Full wwPDB X-ray Structure Validation Report (i)

Apr 16, 2024 – 10:04 AM EDT

PDB ID	:	4LTE
Title	:	Structure of Cysteine-free Human Insulin Degrading Enzyme in Complex with Macrocyclic Inhibitor
Authors	:	Foda, Z.H.; Seeliger, M.A.; Saghatelian, A.; Liu, D.R.
Deposited on	:	2013-07-23
Resolution	:	2.71 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 (i) 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 (i)) were used in the production of this report:

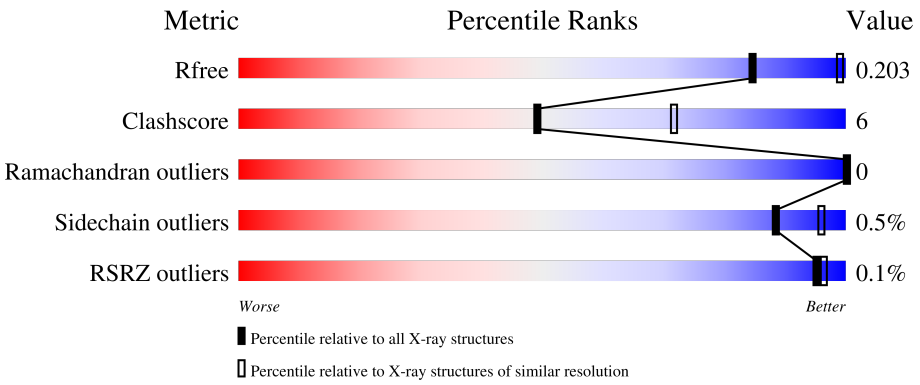
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	978	85% 12% •
1	B	978	85% 12% •
2	M	3	33% 67% 33%
2	N	3	33% 33% 33% 33%

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
5	LYN	M	101	-	-	X	X
5	LYN	N	101	-	-	X	-
6	FUM	M	102	-	X	-	-
6	FUM	N	102	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16250 atoms, of which 34 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	954	7771	5005	1304	1440	22	0	0	0
1	B	954	7760	5002	1302	1434	22	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	LEU	CYS	engineered mutation	UNP P14735
A	111	GLN	GLU	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	111	GLN	GLU	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735

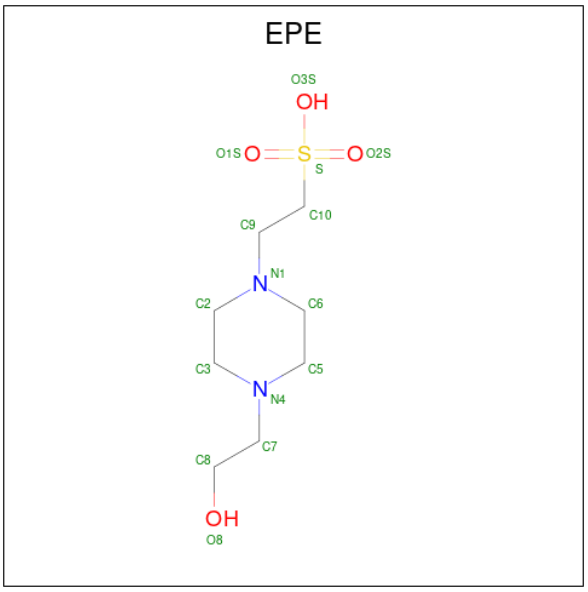
- Molecule 2 is a protein called Macrocyclic Inhibitor.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	M	2	29	25	1	3	0	0	0
			Total	C	N	O			
2	N	2	29	25	1	3	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
			Total	Zn		
3	B	1	1	1	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
4	A	1	32	8	17	2	4	1	0	0

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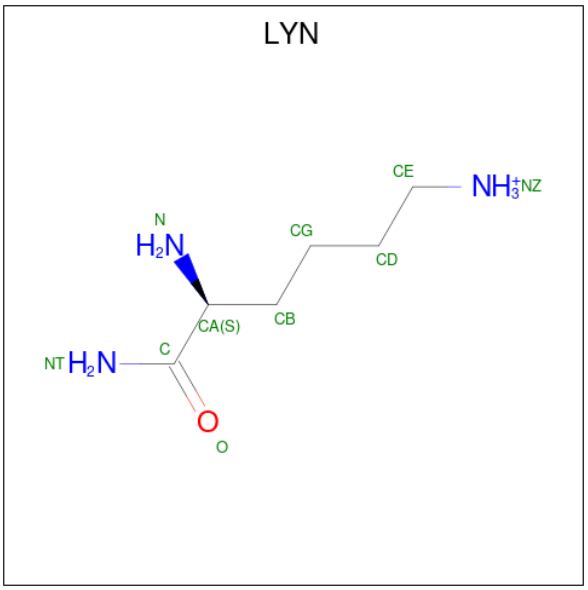
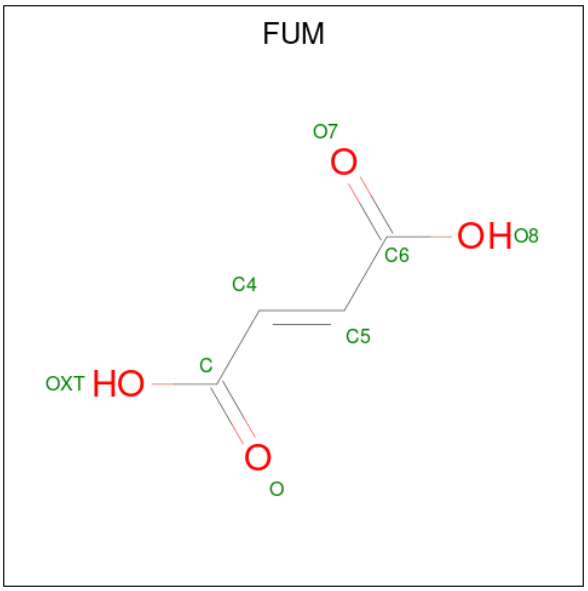
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
4	B	1	32	8	17	2	4	1	0	0

