Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:32 PM GMT

PDB ID	:	4IME
Title	:	Crystal Structure of Pasteurella multocida N-Acetyl-D-Neuraminic acid lyase K164A Mutant
Authors	:	Fisher, A.J.; Huynh, N.
Deposited on	:	2013-01-02
Resolution	:	1.75 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

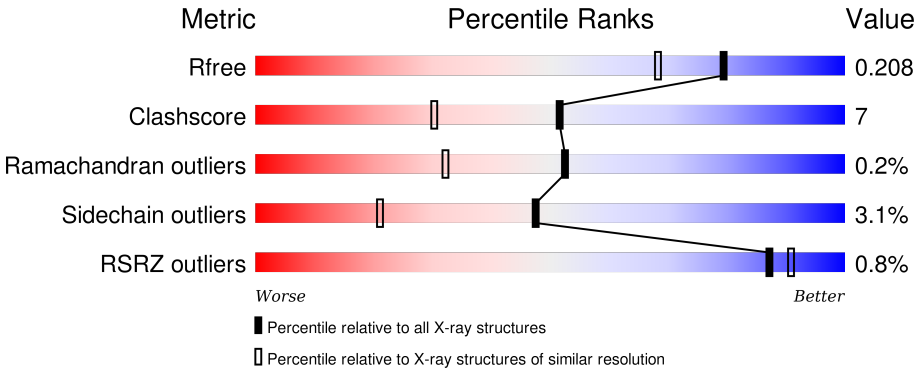
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.75 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}	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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. 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	293	87% 11%
1	B	293	89% 10%
1	C	293	87% 12%
1	D	293	90% 9%
1	E	293	90% 8%

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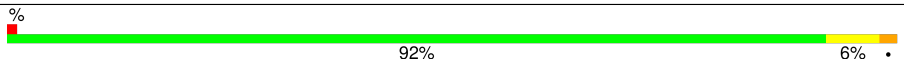
Mol	Chain	Length	Quality of chain
1	F	293	
1	G	293	
1	H	293	

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
2	ME2	B	302	-	-	X	X
2	ME2	C	5001	-	-	X	-
2	ME2	D	301	-	-	-	X
2	ME2	E	302	-	-	-	X
2	ME2	G	301	-	-	X	-
3	PG6	G	302	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 21389 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 N-acetylneuraminate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	2	0
			2311	1495	370	438	8			
1	B	293	Total	C	N	O	S	0	0	0
			2295	1485	367	435	8			
1	C	293	Total	C	N	O	S	0	3	0
			2322	1504	371	439	8			
1	D	293	Total	C	N	O	S	0	3	0
			2322	1504	371	439	8			
1	E	293	Total	C	N	O	S	0	3	0
			2322	1504	371	439	8			
1	F	293	Total	C	N	O	S	0	2	0
			2314	1500	369	437	8			
1	G	293	Total	C	N	O	S	0	2	0
			2311	1495	370	438	8			
1	H	293	Total	C	N	O	S	0	3	0
			2319	1503	370	438	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
A	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
B	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
B	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
C	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
C	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
D	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
D	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
E	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
E	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
F	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
F	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
G	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0

