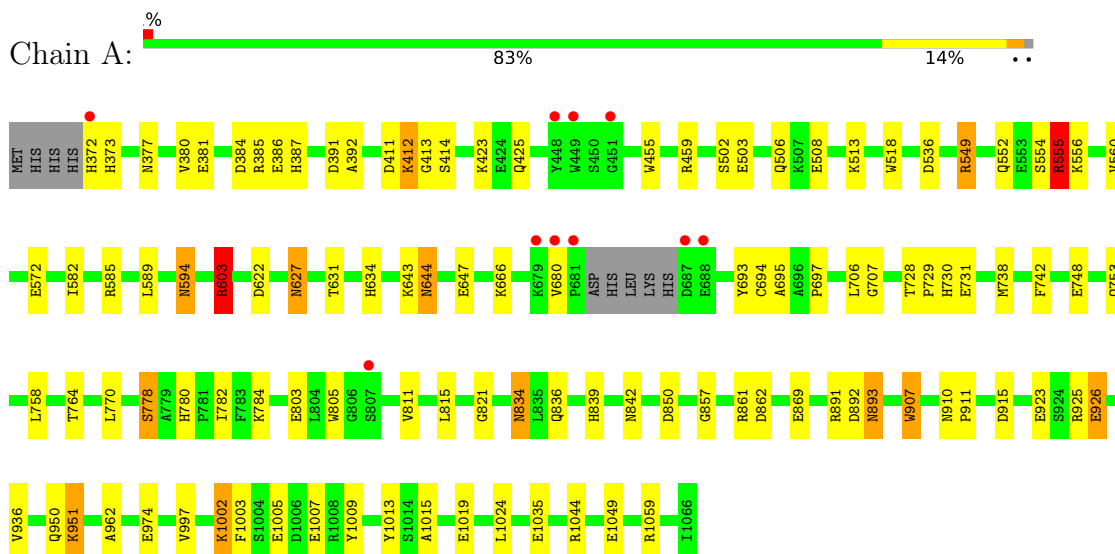
- Molecule 7 is water.

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

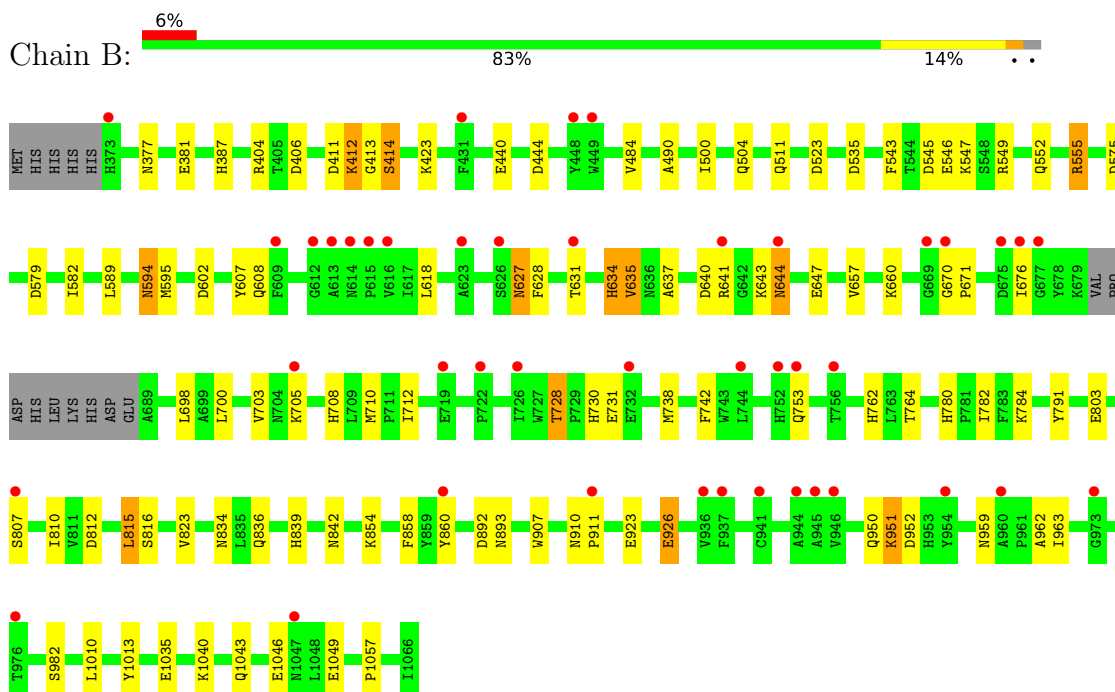
### 3 Residue-property plots [i](#)

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.