- Molecule 5 is 2,6-DIAMINO-HEXANOIC ACID AMIDE (three-letter code: LYN) (formula: $C_6H_{16}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	M	1	10	6	3	1	0	0
5	N	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 6 is FUMARIC ACID (three-letter code: FUM) (formula: $C_4H_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	M	1	Total C O 6 4 2	0	0
6	N	1	Total C O 6 4 2	0	0

- Molecule 7 is water.

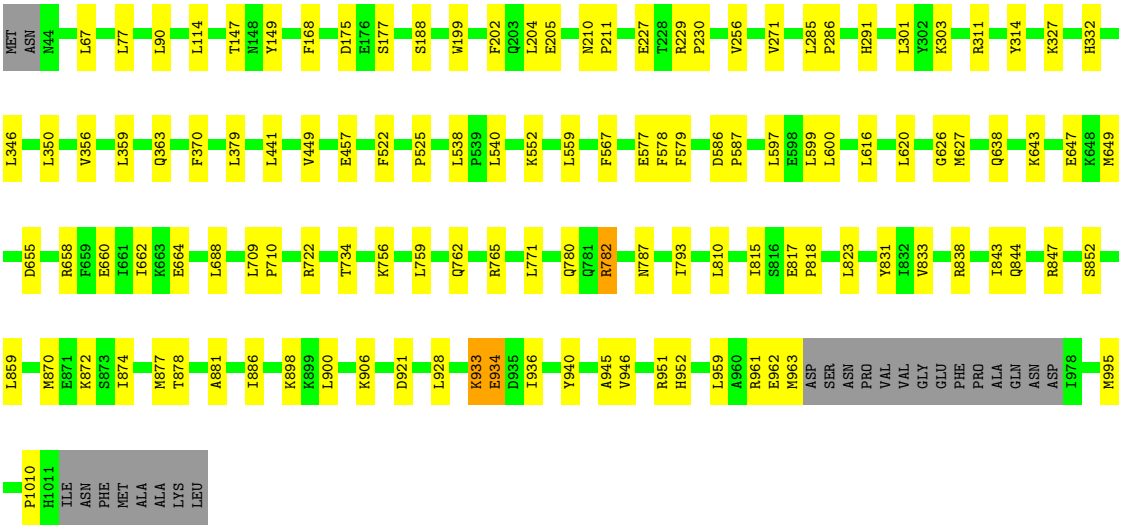
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	294	Total O 294 294	0	0
7	B	268	Total O 268 268	0	0
7	M	1	Total O 1 1	0	0

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.

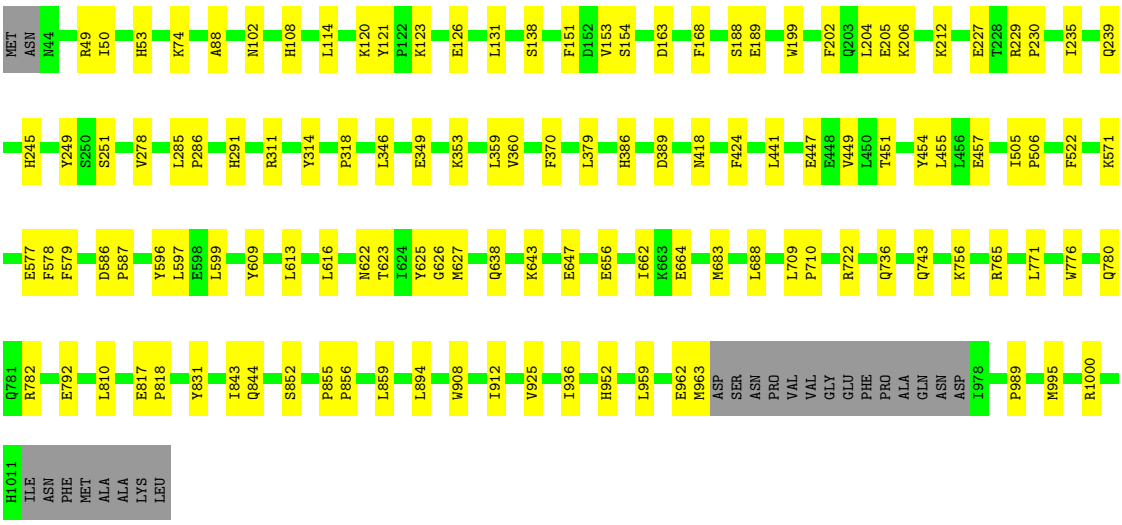
- Molecule 1: Insulin-degrading enzyme

Chain A:



- Molecule 1: Insulin-degrading enzyme

Chain B:

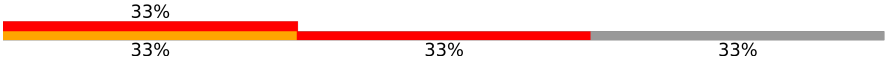


• Molecule 2: Macrocyclic Inhibitor

Chain M:

• Molecule 2: Macrocyclic Inhibitor

Chain N:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	261.97Å 261.97Å 90.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	130.99 – 2.71 226.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (130.99-2.71) 95.3 (226.88-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.158 , 0.200 0.164 , 0.203	Depositor DCC
R_{free} test set	2217 reflections (2.28%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16250	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, DFF, FUM, LYN, EPE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.51	0/7966	0.63	1/10784 (0.0%)
1	B	0.53	0/7955	0.63	1/10770 (0.0%)
2	M	6.45	6/10 (60.0%)	8.01	6/11 (54.5%)
2	N	6.40	6/10 (60.0%)	8.90	6/11 (54.5%)
All	All	0.57	12/15941 (0.1%)	0.69	14/21576 (0.1%)

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
2	M	0	1
2	N	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	1	PHE	CG-CD2	9.78	1.53	1.38
2	N	1	PHE	CG-CD2	9.30	1.52	1.38
2	M	1	PHE	CD2-CE2	9.12	1.57	1.39
2	N	1	PHE	CG-CD1	9.02	1.52	1.38
2	N	1	PHE	CD2-CE2	8.64	1.56	1.39
2	M	1	PHE	CE1-CZ	7.90	1.52	1.37
2	N	1	PHE	CD1-CE1	7.86	1.54	1.39
2	M	1	PHE	CG-CD1	7.86	1.50	1.38
2	M	1	PHE	CD1-CE1	7.77	1.54	1.39
2	N	1	PHE	CE1-CZ	7.74	1.52	1.37
2	M	1	PHE	CE2-CZ	6.82	1.50	1.37
2	N	1	PHE	CE2-CZ	6.30	1.49	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	1	PHE	CB-CG-CD2	-16.78	109.06	120.80
2	N	1	PHE	CB-CG-CD1	-16.62	109.16	120.80
2	M	1	PHE	CB-CG-CD2	-16.23	109.44	120.80
2	M	1	PHE	CB-CG-CD1	-14.24	110.83	120.80
2	N	1	PHE	CG-CD2-CE2	-10.80	108.92	120.80
2	M	1	PHE	CD1-CG-CD2	-8.79	106.87	118.30
2	N	1	PHE	CE1-CZ-CE2	-8.05	105.52	120.00
2	M	1	PHE	CG-CD1-CE1	-7.64	112.39	120.80
2	N	1	PHE	CD1-CG-CD2	-7.60	108.42	118.30
1	B	625	TYR	N-CA-C	6.37	128.21	111.00
2	M	1	PHE	CE1-CZ-CE2	-6.12	108.98	120.00
1	A	67	LEU	CA-CB-CG	5.78	128.60	115.30
2	N	1	PHE	CD1-CE1-CZ	-5.52	113.48	120.10
2	M	1	PHE	CG-CD2-CE2	-5.14	115.14	120.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	M	1	PHE	Sidechain
2	N	1	PHE	Sidechain

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	7771	0	7665	85	3
1	B	7760	0	7663	87	3
2	M	29	0	20	5	0
2	N	29	0	20	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	17	17	1	0
4	B	15	17	17	0	0
5	M	10	0	13	12	0
5	N	10	0	13	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	M	6	0	1	2	0
6	N	6	0	1	2	0
7	A	294	0	0	5	0
7	B	268	0	0	3	0
7	M	1	0	0	0	0
All	All	16216	34	15430	182	3

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 6.

