



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 07:24 AM GMT

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 wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

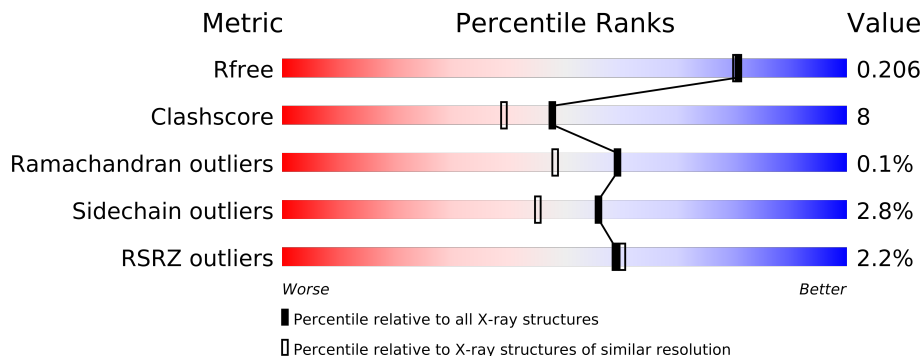
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	696	
1	B	696	
1	C	696	
1	D	696	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	ACY	A	2200[A]	-	X
4	ACY	A	2200[B]	-	X
4	ACY	A	2203	-	X
4	ACY	A	2204	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	ACY	A	2218	-	X
4	ACY	A	2222	-	X
4	ACY	B	2205	-	X
4	ACY	B	2206	-	X
4	ACY	B	2207	-	X
4	ACY	C	2209[A]	-	X
4	ACY	C	2209[B]	-	X
4	ACY	C	2211	-	X
4	ACY	C	2213	-	X
4	ACY	C	2221	-	X
4	ACY	D	2214	-	X
4	ACY	D	2216	-	X
4	ACY	D	2219	-	X
5	GOL	A	2307	-	X
5	GOL	A	2308	-	X
5	GOL	A	2320[A]	-	X
5	GOL	A	2320[B]	-	X
5	GOL	C	2317	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25025 atoms, of which 0 are hydrogen and 0 are deuterium.

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-lipoxygenaseprotein.

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	UNP O16025
A	414	SER	ASP	ENGINEERED	UNP O16025
A	782	ILE	VAL	SEE REMARK 999	UNP O16025
A	805	TRP	ILE	ENGINEERED	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	UNP O16025
B	414	SER	ASP	ENGINEERED	UNP O16025
B	782	ILE	VAL	SEE REMARK 999	UNP O16025
B	805	TRP	ILE	ENGINEERED	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	UNP O16025
C	414	SER	ASP	ENGINEERED	UNP O16025
C	782	ILE	VAL	SEE REMARK 999	UNP O16025
C	805	TRP	ILE	ENGINEERED	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	UNP O16025
D	414	SER	ASP	ENGINEERED	UNP O16025
D	782	ILE	VAL	SEE REMARK 999	UNP O16025
D	805	TRP	ILE	ENGINEERED	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	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0

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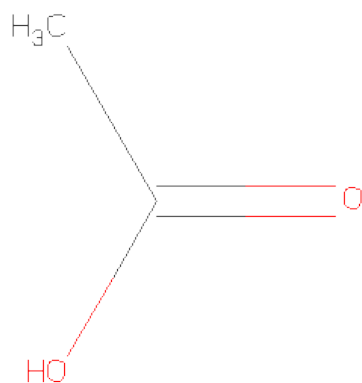
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

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

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

- Molecule 4 is ACETIC ACID (three-letter code: ACY) (formula: C₂H₄O₂).



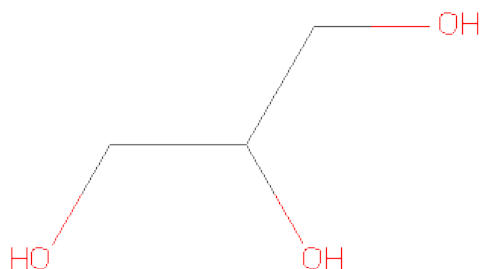
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			8	4	4		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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	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	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	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is water.