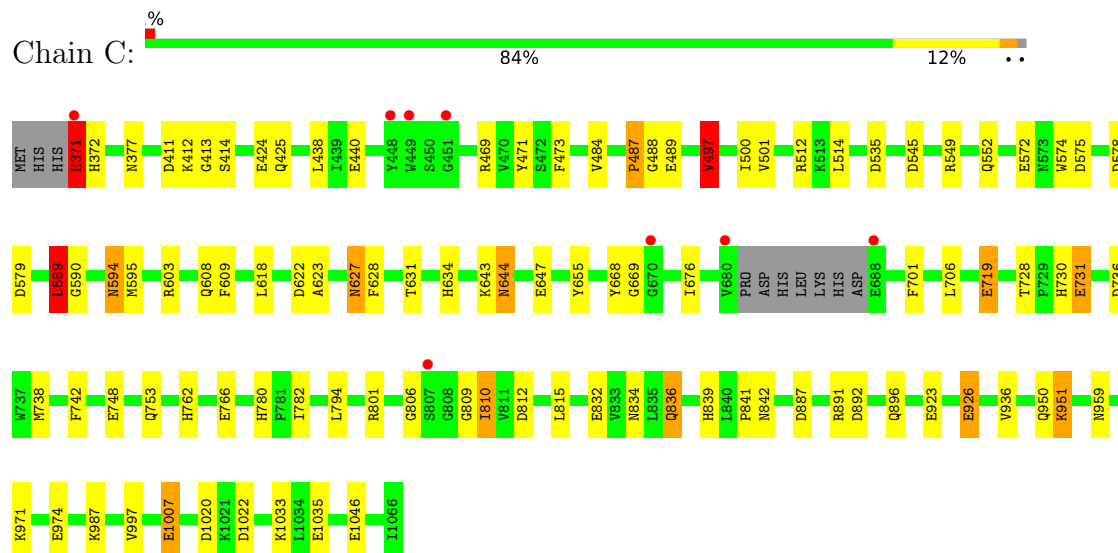
- Molecule 1: Allene oxide synthase-lipoxygenase protein



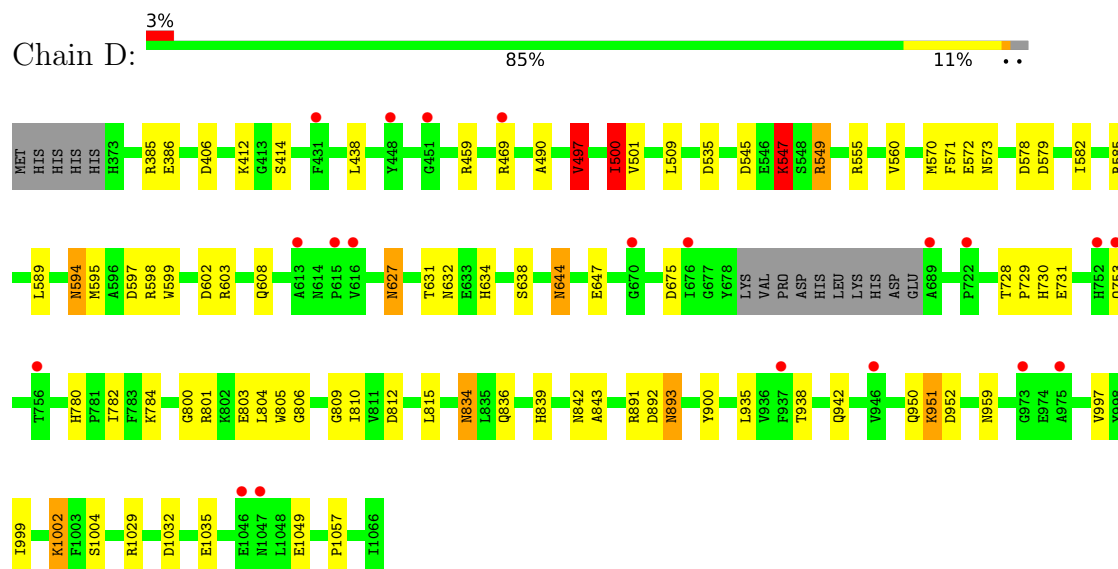
- Molecule 1: Allene oxide synthase-lipoxygenase protein



- Molecule 1: Allene oxide synthase-lipoxygenase protein



- Molecule 1: Allene oxide synthase-lipoxygenase protein



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.70Å 170.21Å 104.20Å 90.00° 96.13° 90.00°	Depositor
Resolution (Å)	34.54 – 1.90 34.03 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.54-1.90) 98.4 (34.03-1.90)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.89Å)	Xtrriage
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 <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.177	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.098 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	25025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, FE2, CL, CA, ACY