All (182) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:946:VAL:HA	1:A:951:ARG:NH1	1.70	1.06
1:A:780:GLN:HE21	1:A:959:LEU:HD11	1.32	0.95
5:M:101:LYN:HB2	6:M:102:FUM:C4	2.03	0.88
1:B:49:ARG:NH2	1:B:447:GLU:OE2	2.07	0.87
1:A:780:GLN:NE2	1:A:959:LEU:HD11	1.95	0.82
1:B:596:TYR:HE2	1:B:627:MET:HE1	1.49	0.78
1:A:204:LEU:HD23	2:M:2:DFF:H5	1.64	0.78
1:B:597:LEU:HD21	1:B:627:MET:HE2	1.67	0.77
5:N:101:LYN:HE3	6:N:102:FUM:C4	2.14	0.77
1:B:959:LEU:HD22	1:B:963:MET:CE	2.16	0.76
5:M:101:LYN:HE3	6:M:102:FUM:C4	2.16	0.75
1:A:199:TRP:CZ2	5:M:101:LYN:HA	2.23	0.73
1:B:202:PHE:HB2	5:N:101:LYN:HG2	1.68	0.73
1:B:623:THR:OG1	1:B:626:GLY:HA2	1.87	0.73
1:A:597:LEU:HD11	1:A:627:MET:HG2	1.71	0.72
1:A:946:VAL:HA	1:A:951:ARG:HH11	1.52	0.72
1:A:199:TRP:CE2	5:M:101:LYN:HA	2.28	0.69
1:B:199:TRP:CE2	5:N:101:LYN:HA	2.29	0.68
1:B:579:PHE:CE2	1:B:765:ARG:NH1	2.62	0.68
1:A:961:ARG:NH1	1:A:962:GLU:OE1	2.27	0.67
1:B:239:GLN:NE2	7:B:1201:HOH:O	2.26	0.67
1:B:597:LEU:HD21	1:B:627:MET:CE	2.24	0.67
1:B:360:VAL:CG1	2:N:1:PHE:HE2	2.07	0.67
5:N:101:LYN:HB2	6:N:102:FUM:C4	2.25	0.66
1:A:202:PHE:HB2	5:M:101:LYN:HD2	1.77	0.66
1:B:204:LEU:HD23	2:N:2:DFF:H5	1.76	0.66
1:A:311:ARG:NH2	1:A:664:GLU:OE2	2.29	0.65
1:B:311:ARG:NH2	1:B:664:GLU:OE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:GLU:HG2	1:B:579:PHE:CZ	2.31	0.65
1:A:782:ARG:HH12	1:A:963:MET:C	2.01	0.64
1:A:441:LEU:HD23	1:A:449:VAL:HG11	1.79	0.63
1:A:332:HIS:CE1	1:A:363:GLN:HE21	2.15	0.63
1:B:360:VAL:CG1	2:N:1:PHE:CE2	2.82	0.62
1:B:123:LYS:HB3	1:B:126:GLU:HB2	1.81	0.62
1:A:311:ARG:HB3	1:A:379:LEU:HB2	1.82	0.61
5:N:101:LYN:CD	5:N:101:LYN:C	2.80	0.59
1:B:74:LYS:HD2	7:B:1283:HOH:O	2.02	0.59
1:B:199:TRP:CZ2	5:N:101:LYN:HA	2.37	0.59
1:B:810:LEU:HD23	1:B:936:ILE:HD11	1.84	0.58
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.86	0.58
1:B:441:LEU:HD23	1:B:449:VAL:HG11	1.85	0.58
1:A:229:ARG:HD2	7:A:1360:HOH:O	2.04	0.58
1:B:360:VAL:HG11	2:N:1:PHE:CE2	2.39	0.58
1:B:360:VAL:HG12	2:N:1:PHE:HE2	1.69	0.57
1:B:616:LEU:HD11	1:B:638:GLN:HG3	1.85	0.57
1:A:229:ARG:HB3	1:A:230:PRO:HD3	1.87	0.57
1:A:577:GLU:HG2	1:A:579:PHE:CZ	2.39	0.57
1:B:188:SER:HB2	1:B:831:TYR:HB2	1.85	0.57
1:A:205:GLU:HB2	2:M:2:DFF:H3	1.86	0.57
1:B:386:HIS:HD2	1:B:389:ASP:OD2	1.88	0.57
1:B:599:LEU:HD23	1:B:662:ILE:HD12	1.87	0.57
1:A:810:LEU:HD23	1:A:936:ILE:HD11	1.87	0.56
1:B:212:LYS:HE3	7:B:1276:HOH:O	2.05	0.56
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.86	0.56
1:A:872:LYS:NZ	7:A:1204:HOH:O	2.38	0.56
1:B:959:LEU:HD22	1:B:963:MET:HE2	1.88	0.55
1:B:311:ARG:HH22	1:B:664:GLU:CD	2.10	0.55
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.88	0.54
1:B:578:PHE:HB2	1:B:627:MET:HB2	1.89	0.54