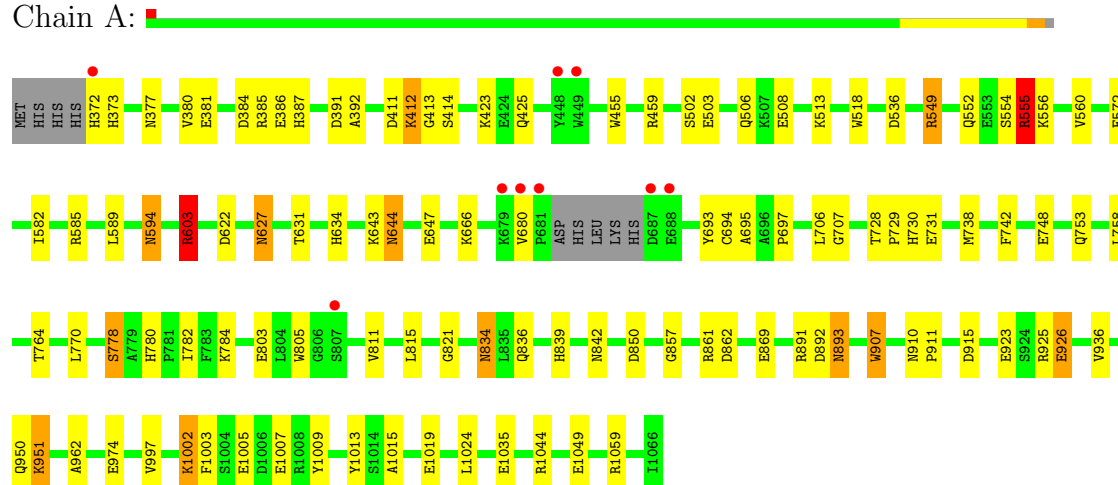
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	748	Total	O	0	0
			748	748		
7	B	526	Total	O	0	0
			526	526		
7	C	672	Total	O	0	0
			672	672		
7	D	539	Total	O	0	0
			539	539		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

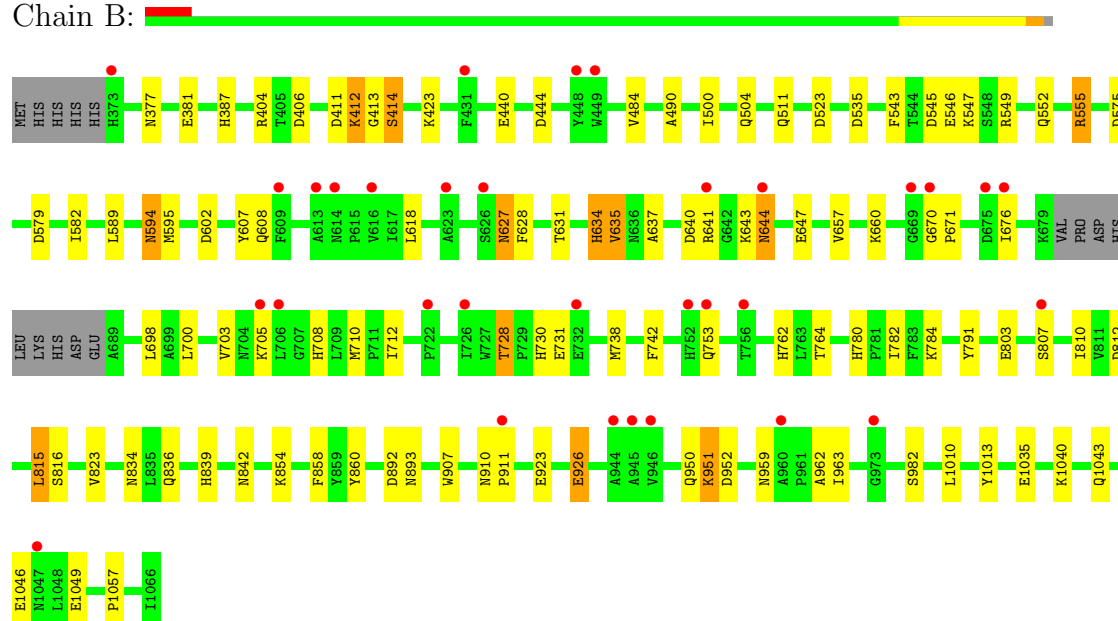
- Molecule 1: Allene oxide synthase-lipoxygenaseprotein

Chain A:



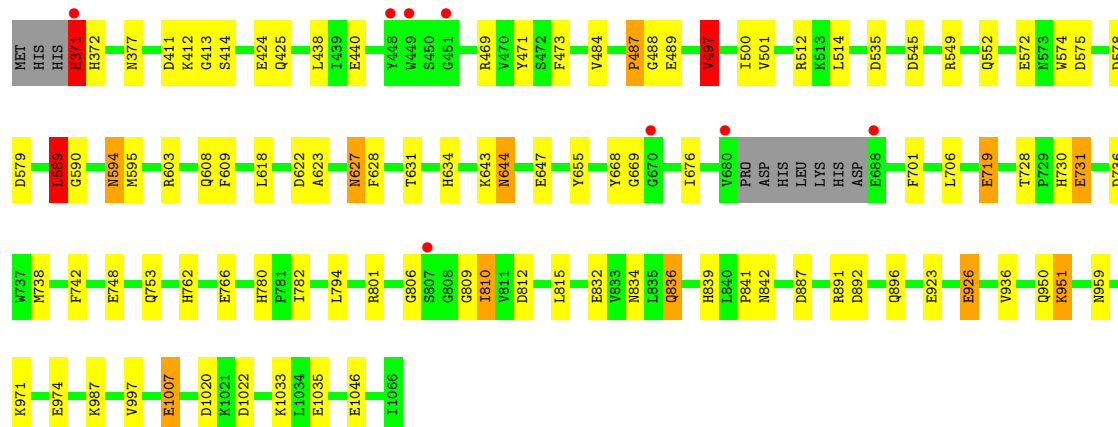
- Molecule 1: Allene oxide synthase-lipoxygenaseprotein

Chain B:



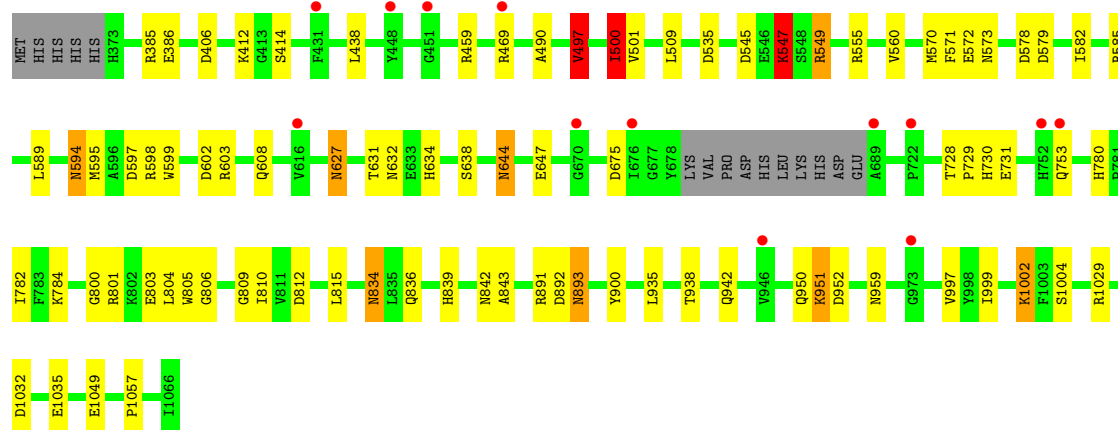
- Molecule 1: Allene oxide synthase-lipoxygenaseprotein

Chain C:



- Molecule 1: Allene oxide synthase-lipoxygenaseprotein

Chain D:



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 34.03 – 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
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.162 , 0.206 0.163 , 0.206	Depositor DCC
R_{free} test set	14029 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.7	EDS
Estimated twinning fraction	0.098 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 277934 reflections (0.000%)	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, FE2, ACY, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	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

The worst 5 of 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

The worst 5 of 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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

There are no chirality outliers.

5 of 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

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 349 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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	Distance(Å)	Clash(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%)	50	37
1	C	703/696 (101%)	675 (96%)	26 (4%)	2 (0%)	50	37
1	D	699/696 (100%)	676 (97%)	23 (3%)	0	100	100
All	All	2810/2784 (101%)	2711 (96%)	95 (3%)	4 (0%)	59	48

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%)	589 (97%)	16 (3%)	59	49
1	B	590/602 (98%)	565 (96%)	25 (4%)	40	27
1	C	593/602 (98%)	578 (98%)	15 (2%)	60	50
1	D	585/602 (97%)	569 (97%)	16 (3%)	57	47
All	All	2373/2408 (98%)	2301 (97%)	72 (3%)	56	42