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	1.21	11/5851 (0.2%)	1.00	17/7955 (0.2%)
1	B	1.10	7/5773 (0.1%)	0.91	13/7856 (0.2%)
1	C	1.23	14/5791 (0.2%)	0.98	13/7878 (0.2%)
1	D	1.13	7/5754 (0.1%)	0.97	14/7827 (0.2%)
All	All	1.17	39/23169 (0.2%)	0.97	57/31516 (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 (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	923[A]	GLU	CG-CD	-11.76	1.34	1.51
1	C	923[B]	GLU	CG-CD	-11.76	1.34	1.51
1	C	414	SER	C-N	7.92	1.52	1.34
1	B	414	SER	C-N	7.04	1.50	1.34
1	C	623	ALA	CA-CB	6.66	1.66	1.52
1	A	869	GLU	CB-CG	6.47	1.64	1.52
1	D	900	TYR	CD1-CE1	5.92	1.48	1.39
1	A	693	TYR	CD1-CE1	5.86	1.48	1.39
1	C	1046	GLU	CB-CG	-5.78	1.41	1.52
1	A	1005	GLU	CG-CD	5.75	1.60	1.51
1	B	926[A]	GLU	CB-CG	5.74	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	926[B]	GLU	CB-CG	5.74	1.63	1.52
1	D	414	SER	C-N	5.72	1.47	1.34
1	D	843	ALA	CA-CB	5.71	1.64	1.52
1	D	1002	LYS	CD-CE	5.64	1.65	1.51
1	C	1007	GLU	CD-OE2	5.60	1.31	1.25
1	C	471	TYR	CG-CD1	5.52	1.46	1.39
1	C	926	GLU	CG-CD	5.52	1.60	1.51
1	A	1005	GLU	CB-CG	5.46	1.62	1.52
1	C	701	PHE	CE1-CZ	5.41	1.47	1.37
1	C	669	GLY	N-CA	-5.35	1.38	1.46
1	B	860	TYR	CE1-CZ	5.23	1.45	1.38
1	A	936	VAL	CB-CG2	5.22	1.63	1.52
1	C	936	VAL	CB-CG2	5.21	1.63	1.52
1	D	560	VAL	CB-CG2	5.21	1.63	1.52
1	D	805	TRP	CE3-CZ3	5.20	1.47	1.38
1	A	1009	TYR	CE2-CZ	5.20	1.45	1.38
1	A	1013	TYR	CD1-CE1	5.17	1.47	1.39
1	B	607	TYR	CE1-CZ	5.17	1.45	1.38
1	B	1013	TYR	CE1-CZ	5.14	1.45	1.38
1	C	731	GLU	CD-OE1	5.13	1.31	1.25
1	C	628	PHE	CE2-CZ	5.12	1.47	1.37
1	D	547	LYS	CG-CD	5.10	1.69	1.52
1	A	694	CYS	CB-SG	5.09	1.91	1.82
1	A	560	VAL	CB-CG2	5.08	1.63	1.52
1	A	1002	LYS	CD-CE	5.08	1.64	1.51
1	A	907	TRP	CE3-CZ3	5.07	1.47	1.38
1	B	546	GLU	CG-CD	5.03	1.59	1.51
1	C	836	GLN	CG-CD	5.02	1.62	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	549	ARG	NE-CZ-NH2	-16.30	112.15	120.30
1	D	549	ARG	NE-CZ-NH1	12.25	126.42	120.30
1	B	549	ARG	NE-CZ-NH2	-11.57	114.52	120.30
1	D	585	ARG	NE-CZ-NH1	-10.28	115.16	120.30
1	A	549	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	535	ASP	CB-CG-OD2	8.39	125.85	118.30
1	D	535	ASP	CB-CG-OD2	8.37	125.83	118.30
1	D	585	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	C	549	ARG	NE-CZ-NH2	-7.99	116.30	120.30
1	D	497	VAL	CG1-CB-CG2	7.74	123.28	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1044	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	A	555	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	C	438	LEU	CA-CB-CG	7.50	132.56	115.30
1	B	523	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	549	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	603[A]	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	603[B]	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	B	549	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	555	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	C	578	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	497	VAL	CG1-CB-CG2	6.48	121.27	110.90
1	D	385	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	C	438	LEU	CB-CG-CD1	-6.42	100.08	111.00
1	C	512	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	A	925	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	D	535	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	536[A]	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	536[B]	ASP	CB-CG-OD1	6.19	123.87	118.30
1	B	414	SER	O-C-N	-6.07	112.99	122.70
1	D	602	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	589	LEU	CA-C-N	5.92	128.05	116.20
1	B	1010	LEU	CB-CG-CD2	-5.90	100.96	111.00
1	D	935	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	C	372	HIS	N-CA-C	5.85	126.79	111.00
1	A	555	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	406[A]	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	406[B]	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	622	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	523	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	385	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	812	ASP	CB-CA-C	-5.49	99.42	110.40
1	B	444	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	923[A]	GLU	CB-CG-CD	5.41	128.80	114.20
1	C	923[B]	GLU	CB-CG-CD	5.41	128.80	114.20
1	A	915	ASP	CB-CG-OD1	-5.30	113.53	118.30
1	D	597	ASP	CB-CG-OD2	5.28	123.06	118.30
1	C	535	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	925	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	500	ILE	CG1-CB-CG2	5.23	122.91	111.40
1	C	736	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	589	LEU	N-CA-C	5.17	124.97	111.00
1	A	861	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	602	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	675	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	862	ASP	CB-CG-OD2	5.07	122.87	118.30
1	D	1029	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	A	1024	LEU	CB-CG-CD1	-5.03	102.46	111.00