1:A:660:GLU:HG3	7:A:1220:HOH:O	2.07	0.54
5:N:101:LYN:HG3	5:N:101:LYN:NT	2.23	0.54
1:B:643:LYS:HE2	1:B:647:GLU:OE1	2.08	0.54
1:A:874:ILE:O	1:A:933:LYS:HE3	2.08	0.54
1:A:204:LEU:CD2	2:M:2:DFF:H5	2.37	0.53
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.11	0.53
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.90	0.53
1:A:600:LEU:HD23	1:A:620:LEU:HD21	1.91	0.53
1:B:202:PHE:HB2	5:N:101:LYN:CG	2.38	0.53
1:B:596:TYR:CE2	1:B:627:MET:HE1	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.91	0.53
1:A:815:ILE:HG22	1:A:870:MET:HG3	1.92	0.52
1:B:120:LYS:HD3	1:B:121:TYR:CE2	2.45	0.52
5:M:101:LYN:CD	5:M:101:LYN:C	2.87	0.52
1:A:285:LEU:HD12	1:A:286:PRO:HD2	1.92	0.51
1:A:838:ARG:HB2	1:A:847:ARG:HD3	1.93	0.51
5:N:101:LYN:C	5:N:101:LYN:HD3	2.41	0.51
1:B:609:TYR:CE2	1:B:613:LEU:HD11	2.46	0.51
1:A:722:ARG:HA	1:A:756:LYS:O	2.11	0.51
1:B:88:ALA:HB3	1:B:151:PHE:CE2	2.46	0.50
1:B:229:ARG:HB3	1:B:230:PRO:HD3	1.94	0.50
1:B:451:THR:HB	1:B:455:LEU:HD12	1.94	0.50
1:A:525:PRO:HD3	7:A:1287:HOH:O	2.11	0.50
1:A:586:ASP:HB2	1:A:587:PRO:HD2	1.93	0.50
1:B:418:ASN:ND2	1:B:454:TYR:O	2.45	0.50
1:A:114:LEU:HD13	1:A:168:PHE:HB3	1.93	0.50
1:A:940:TYR:CE2	1:A:945:ALA:HB2	2.47	0.50
1:B:688:LEU:HD13	1:B:995:MET:HE1	1.92	0.50
1:B:780:GLN:HE21	1:B:959:LEU:HD11	1.76	0.49
1:A:359:LEU:C	1:A:359:LEU:HD23	2.33	0.49
1:A:314:TYR:CD2	2:M:2:DFF:H14	2.48	0.49
1:B:908:TRP:O	1:B:912:ILE:HG12	2.11	0.49
1:B:245:HIS:O	1:B:249:TYR:HB2	2.12	0.49
1:A:843:ILE:HG22	1:A:844:GLN:N	2.27	0.49
1:A:441:LEU:CD2	1:A:449:VAL:HG11	2.42	0.49
1:B:311:ARG:HB3	1:B:379:LEU:HB2	1.94	0.49
1:B:596:TYR:CE2	1:B:627:MET:CE	2.96	0.49
1:A:599:LEU:HD23	1:A:662:ILE:HD12	1.94	0.49
1:B:586:ASP:HB2	1:B:587:PRO:HD2	1.94	0.49
1:A:578:PHE:O	1:A:626:GLY:HA3	2.12	0.48
1:A:852:SER:HB3	1:A:859:LEU:HD11	1.96	0.48
1:A:787:ASN:HB2	1:A:961:ARG:NH2	2.28	0.48
4:A:1102:EPE:H71	7:A:1434:HOH:O	2.12	0.48
1:B:131:LEU:CD1	1:B:138:SER:HB2	2.44	0.48
1:B:776:TRP:CE3	1:B:989:PRO:HB3	2.49	0.48
1:A:202:PHE:HB2	5:M:101:LYN:CD	2.42	0.47
1:A:291:HIS:CD2	1:A:370:PHE:HB2	2.49	0.47
1:A:688:LEU:HD13	1:A:995:MET:HE1	1.96	0.47
1:A:759:LEU:CD1	1:B:587:PRO:HG2	2.44	0.47
1:B:49:ARG:HG2	1:B:50:ILE:N	2.29	0.47
1:B:843:ILE:HG22	1:B:844:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:LYS:NZ	1:A:921:ASP:OD2	2.34	0.47
1:A:188:SER:HB2	1:A:831:TYR:HB2	1.97	0.47
1:B:441:LEU:CD2	1:B:449:VAL:HG11	2.45	0.47
1:B:656:GLU:HG3	1:B:709:LEU:HD22	1.97	0.47
1:B:780:GLN:NE2	1:B:959:LEU:HD11	2.30	0.47
1:A:709:LEU:HB3	1:A:710:PRO:HD3	1.96	0.47
1:B:346:LEU:HA	1:B:522:PHE:CE1	2.50	0.47
1:A:759:LEU:HB2	1:A:762:GLN:HG3	1.97	0.47
5:M:101:LYN:C	5:M:101:LYN:HD3	2.44	0.47
1:A:567:PHE:CE2	1:A:900:LEU:HA	2.50	0.46