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	823	VAL
1	B	1057	PRO
1	D	815	LEU
1	B	854	LYS
1	B	926[A]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	947	ASN
1	C	614	ASN
1	D	905	ASN
1	B	950	GLN
1	C	377	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	2200[A]	-	3,3,3	0.55	0	3,3,3	1.25	0
4	ACY	A	2200[B]	-	3,3,3	0.78	0	3,3,3	0.84	0
4	ACY	A	2201	-	3,3,3	0.61	0	3,3,3	1.11	0
4	ACY	A	2202	-	3,3,3	0.87	0	3,3,3	2.63	2 (66%)
4	ACY	A	2203	-	3,3,3	0.40	0	3,3,3	1.18	0
4	ACY	A	2204	-	3,3,3	0.47	0	3,3,3	1.45	0
4	ACY	A	2218	-	3,3,3	0.78	0	3,3,3	0.45	0
4	ACY	A	2220	-	3,3,3	0.86	0	3,3,3	0.88	0
4	ACY	A	2222	-	3,3,3	0.53	0	3,3,3	1.04	0
5	GOL	A	2301	-	5,5,5	0.65	0	5,5,5	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	2302	-	5,5,5	0.48	0	5,5,5	0.56	0
5	GOL	A	2303	-	5,5,5	0.68	0	5,5,5	0.81	0
5	GOL	A	2304	-	5,5,5	0.97	0	5,5,5	1.40	2 (40%)
5	GOL	A	2305	-	5,5,5	0.34	0	5,5,5	1.88	1 (20%)
5	GOL	A	2306	-	5,5,5	0.27	0	5,5,5	1.96	2 (40%)
5	GOL	A	2307	-	5,5,5	0.80	0	5,5,5	1.10	0
5	GOL	A	2308	-	5,5,5	0.40	0	5,5,5	0.36	0
5	GOL	A	2320[A]	-	5,5,5	0.42	0	5,5,5	0.96	0
5	GOL	A	2320[B]	-	5,5,5	0.48	0	5,5,5	1.15	0
4	ACY	B	2205	-	3,3,3	0.63	0	3,3,3	1.01	0
4	ACY	B	2206	-	3,3,3	0.55	0	3,3,3	1.52	1 (33%)
4	ACY	B	2207	-	3,3,3	0.61	0	3,3,3	0.87	0
4	ACY	B	2208	-	3,3,3	0.73	0	3,3,3	0.37	0
5	GOL	B	2309	-	5,5,5	0.47	0	5,5,5	0.28	0
5	GOL	B	2310	-	5,5,5	0.70	0	5,5,5	2.82	2 (40%)
5	GOL	B	2311	-	5,5,5	0.45	0	5,5,5	1.40	1 (20%)
5	GOL	B	2312	-	5,5,5	0.45	0	5,5,5	0.92	0
4	ACY	C	2209[A]	-	3,3,3	0.50	0	3,3,3	2.03	2 (66%)
4	ACY	C	2209[B]	-	3,3,3	0.94	0	3,3,3	0.49	0
4	ACY	C	2210	-	3,3,3	0.78	0	3,3,3	0.29	0
4	ACY	C	2211	-	3,3,3	0.56	0	3,3,3	1.29	0
4	ACY	C	2212	-	3,3,3	0.44	0	3,3,3	1.34	0
4	ACY	C	2213	-	3,3,3	0.55	0	3,3,3	1.68	1 (33%)
4	ACY	C	2221	-	3,3,3	0.62	0	3,3,3	0.78	0
5	GOL	C	2313	-	5,5,5	0.78	0	5,5,5	1.30	0
5	GOL	C	2314	-	5,5,5	0.34	0	5,5,5	0.54	0
5	GOL	C	2315	-	5,5,5	0.70	0	5,5,5	0.60	0
5	GOL	C	2317	-	5,5,5	0.39	0	5,5,5	1.22	1 (20%)
5	GOL	C	2321	-	5,5,5	0.84	0	5,5,5	1.42	1 (20%)
5	GOL	C	2322	-	5,5,5	0.95	0	5,5,5	2.77	2 (40%)
4	ACY	D	2214	-	3,3,3	0.85	0	3,3,3	0.43	0
4	ACY	D	2215	-	3,3,3	0.47	0	3,3,3	2.09	1 (33%)
4	ACY	D	2216	-	3,3,3	0.69	0	3,3,3	0.86	0
4	ACY	D	2217	-	3,3,3	0.75	0	3,3,3	0.67	0
4	ACY	D	2219	-	3,3,3	0.73	0	3,3,3	0.19	0
5	GOL	D	2318	-	5,5,5	0.42	0	5,5,5	0.58	0
5	GOL	D	2319	-	5,5,5	1.03	0	5,5,5	1.14	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