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 [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	5624	0	5393	107	0
1	B	5552	0	5281	79	0
1	C	5576	0	5311	84	1
1	D	5538	0	5281	68	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	11	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	29	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	349	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 (349) 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:B:387:HIS:ND1	7:B:2320:HOH:O	1.79	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:A:387:HIS:ND1	7:A:2318:HOH:O	1.91	1.04
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:547:LYS:HD2	1:B:791[B]:TYR:HH	1.36	0.86
1:D:608:GLN:HB2	4:D:2214:ACY:H3	1.56	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: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:C:579:ASP:CG	5:C:2322:GOL:H11	2.04	0.77
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: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
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
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
1:B:839:HIS:HE1	7:B:1471:HOH:O	1.84	0.60
1:C:1035:GLU:CD	5:C:2321:GOL:H31	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:497:VAL:HG13	1:D:501:VAL:HB	1.85	0.58
1:D:644:ASN:C	1:D:644:ASN:HD22	2.07	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:D:579:ASP:CG	5:D:2319:GOL:H2	2.23	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: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
5:A:2303:GOL:HO1	5:B:2310:GOL:H2	1.72	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:C:627:ASN:H	1:C:627:ASN:ND2	2.00	0.53
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:A:585:ARG:HE	1:D:572:GLU:CD	2.12	0.53
1:C:575:ASP:OD1	5:C:2322:GOL:H12	2.09	0.53
1:D:891:ARG:HD3	7:D:2372:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:738:MET:HG3	1:C:742:PHE:CE1	2.44	0.53
1:A:413:GLY:C	5:B:2310:GOL:H12	2.29	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: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: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:D:386[A]:GLU:CD	1:D:549:ARG:HH22	2.14	0.51
1:A:1003:PHE:CE1	4:A:2204:ACY:CH3	2.93	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:GLU:CB	1:C:1020[B]:ASP:CG	2.78	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:502:SER:O	1:A:506[B]:GLN:HG3	2.14	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: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
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: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
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:594:ASN:C	1:C:594:ASN:HD22	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:710:MET:HE3	7:B:1220:HOH:O	2.16	0.44
1:B:784:LYS:HE3	7:B:2387:HOH:O	2.17	0.44
1:A:695:ALA:C	1:A:697:PRO:HD3	2.38	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: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:B:579:ASP:OD1	5:B:2311:GOL:O2	2.37	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
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:594:ASN:C	1:A:594:ASN:HD22	2.22	0.42
1:A:643:LYS:HB3	1:A:647:GLU:HB2	2.01	0.42
1:A:926[A]:GLU:CD	1:A:926[A]:GLU:H	2.22	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:594:ASN:C	1:D:594:ASN:HD22	2.22	0.42
1:D:810:ILE:CG2	7:D:2148:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:386:GLU:CD	1:A:549:ARG:HH22	2.23	0.40
1:A:513:LYS:NZ	7:A:1375:HOH:O	2.43	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 [i](#)

#### 5.3.1 Protein backbone [i](#)

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%)	41	31
1	C	703/696 (101%)	675 (96%)	26 (4%)	2 (0%)	41	31
1	D	699/696 (100%)	676 (97%)	23 (3%)	0	100	100
All	All	2810/2784 (101%)	2711 (96%)	95 (3%)	4 (0%)	51	42

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 [i](#)

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%)	589 (97%)	16 (3%)	46	39
1	B	590/602 (98%)	565 (96%)	25 (4%)	30	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	593/602 (98%)	578 (98%)	15 (2%)	47	41
1	D	585/602 (97%)	569 (97%)	16 (3%)	44	38
All	All	2373/2408 (98%)	2301 (97%)	72 (3%)	43	33

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

Mol	Chain	Res	Type
1	A	412	LYS
1	A	555	ARG
1	A	594	ASN
1	A	603[A]	ARG
1	A	603[B]	ARG
1	A	627	ASN
1	A	644[A]	ASN
1	A	644[B]	ASN
1	A	778[A]	SER
1	A	778[B]	SER
1	A	834	ASN
1	A	893	ASN
1	A	923	GLU
1	A	926[A]	GLU
1	A	926[B]	GLU
1	A	951	LYS
1	B	404	ARG
1	B	412	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
1	B	676	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