1:B:579:PHE:CZ	1:B:765:ARG:NH1	2.83	0.46
1:B:205:GLU:HB2	2:N:2:DFF:H3	1.97	0.46
1:B:894:LEU:HG	1:B:925:VAL:HG21	1.97	0.46
1:A:90:LEU:HD12	1:A:256:VAL:HG22	1.97	0.46
1:A:199:TRP:HA	5:M:101:LYN:HG2	1.97	0.46
1:B:709:LEU:HB3	1:B:710:PRO:HD3	1.98	0.46
1:A:346:LEU:HA	1:A:522:PHE:CE1	2.51	0.46
1:A:314:TYR:CG	2:M:2:DFF:H14	2.51	0.45
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.98	0.45
1:A:771:LEU:HB2	1:A:952:HIS:HB3	1.98	0.45
1:A:578:PHE:HB2	1:A:627:MET:HB2	1.98	0.45
1:B:683:MET:HA	1:B:792:GLU:OE1	2.16	0.45
1:A:600:LEU:HD23	1:A:620:LEU:CD2	2.45	0.45
1:B:349:GLU:HA	1:B:349:GLU:OE1	2.17	0.45
1:B:121:TYR:OH	1:B:163:ASP:OD2	2.23	0.45
1:A:793:ILE:O	1:A:847:ARG:HA	2.17	0.44
1:B:202:PHE:CB	5:N:101:LYN:HG2	2.42	0.44
1:B:202:PHE:CZ	1:B:206:LYS:HE3	2.53	0.44
5:M:101:LYN:HB2	5:M:101:LYN:HE3	1.45	0.44
1:A:147:THR:HG22	1:A:149:TYR:CE1	2.53	0.43
1:A:877:MET:HG3	1:A:881:ALA:HB3	1.99	0.43
1:A:175:ASP:OD2	1:A:177:SER:HB3	2.18	0.43
1:B:108:HIS:CE1	1:B:189:GLU:OE1	2.71	0.43
1:A:759:LEU:HD12	1:B:587:PRO:HG2	2.00	0.43
1:A:579:PHE:CE2	1:A:765:ARG:NH2	2.86	0.43
1:A:1010:PRO:HD3	1:B:1000:ARG:HH21	1.83	0.43
1:A:643:LYS:HE2	1:A:647:GLU:OE1	2.18	0.43
1:B:314:TYR:CG	2:N:2:DFF:H14	2.54	0.43
1:B:597:LEU:HD12	1:B:622:ASN:N	2.34	0.43
1:B:227:GLU:C	1:B:230:PRO:HD2	2.39	0.43
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:LEU:HB2	1:B:952:HIS:HB3	2.01	0.42
1:A:540:LEU:HD12	1:A:540:LEU:HA	1.58	0.42
1:A:620:LEU:HD11	1:A:649:MET:CE	2.49	0.42
1:B:424:PHE:O	1:B:571:LYS:NZ	2.51	0.42
5:N:101:LYN:HE3	5:N:101:LYN:HB2	1.45	0.42
1:B:359:LEU:C	1:B:359:LEU:HD23	2.40	0.42
1:A:655:ASP:OD2	1:A:658:ARG:HG2	2.19	0.42
1:A:579:PHE:CZ	1:A:765:ARG:NH2	2.88	0.42
1:A:823:LEU:HB2	1:A:833:VAL:HG11	2.02	0.42
1:A:843:ILE:HG22	1:A:844:GLN:H	1.85	0.42
1:B:505:ILE:HA	1:B:506:PRO:HD3	1.87	0.42
1:B:855:PRO:HA	1:B:856:PRO:HD3	1.93	0.41
1:A:227:GLU:C	1:A:230:PRO:HD2	2.40	0.41
1:A:77:LEU:HD21	1:A:271:VAL:HG21	2.03	0.41
1:A:597:LEU:HD23	1:A:597:LEU:HA	1.80	0.41
5:M:101:LYN:HE2	5:M:101:LYN:H	1.85	0.41
1:B:102:ASN:ND2	1:B:235:ILE:HD11	2.35	0.41
1:B:959:LEU:CD2	1:B:963:MET:CE	2.95	0.41
1:A:202:PHE:HB2	5:M:101:LYN:CG	2.51	0.41
1:A:210:ASN:HA	1:A:211:PRO:HD3	1.84	0.41
1:A:350:LEU:HB3	1:A:356:VAL:HG22	2.03	0.41
1:A:552:LYS:HB3	1:A:559:LEU:HB3	2.02	0.41
1:B:586:ASP:HB2	1:B:587:PRO:CD	2.51	0.41
1:A:327:LYS:HB3	1:A:457:GLU:HB2	2.03	0.40
1:A:886:ILE:HG23	1:A:928:LEU:HG	2.02	0.40
1:B:251:SER:HB3	1:B:278:VAL:HG12	2.02	0.40
1:B:722:ARG:HA	1:B:756:LYS:O	2.21	0.40
1:A:301:LEU:HD21	1:A:303:LYS:HE3	2.04	0.40
1:B:153:VAL:HG22	1:B:154:SER:N	2.36	0.40
1:B:291:HIS:CE1	1:B:318:PRO:HB3	2.56	0.40
1:B:852:SER:HB3	1:B:859:LEU:HD11	2.03	0.40