4	ACY	A	2200[A]	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2200[B]	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2201	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2202	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2203	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2204	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2218	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2220	-	-	0/0/0/0	0/0/0/0
4	ACY	A	2222	-	-	0/0/0/0	0/0/0/0
5	GOL	A	2301	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2302	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2303	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2304	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2305	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2306	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2307	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2308	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2320[A]	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2320[B]	-	-	0/4/4/4	0/0/0/0
4	ACY	B	2205	-	-	0/0/0/0	0/0/0/0
4	ACY	B	2206	-	-	0/0/0/0	0/0/0/0
4	ACY	B	2207	-	-	0/0/0/0	0/0/0/0
4	ACY	B	2208	-	-	0/0/0/0	0/0/0/0
5	GOL	B	2309	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2310	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2311	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2312	-	-	0/4/4/4	0/0/0/0
4	ACY	C	2209[A]	-	-	0/0/0/0	0/0/0/0
4	ACY	C	2209[B]	-	-	0/0/0/0	0/0/0/0
4	ACY	C	2210	-	-	0/0/0/0	0/0/0/0
4	ACY	C	2211	-	-	0/0/0/0	0/0/0/0
4	ACY	C	2212	-	-	0/0/0/0	0/0/0/0
4	ACY	C	2213	-	-	0/0/0/0	0/0/0/0
4	ACY	C	2221	-	-	0/0/0/0	0/0/0/0
5	GOL	C	2313	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2314	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2315	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2317	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2321	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2322	-	-	0/4/4/4	0/0/0/0
4	ACY	D	2214	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACY	D	2215	-	-	0/0/0/0	0/0/0/0
4	ACY	D	2216	-	-	0/0/0/0	0/0/0/0
4	ACY	D	2217	-	-	0/0/0/0	0/0/0/0
4	ACY	D	2219	-	-	0/0/0/0	0/0/0/0
5	GOL	D	2318	-	-	0/4/4/4	0/0/0/0
5	GOL	D	2319	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2322	GOL	C3-C2-C1	-4.88	89.71	111.26
5	B	2310	GOL	O3-C3-C2	-4.26	88.94	109.71
5	B	2310	GOL	O2-C2-C1	4.02	126.53	108.22
5	A	2305	GOL	O1-C1-C2	-3.66	91.85	109.71
4	A	2202	ACY	O-C-CH3	-3.46	106.98	122.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	687/696 (98%)	-0.39	9 (1%) 74 75	14, 22, 36, 71	5 (0%)
1	B	682/696 (97%)	-0.01	32 (4%) 30 30	18, 29, 52, 67	7 (1%)
1	C	686/696 (98%)	-0.39	8 (1%) 75 78	15, 23, 37, 58	13 (1%)
1	D	681/696 (97%)	-0.12	13 (1%) 64 65	17, 27, 44, 52	6 (0%)
All	All	2736/2784 (98%)	-0.23	62 (2%) 59 59	14, 25, 45, 71	31 (1%)