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Mol	Chain	Res	Type
1	B	858	PHE
1	B	923	GLU
1	B	926[A]	GLU
1	B	926[B]	GLU
1	B	951	LYS
1	B	982	SER
1	B	1057	PRO
1	C	371	HIS
1	C	497	VAL
1	C	514	LEU
1	C	545	ASP
1	C	594	ASN
1	C	603	ARG
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	951	LYS
1	C	987	LYS
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	594	ASN
1	D	603	ARG
1	D	627	ASN
1	D	644	ASN
1	D	815	LEU
1	D	834	ASN
1	D	893[A]	ASN
1	D	893[B]	ASN
1	D	951	LYS
1	D	1057	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	377	ASN
1	A	429	GLN
1	A	458	ASN
1	A	467	GLN
1	A	594	ASN
1	A	614	ASN
1	A	627	ASN
1	A	634	HIS
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	905	ASN
1	A	947	ASN
1	A	950	GLN
1	B	377	ASN
1	B	458	ASN
1	B	504	GLN
1	B	594	ASN
1	B	614	ASN
1	B	627	ASN
1	B	634	HIS
1	B	730	HIS
1	B	750	ASN
1	B	780	HIS
1	B	834	ASN
1	B	839	HIS
1	B	842	ASN
1	B	905	ASN
1	B	947	ASN
1	B	950	GLN
1	B	959	ASN
1	B	1043	GLN
1	C	377	ASN
1	C	458	ASN
1	C	504	GLN
1	C	594	ASN
1	C	614	ASN
1	C	627	ASN

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Mol	Chain	Res	Type
1	C	634	HIS
1	C	715	GLN
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	905	ASN
1	C	947	ASN
1	C	950	GLN
1	C	959	ASN
1	D	458	ASN
1	D	517	GLN
1	D	594	ASN
1	D	614	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	905	ASN
1	D	947	ASN
1	D	950	GLN
1	D	959	ASN
1	D	966	HIS
1	D	1043	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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
5	GOL	A	2304	-	5,5,5	0.97	0	5,5,5	1.47	2 (40%)
5	GOL	C	2321	-	5,5,5	0.90	0	5,5,5	1.36	1 (20%)
4	ACY	C	2213	-	3,3,3	0.69	0	3,3,3	1.91	1 (33%)
4	ACY	C	2209[A]	-	3,3,3	0.62	0	3,3,3	2.29	2 (66%)
5	GOL	C	2315	-	5,5,5	0.77	0	5,5,5	0.58	0
5	GOL	C	2322	-	5,5,5	0.91	0	5,5,5	3.05	2 (40%)
4	ACY	C	2210	-	3,3,3	0.91	0	3,3,3	0.35	0
5	GOL	A	2301	-	5,5,5	0.70	0	5,5,5	0.87	0
4	ACY	A	2201	-	3,3,3	0.72	0	3,3,3	1.24	0
4	ACY	D	2217	-	3,3,3	0.88	0	3,3,3	0.80	0
5	GOL	A	2320[A]	-	5,5,5	0.52	0	5,5,5	1.00	0
5	GOL	B	2309	-	5,5,5	0.53	0	5,5,5	0.25	0
4	ACY	A	2218	-	3,3,3	0.93	0	3,3,3	0.47	0
4	ACY	B	2208	-	3,3,3	0.86	0	3,3,3	0.46	0
4	ACY	A	2200[B]	-	3,3,3	0.92	0	3,3,3	0.97	0
4	ACY	B	2205	-	3,3,3	0.72	0	3,3,3	1.17	0
5	GOL	C	2313	-	5,5,5	0.84	0	5,5,5	1.34	1 (20%)
4	ACY	D	2216	-	3,3,3	0.83	0	3,3,3	1.01	0
4	ACY	C	2212	-	3,3,3	0.56	0	3,3,3	1.55	1 (33%)
5	GOL	B	2311	-	5,5,5	0.53	0	5,5,5	1.44	1 (20%)
4	ACY	C	2221	-	3,3,3	0.76	0	3,3,3	0.89	0
5	GOL	B	2310	-	5,5,5	0.75	0	5,5,5	2.88	2 (40%)
4	ACY	C	2211	-	3,3,3	0.65	0	3,3,3	1.49	0
4	ACY	D	2214	-	3,3,3	0.97	0	3,3,3	0.49	0
4	ACY	A	2202	-	3,3,3	1.01	0	3,3,3	2.96	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACY	A	2204	-	3,3,3	0.60	0	3,3,3	1.64	1 (33%)
4	ACY	A	2222	-	3,3,3	0.66	0	3,3,3	1.21	0
4	ACY	B	2206	-	3,3,3	0.65	0	3,3,3	1.76	1 (33%)
4	ACY	C	2209[B]	-	3,3,3	1.12	0	3,3,3	0.53	0
5	GOL	A	2305	-	5,5,5	0.36	0	5,5,5	1.97	1 (20%)
5	GOL	A	2308	-	5,5,5	0.42	0	5,5,5	0.44	0
5	GOL	A	2307	-	5,5,5	0.86	0	5,5,5	1.23	0
5	GOL	C	2314	-	5,5,5	0.38	0	5,5,5	0.64	0
5	GOL	A	2320[B]	-	5,5,5	0.57	0	5,5,5	1.12	0
4	ACY	D	2215	-	3,3,3	0.59	0	3,3,3	2.37	1 (33%)
5	GOL	C	2317	-	5,5,5	0.42	0	5,5,5	1.16	1 (20%)
4	ACY	A	2200[A]	-	3,3,3	0.67	0	3,3,3	1.43	0
5	GOL	A	2302	-	5,5,5	0.54	0	5,5,5	0.62	0
4	ACY	A	2220	-	3,3,3	0.99	0	3,3,3	1.03	0
5	GOL	A	2306	-	5,5,5	0.34	0	5,5,5	1.90	2 (40%)
4	ACY	B	2207	-	3,3,3	0.74	0	3,3,3	1.03	0
4	ACY	A	2203	-	3,3,3	0.51	0	3,3,3	1.38	0
5	GOL	D	2318	-	5,5,5	0.44	0	5,5,5	0.53	0
5	GOL	B	2312	-	5,5,5	0.46	0	5,5,5	0.89	0
4	ACY	D	2219	-	3,3,3	0.87	0	3,3,3	0.23	0
5	GOL	D	2319	-	5,5,5	1.05	0	5,5,5	1.16	0
5	GOL	A	2303	-	5,5,5	0.77	0	5,5,5	0.82	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	A	2304	-	-	2/4/4/4	-
5	GOL	C	2321	-	-	2/4/4/4	-
5	GOL	C	2315	-	-	2/4/4/4	-
5	GOL	C	2322	-	-	4/4/4/4	-
5	GOL	A	2301	-	-	0/4/4/4	-
5	GOL	A	2320[A]	-	-	3/4/4/4	-
5	GOL	B	2309	-	-	0/4/4/4	-
5	GOL	C	2313	-	-	0/4/4/4	-
5	GOL	B	2311	-	-	4/4/4/4	-
5	GOL	B	2310	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	2305	-	-	3/4/4/4	-
5	GOL	A	2308	-	-	0/4/4/4	-
5	GOL	A	2307	-	-	2/4/4/4	-
5	GOL	C	2314	-	-	0/4/4/4	-
5	GOL	A	2320[B]	-	-	4/4/4/4	-
5	GOL	C	2317	-	-	2/4/4/4	-
5	GOL	A	2302	-	-	0/4/4/4	-
5	GOL	A	2306	-	-	2/4/4/4	-
5	GOL	D	2318	-	-	2/4/4/4	-
5	GOL	B	2312	-	-	4/4/4/4	-
5	GOL	D	2319	-	-	4/4/4/4	-
5	GOL	A	2303	-	-	0/4/4/4	-