All (3) 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:A:934:GLU:OE2	1:B:53:HIS:CD2[6_554]	1.52	0.68
1:A:934:GLU:OE2	1:B:53:HIS:NE2[6_554]	1.66	0.54
1:A:878:THR:OG1	1:B:457:GLU:OE2[6_554]	2.09	0.11

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	950/978 (97%)	928 (98%)	22 (2%)	0	100	100
1	B	950/978 (97%)	928 (98%)	22 (2%)	0	100	100
All	All	1900/1956 (97%)	1856 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	840/870 (97%)	836 (100%)	4 (0%)	88	96
1	B	838/870 (96%)	833 (99%)	5 (1%)	86	95
All	All	1678/1740 (96%)	1669 (100%)	9 (0%)	88	96

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	782	ARG
1	A	898	LYS
1	A	933	LYS
1	A	934	GLU
1	B	353	LYS
1	B	736	GLN
1	B	743	GLN
1	B	782	ARG

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Mol	Chain	Res	Type
1	B	962	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	363	GLN
1	A	724	HIS
1	A	780	GLN
1	B	386	HIS
1	B	780	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)

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	LYN	N	101	2,6	9,9,9	1.99	1 (11%)	9,10,10	2.21	2 (22%)
2	DFF	N	2	5,2	19,20,21	0.87	1 (5%)	23,26,28	1.79	4 (17%)
5	LYN	M	101	2,6	9,9,9	1.83	1 (11%)	9,10,10	1.64	1 (11%)
2	DFF	M	2	5,2	19,20,21	1.05	2 (10%)	23,26,28	1.64	2 (8%)

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	LYN	N	101	2,6	-	4/9/9/9	-
2	DFF	N	2	5,2	-	6/13/14/16	0/2/2/2
5	LYN	M	101	2,6	-	5/9/9/9	-
2	DFF	M	2	5,2	-	6/13/14/16	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	101	LYN	C-NT	5.74	1.47	1.32
5	M	101	LYN	C-NT	5.28	1.46	1.32
2	M	2	DFF	CZ-C7	2.46	1.53	1.49
2	M	2	DFF	C4-C7	2.21	1.53	1.49
2	N	2	DFF	CZ-C7	2.12	1.53	1.49

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	2	DFF	CG-CB-CA	-4.75	104.48	114.10
5	N	101	LYN	CA-C-NT	4.66	124.67	116.68
2	M	2	DFF	CG-CB-CA	-4.49	105.01	114.10
2	M	2	DFF	CB-CA-C	-4.29	103.43	111.47
2	N	2	DFF	CB-CA-C	-4.05	103.88	111.47
5	N	101	LYN	O-C-NT	-3.57	116.78	123.00
5	M	101	LYN	O-C-NT	-3.16	117.51	123.00
2	N	2	DFF	CB-CG-CD2	-2.13	116.68	120.91
2	N	2	DFF	C2-C3-C4	-2.05	117.92	120.34

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	M	101	LYN	NT-C-CA-N
2	M	2	DFF	C-CA-CB-CG
2	N	2	DFF	C-CA-CB-CG
5	N	101	LYN	CE-CD-CG-CB
5	M	101	LYN	CE-CD-CG-CB
2	M	2	DFF	O1-C7-CZ-CE2
2	N	2	DFF	O1-C7-CZ-CE2
2	N	2	DFF	O1-C7-CZ-CE1
2	M	2	DFF	O1-C7-CZ-CE1
2	M	2	DFF	C4-C7-CZ-CE2

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Mol	Chain	Res	Type	Atoms
2	M	2	DFF	C4-C7-CZ-CE1
2	N	2	DFF	C4-C7-CZ-CE2
2	N	2	DFF	C4-C7-CZ-CE1
5	N	101	LYN	C-CA-CB-CG
2	N	2	DFF	N-CA-CB-CG
5	M	101	LYN	O-C-CA-N
2	M	2	DFF	N-CA-CB-CG
5	N	101	LYN	CG-CD-CE-NZ
5	M	101	LYN	C-CA-CB-CG
5	M	101	LYN	CG-CD-CE-NZ
5	N	101	LYN	CA-CB-CG-CD

There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	101	LYN	11	0
2	N	2	DFF	3	0
5	M	101	LYN	12	0
2	M	2	DFF	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
6	FUM	N	102	5	5,5,7	2.32	2 (40%)	4,4,8	1.92	2 (50%)
4	EPE	B	1102	-	15,15,15	0.78	1 (6%)	18,20,20	2.16	5 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	LYN	N	101	2,6	9,9,9	1.99	1 (11%)	9,10,10	2.21	2 (22%)
5	LYN	M	101	2,6	9,9,9	1.83	1 (11%)	9,10,10	1.64	1 (11%)
4	EPE	A	1102	-	15,15,15	0.64	0	18,20,20	2.29	7 (38%)
6	FUM	M	102	5	5,5,7	2.24	2 (40%)	4,4,8	2.08	2 (50%)