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	680	VAL	8.8
1	A	681	PRO	5.9
1	C	680	VAL	4.8
1	D	448	TYR	4.2
1	C	449	TRP	4.2

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	A	2308	6/6	0.16	6.64	47,51,52,53	0
4	ACY	A	2218	4/4	0.15	5.13	40,41,41,42	0
5	GOL	A	2307	6/6	0.20	4.90	39,49,49,51	0
4	ACY	C	2221	4/4	0.13	4.86	41,43,44,44	0
4	ACY	D	2219	4/4	0.18	4.53	43,44,46,48	0
4	ACY	A	2222	4/4	0.12	4.41	50,53,53,53	0
4	ACY	C	2211	4/4	0.12	4.15	45,47,48,48	0
4	ACY	C	2209[A]	4/4	0.19	3.55	16,16,16,18	4
4	ACY	C	2209[B]	4/4	0.19	3.23	18,20,20,21	4
4	ACY	B	2206	4/4	0.14	3.21	45,49,49,50	0
4	ACY	B	2207	4/4	0.12	2.99	40,43,43,43	0
4	ACY	D	2214	4/4	0.25	2.88	34,36,37,39	0
4	ACY	A	2200[B]	4/4	0.16	2.80	18,18,19,21	4
4	ACY	B	2205	4/4	0.29	2.77	39,39,40,41	0
4	ACY	A	2200[A]	4/4	0.16	2.63	17,17,17,20	4
4	ACY	C	2213	4/4	0.18	2.53	39,40,42,43	0
4	ACY	A	2203	4/4	0.12	2.53	44,44,45,45	0
4	ACY	A	2204	4/4	0.10	2.51	49,50,50,50	0
4	ACY	D	2216	4/4	0.11	2.39	44,46,46,46	0
5	GOL	A	2320[B]	6/6	0.16	2.31	25,30,31,34	6
5	GOL	A	2320[A]	6/6	0.16	2.08	15,23,27,30	6
5	GOL	C	2317	6/6	0.15	2.06	31,37,38,41	0
4	ACY	C	2212	4/4	0.12	1.88	38,39,40,40	0
5	GOL	C	2314	6/6	0.11	1.87	27,29,30,32	0
4	ACY	A	2220	4/4	0.15	1.76	37,40,41,43	0
4	ACY	C	2210	4/4	0.14	1.73	45,46,46,46	0
4	ACY	A	2202	4/4	0.17	1.64	36,38,41,41	0
4	ACY	D	2217	4/4	0.15	1.55	50,51,51,52	0
5	GOL	A	2304	6/6	0.14	1.31	24,33,38,43	0
5	GOL	C	2313	6/6	0.10	1.29	26,30,37,39	0
6	CL	A	2402	1/1	0.07	1.21	44,44,44,44	0
4	ACY	A	2201	4/4	0.12	1.21	47,47,48,50	0
5	GOL	C	2321	6/6	0.14	1.19	24,40,43,50	0
5	GOL	B	2310	6/6	0.19	1.13	30,38,42,44	0
4	ACY	D	2215	4/4	0.22	1.09	40,42,44,44	0
5	GOL	C	2322	6/6	0.14	1.09	12,36,37,38	0
4	ACY	B	2208	4/4	0.14	1.02	53,53,54,54	0
5	GOL	A	2306	6/6	0.12	0.95	24,36,39,49	0
5	GOL	A	2303	6/6	0.15	0.93	28,41,41,46	0
5	GOL	D	2318	6/6	0.12	0.68	29,30,31,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	GOL	B	2309	6/6	0.10	0.48	29,31,35,35	0
5	GOL	B	2312	6/6	0.11	0.12	39,45,47,47	0
5	GOL	D	2319	6/6	0.12	0.09	30,38,41,41	0
5	GOL	A	2305	6/6	0.12	-0.01	20,36,40,41	0
5	GOL	A	2301	6/6	0.08	-0.07	26,34,36,39	0
6	CL	B	2401	1/1	0.08	-0.13	28,28,28,28	0
3	CA	A	1067	1/1	0.07	-0.21	22,22,22,22	0
5	GOL	C	2315	6/6	0.08	-0.24	24,34,37,43	0
5	GOL	A	2302	6/6	0.07	-0.30	25,30,35,35	0
5	GOL	B	2311	6/6	0.14	-0.34	28,46,50,53	0
3	CA	C	1067	1/1	0.06	-0.39	23,23,23,23	0
3	CA	A	1501	1/1	0.05	-0.62	23,23,23,23	0
3	CA	A	1502	1/1	0.06	-0.73	21,21,21,21	0
6	CL	D	2401	1/1	0.06	-0.87	28,28,28,28	0
3	CA	C	1502	1/1	0.05	-0.92	21,21,21,21	0
6	CL	A	2401	1/1	0.05	-1.18	26,26,26,26	0
2	FE2	D	1500	1/1	0.08	-1.84	20,20,20,20	0
2	FE2	C	1500	1/1	0.06	-1.99	18,18,18,18	0
2	FE2	A	1500	1/1	0.07	-1.99	17,17,17,17	0
3	CA	D	1501	1/1	0.03	-2.11	23,23,23,23	0
3	CA	B	1501	1/1	0.04	-2.55	23,23,23,23	0
2	FE2	B	1500	1/1	0.07	-2.67	22,22,22,22	0
3	CA	C	1501	1/1	0.03	-2.83	24,24,24,24	0
6	CL	C	2402	1/1	0.03	-3.30	38,38,38,38	0
6	CL	C	2401	1/1	0.03	-3.41	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.