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2322	GOL	C3-C2-C1	-5.66	89.71	111.70
5	B	2310	GOL	O3-C3-C2	-4.43	88.94	110.20
5	B	2310	GOL	O2-C2-C1	3.95	126.53	109.12
4	A	2202	ACY	O-C-CH3	-3.94	106.98	122.33
5	A	2305	GOL	O1-C1-C2	-3.83	91.85	110.20
4	D	2215	ACY	O-C-CH3	-3.32	109.41	122.33
5	C	2322	GOL	O2-C2-C3	3.21	123.25	109.12
4	A	2202	ACY	OXT-C-O	3.09	133.45	122.05
5	A	2306	GOL	O2-C2-C1	3.05	122.55	109.12
4	C	2209[A]	ACY	O-C-CH3	-3.03	110.52	122.33
4	C	2213	ACY	O-C-CH3	-2.68	111.92	122.33
5	C	2321	GOL	O2-C2-C1	2.51	120.17	109.12
5	A	2306	GOL	O2-C2-C3	2.49	120.09	109.12
4	C	2209[A]	ACY	OXT-C-O	2.45	131.07	122.05
5	C	2317	GOL	O2-C2-C1	2.36	119.51	109.12
4	B	2206	ACY	O-C-CH3	-2.34	113.22	122.33
5	A	2304	GOL	O3-C3-C2	-2.27	99.33	110.20
4	A	2204	ACY	O-C-CH3	-2.21	113.73	122.33
4	C	2212	ACY	O-C-CH3	-2.07	114.25	122.33
5	A	2304	GOL	O1-C1-C2	2.07	120.12	110.20
5	C	2313	GOL	O1-C1-C2	-2.05	100.37	110.20
5	B	2311	GOL	O2-C2-C1	2.04	118.09	109.12

There are no chirality outliers.