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
6	FUM	N	102	5	-	2/3/3/5	-
4	EPE	B	1102	-	-	2/9/19/19	0/1/1/1
5	LYN	N	101	2,6	-	4/9/9/9	-
5	LYN	M	101	2,6	-	5/9/9/9	-
4	EPE	A	1102	-	-	7/9/19/19	0/1/1/1
6	FUM	M	102	5	-	2/3/3/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	101	LYN	C-NT	5.74	1.47	1.32
5	M	101	LYN	C-NT	5.28	1.46	1.32
6	N	102	FUM	C4-C	3.93	1.56	1.44
6	M	102	FUM	C4-C	3.83	1.55	1.44
6	N	102	FUM	C5-C6	3.11	1.53	1.44
6	M	102	FUM	C5-C6	3.01	1.53	1.44
4	B	1102	EPE	C10-S	2.57	1.81	1.77

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	EPE	C5-N4-C3	5.77	121.81	108.83
5	N	101	LYN	CA-C-NT	4.66	124.67	116.68
4	B	1102	EPE	C5-N4-C3	4.46	118.87	108.83
4	B	1102	EPE	O2S-S-C10	4.13	111.89	106.92
4	B	1102	EPE	C7-N4-C5	3.73	120.76	111.23
4	A	1102	EPE	C7-N4-C3	3.70	120.69	111.23
5	N	101	LYN	O-C-NT	-3.57	116.78	123.00
4	B	1102	EPE	C7-N4-C3	3.56	120.34	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1102	EPE	O1S-S-C10	3.54	111.18	106.92
5	M	101	LYN	O-C-NT	-3.16	117.51	123.00
6	N	102	FUM	C4-C5-C6	-3.07	117.41	121.70
6	M	102	FUM	C4-C5-C6	-2.94	117.59	121.70
4	A	1102	EPE	O3S-S-C10	2.67	110.09	105.77
4	B	1102	EPE	O1S-S-C10	2.64	110.10	106.92
4	A	1102	EPE	C9-N1-C2	2.63	117.95	111.23
4	A	1102	EPE	C7-N4-C5	2.41	117.39	111.23
6	N	102	FUM	O-C-C4	-2.17	118.26	125.67
6	M	102	FUM	O-C-C4	-2.16	118.29	125.67
4	A	1102	EPE	C2-C3-N4	2.10	114.96	110.64

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	EPE	C10-C9-N1-C2
4	A	1102	EPE	C8-C7-N4-C5
5	M	101	LYN	NT-C-CA-N
6	M	102	FUM	O-C-C4-C5
6	M	102	FUM	C4-C5-C6-O7
6	N	102	FUM	O-C-C4-C5
6	N	102	FUM	C4-C5-C6-O7
5	N	101	LYN	CE-CD-CG-CB
5	M	101	LYN	CE-CD-CG-CB
4	A	1102	EPE	C9-C10-S-O3S
5	N	101	LYN	C-CA-CB-CG
4	B	1102	EPE	N4-C7-C8-O8
4	A	1102	EPE	C10-C9-N1-C6
4	A	1102	EPE	C9-C10-S-O1S
4	A	1102	EPE	C9-C10-S-O2S
4	A	1102	EPE	N4-C7-C8-O8
5	M	101	LYN	O-C-CA-N
5	N	101	LYN	CG-CD-CE-NZ
5	M	101	LYN	C-CA-CB-CG
5	M	101	LYN	CG-CD-CE-NZ
5	N	101	LYN	CA-CB-CG-CD
4	B	1102	EPE	C8-C7-N4-C5

There are no ring outliers.

5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	N	102	FUM	2	0
5	N	101	LYN	11	0
5	M	101	LYN	12	0
4	A	1102	EPE	1	0
6	M	102	FUM	2	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 (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, 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	954/978 (97%)	-0.17	0	100	100	17, 28, 49, 83	0
1	B	954/978 (97%)	-0.25	0	100	100	18, 29, 49, 84	0
2	M	1/3 (33%)	3.68	1 (100%)	0	0	79, 79, 79, 79	0
2	N	1/3 (33%)	3.42	1 (100%)	0	0	75, 75, 75, 75	0
All	All	1910/1962 (97%)	-0.21	2 (0%)	95	96	17, 29, 49, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	1	PHE	3.7
2	N	1	PHE	3.4

6.2 Non-standard residues in protein, DNA, RNA chains (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
5	LYN	M	101	10/10	0.76	0.56	68,87,101,101	0
5	LYN	N	101	10/10	0.80	0.56	73,85,103,113	0
2	DFF	M	2	19/20	0.88	0.35	34,67,96,97	0
2	DFF	N	2	19/20	0.89	0.34	31,61,104,109	0

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, 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
5	LYN	M	101	10/10	0.76	0.56	68,87,101,101	0
5	LYN	N	101	10/10	0.80	0.56	73,85,103,113	0
6	FUM	M	102	6/8	0.81	0.46	68,81,91,94	0
6	FUM	N	102	6/8	0.84	0.25	66,68,71,74	0
4	EPE	B	1102	15/15	0.96	0.21	40,51,61,62	0
4	EPE	A	1102	15/15	0.98	0.19	29,47,56,66	0
3	ZN	B	1101	1/1	0.98	0.14	44,44,44,44	0
3	ZN	A	1101	1/1	0.99	0.16	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.