All (44) 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
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	C	2322	GOL	C1-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	A	2304	GOL	O2-C2-C3-O3
5	C	2322	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	D	2318	GOL	O2-C2-C3-O3
5	B	2311	GOL	O1-C1-C2-C3
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
5	A	2304	GOL	1	0
5	C	2321	GOL	5	0
4	C	2213	ACY	2	0
4	C	2209[A]	ACY	3	0
5	C	2315	GOL	7	0
5	C	2322	GOL	8	0
4	C	2210	ACY	4	0
4	A	2201	ACY	3	0
5	A	2320[A]	GOL	2	0
4	B	2208	ACY	1	0
4	A	2200[B]	ACY	2	0
4	B	2205	ACY	1	0
5	B	2311	GOL	2	0
5	B	2310	GOL	9	0
4	D	2214	ACY	1	0
4	A	2202	ACY	1	0
4	A	2204	ACY	3	0
4	A	2222	ACY	2	0
5	A	2305	GOL	2	0
5	A	2320[B]	GOL	2	0
4	D	2215	ACY	1	0
5	A	2306	GOL	6	0
4	D	2219	ACY	2	0
5	D	2319	GOL	3	0
5	A	2303	GOL	4	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	687/696 (98%)	-0.40	10 (1%) 73 76	14, 22, 36, 71	5 (0%)
1	B	682/696 (97%)	0.02	43 (6%) 20 22	18, 29, 52, 67	7 (1%)
1	C	686/696 (98%)	-0.39	8 (1%) 79 81	15, 23, 37, 58	13 (1%)
1	D	681/696 (97%)	-0.10	20 (2%) 51 54	17, 27, 44, 52	6 (0%)
All	All	2736/2784 (98%)	-0.22	81 (2%) 50 53	14, 25, 45, 71	31 (1%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	9.8
1	A	681	PRO	6.1
1	D	676	ILE	4.9
1	B	676	ILE	4.9
1	C	449	TRP	4.9
1	C	680	VAL	4.8
1	A	448	TYR	4.5
1	D	448	TYR	4.5
1	C	448	TYR	4.5
1	B	722	PRO	4.5
1	D	670	GLY	3.9
1	B	373[A]	HIS	3.8
1	A	688	GLU	3.8
1	B	448	TYR	3.7
1	A	687	ASP	3.6
1	B	623	ALA	3.6
1	D	722	PRO	3.6
1	A	372	HIS	3.5
1	B	613	ALA	3.4
1	D	946	VAL	3.4
1	B	616	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	644[A]	ASN	3.2
1	A	449	TRP	3.1
1	B	753[A]	GLN	3.0
1	C	451	GLY	3.0
1	B	973	GLY	2.9
1	D	689	ALA	2.9
1	D	431	PHE	2.8
1	B	670	GLY	2.8
1	C	688	GLU	2.8
1	B	807	SER	2.8
1	B	641	ARG	2.7
1	B	1047	ASN	2.7
1	B	675[A]	ASP	2.6
1	C	807	SER	2.6
1	B	946	VAL	2.6
1	D	616	VAL	2.6
1	D	973	GLY	2.6
1	B	960	ALA	2.5
1	B	945	ALA	2.5
1	B	614	ASN	2.5
1	D	469[A]	ARG	2.5
1	B	626	SER	2.5
1	B	609	PHE	2.5
1	B	944	ALA	2.5
1	D	753[A]	GLN	2.4
1	C	670	GLY	2.4
1	B	726	ILE	2.4
1	B	756	THR	2.4
1	B	941	CYS	2.3
1	B	976	THR	2.3
1	B	669	GLY	2.3
1	B	752	HIS	2.3
1	D	451	GLY	2.3
1	B	631	THR	2.3
1	D	975	ALA	2.3
1	B	431	PHE	2.2
1	D	1047	ASN	2.2
1	A	807	SER	2.2
1	B	615	PRO	2.2
1	B	705	LYS	2.2
1	A	679	LYS	2.2
1	B	911	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	615	PRO	2.1
1	D	613	ALA	2.1
1	B	937	PHE	2.1
1	D	1046	GLU	2.1
1	D	752	HIS	2.1
1	B	719	GLU	2.1
1	B	860	TYR	2.1
1	B	954	TYR	2.1
1	B	732	GLU	2.0
1	B	936	VAL	2.0
1	A	451	GLY	2.0
1	B	612	GLY	2.0
1	B	744	LEU	2.0
1	D	756	THR	2.0
1	C	371	HIS	2.0
1	B	677	GLY	2.0
1	D	937	PHE	2.0
1	B	449	TRP	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	ACY	D	2219	4/4	0.79	0.18	43,44,46,48	0
4	ACY	C	2210	4/4	0.81	0.14	45,46,46,46	0
4	ACY	C	2221	4/4	0.85	0.14	41,43,44,44	0
4	ACY	A	2220	4/4	0.85	0.15	37,40,41,43	0
5	GOL	C	2321	6/6	0.85	0.14	24,40,43,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	ACY	D	2215	4/4	0.87	0.23	40,42,44,44	0
4	ACY	A	2218	4/4	0.88	0.15	40,41,41,42	0
5	GOL	A	2307	6/6	0.88	0.18	39,49,49,51	0
5	GOL	B	2310	6/6	0.88	0.21	30,38,42,44	0
4	ACY	A	2202	4/4	0.88	0.18	36,38,41,41	0
4	ACY	C	2213	4/4	0.89	0.20	39,40,42,43	0
4	ACY	A	2201	4/4	0.90	0.12	47,47,48,50	0
4	ACY	C	2212	4/4	0.90	0.13	38,39,40,40	0
5	GOL	B	2311	6/6	0.90	0.14	28,46,50,53	0
4	ACY	B	2208	4/4	0.90	0.13	53,53,54,54	0
5	GOL	C	2322	6/6	0.90	0.16	12,36,37,38	0
5	GOL	D	2319	6/6	0.90	0.13	30,38,41,41	0
6	CL	A	2402	1/1	0.90	0.08	44,44,44,44	0
4	ACY	A	2203	4/4	0.91	0.13	44,44,45,45	0
5	GOL	A	2308	6/6	0.91	0.14	47,51,52,53	0
5	GOL	A	2320[A]	6/6	0.91	0.15	15,23,27,30	6
5	GOL	A	2320[B]	6/6	0.91	0.15	25,30,31,34	6
4	ACY	A	2222	4/4	0.91	0.12	50,53,53,53	0
4	ACY	B	2207	4/4	0.92	0.12	40,43,43,43	0
5	GOL	C	2315	6/6	0.92	0.09	24,34,37,43	0
5	GOL	A	2303	6/6	0.92	0.16	28,41,41,46	0
4	ACY	D	2217	4/4	0.92	0.14	50,51,51,52	0
5	GOL	C	2313	6/6	0.93	0.10	26,30,37,39	0
5	GOL	C	2317	6/6	0.93	0.15	31,37,38,41	0
4	ACY	D	2214	4/4	0.93	0.26	34,36,37,39	0
4	ACY	A	2204	4/4	0.93	0.10	49,50,50,50	0
5	GOL	A	2305	6/6	0.93	0.12	20,36,40,41	0
5	GOL	A	2306	6/6	0.93	0.12	24,36,39,49	0
4	ACY	B	2206	4/4	0.93	0.15	45,49,49,50	0
4	ACY	C	2211	4/4	0.94	0.12	45,47,48,48	0
5	GOL	A	2304	6/6	0.94	0.14	24,33,38,43	0
5	GOL	B	2312	6/6	0.94	0.10	39,45,47,47	0
5	GOL	D	2318	6/6	0.94	0.11	29,30,31,34	0
4	ACY	D	2216	4/4	0.94	0.12	44,46,46,46	0
5	GOL	A	2301	6/6	0.94	0.08	26,34,36,39	0
4	ACY	B	2205	4/4	0.95	0.31	39,39,40,41	0
5	GOL	B	2309	6/6	0.96	0.11	29,31,35,35	0
5	GOL	C	2314	6/6	0.97	0.11	27,29,30,32	0
4	ACY	C	2209[A]	4/4	0.97	0.20	16,16,16,18	4
5	GOL	A	2302	6/6	0.97	0.08	25,30,35,35	0
4	ACY	C	2209[B]	4/4	0.97	0.20	18,20,20,21	4
4	ACY	A	2200[A]	4/4	0.98	0.17	17,17,17,20	4

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACY	A	2200[B]	4/4	0.98	0.17	18,18,19,21	4
6	CL	C	2402	1/1	0.98	0.04	38,38,38,38	0
3	CA	C	1502	1/1	0.99	0.06	21,21,21,21	0
3	CA	D	1501	1/1	0.99	0.03	23,23,23,23	0
6	CL	B	2401	1/1	0.99	0.08	28,28,28,28	0
6	CL	C	2401	1/1	0.99	0.04	23,23,23,23	0
2	FE2	B	1500	1/1	0.99	0.07	22,22,22,22	0
2	FE2	A	1500	1/1	1.00	0.07	17,17,17,17	0
3	CA	C	1067	1/1	1.00	0.06	23,23,23,23	0
2	FE2	C	1500	1/1	1.00	0.07	18,18,18,18	0
2	FE2	D	1500	1/1	1.00	0.09	20,20,20,20	0
3	CA	A	1501	1/1	1.00	0.05	23,23,23,23	0
6	CL	A	2401	1/1	1.00	0.06	26,26,26,26	0
3	CA	A	1502	1/1	1.00	0.06	21,21,21,21	0
3	CA	A	1067	1/1	1.00	0.07	22,22,22,22	0
3	CA	B	1501	1/1	1.00	0.04	23,23,23,23	0
3	CA	C	1501	1/1	1.00	0.03	24,24,24,24	0
6	CL	D	2401	1/1	1.00	0.07	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.