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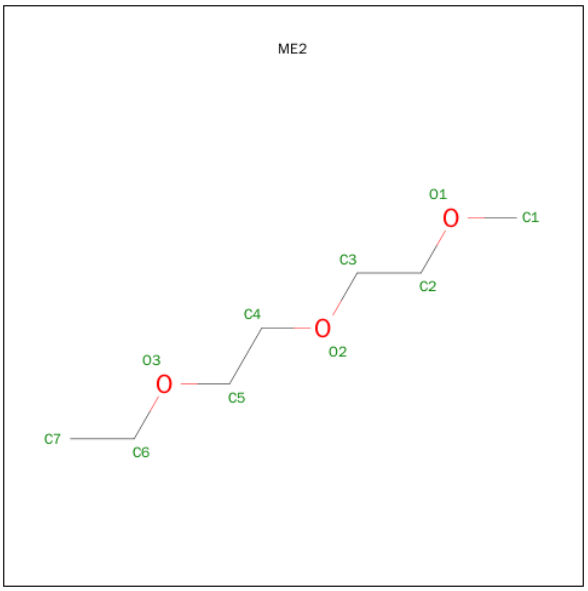
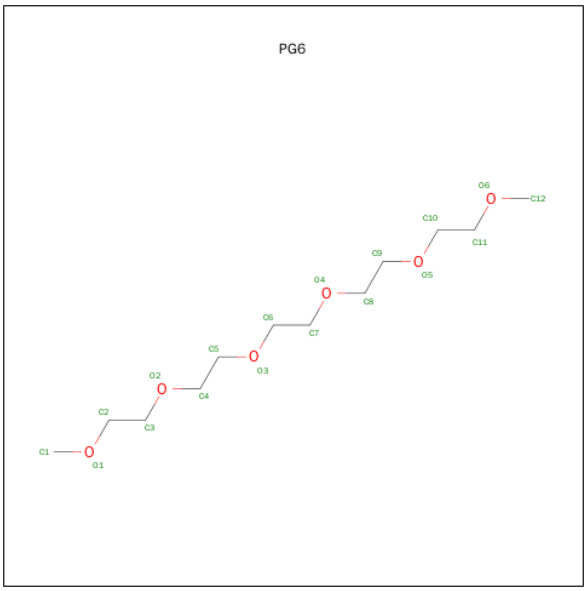
Chain	Residue	Modelled	Actual	Comment	Reference
G	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0
H	164	ALA	LYS	ENGINEERED MUTATION	UNP Q9CKB0
H	278	SER	PRO	SEE REMARK 999	UNP Q9CKB0

- Molecule 2 is 1-ETHOXY-2-(2-METHOXYETHOXY)ETHANE (three-letter code: ME2) (formula: $C_7H_{16}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 7 3	0	0
2	B	1	Total C O 10 7 3	0	0
2	C	1	Total C O 10 7 3	0	0
2	D	1	Total C O 10 7 3	0	0
2	E	1	Total C O 10 7 3	0	0
2	E	1	Total C O 10 7 3	0	0
2	G	1	Total C O 10 7 3	0	0

- Molecule 3 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C O 18 12 6	0	0

- Molecule 4 is water.

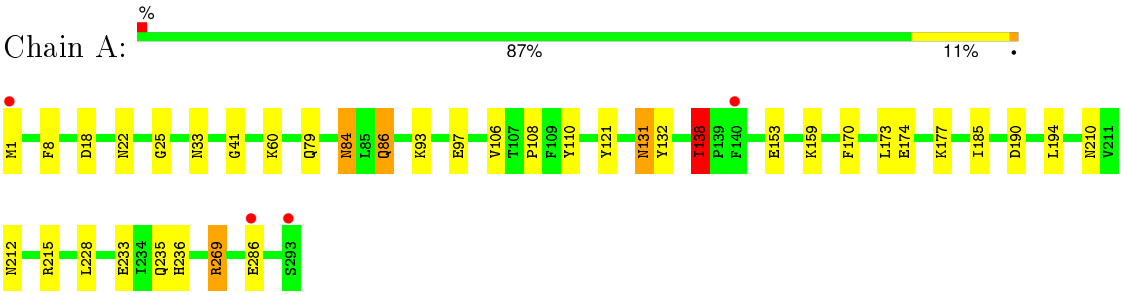
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	305	Total O 305 305	0	0
4	B	383	Total O 383 383	0	0
4	C	358	Total O 358 358	0	0
4	D	369	Total O 369 369	0	0
4	E	316	Total O 316 316	0	0
4	F	366	Total O 366 366	0	0
4	G	313	Total O 313 313	0	0
4	H	375	Total O 375 375	0	0

3 Residue-property plots (i)

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.

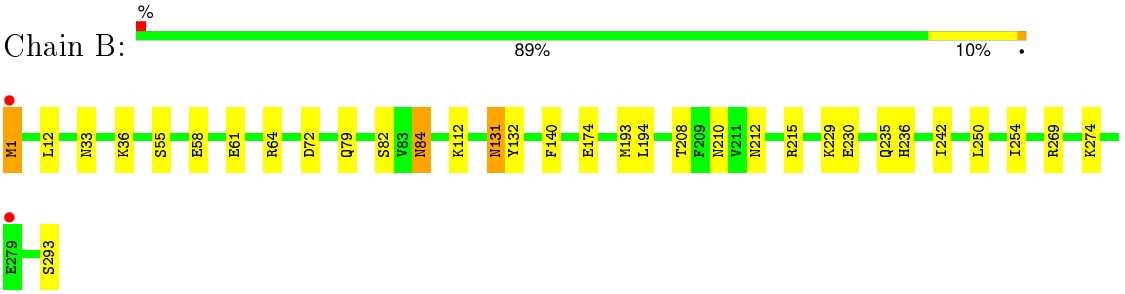
- Molecule 1: N-acetylneuraminate lyase

Chain A:



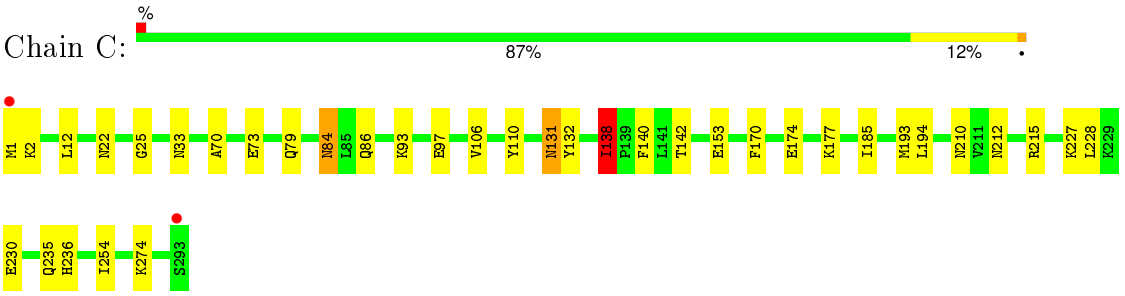
- Molecule 1: N-acetylneuraminate lyase

Chain B:



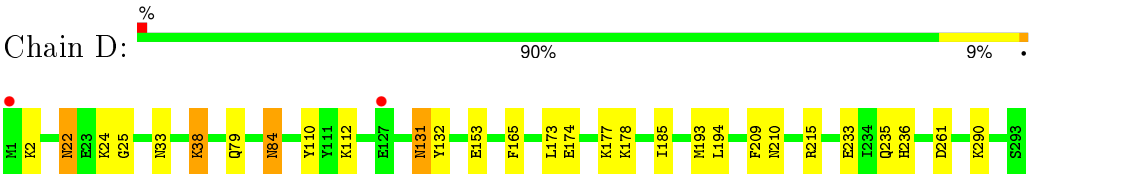
- Molecule 1: N-acetylneuraminate lyase

Chain C:



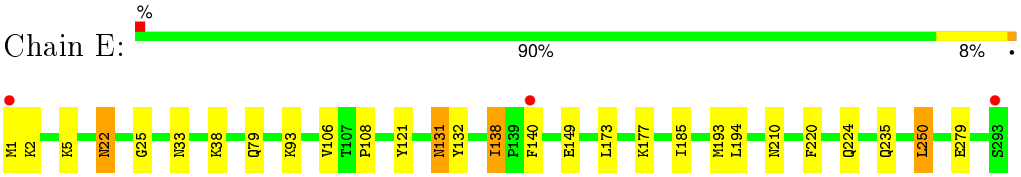
- Molecule 1: N-acetylneuraminate lyase

Chain D:



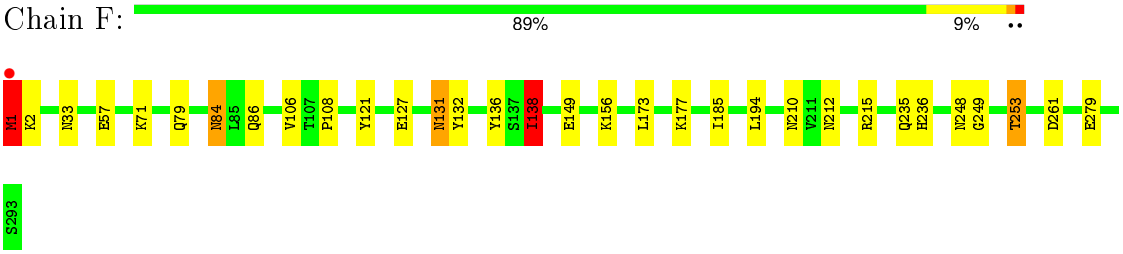
• Molecule 1: N-acetylneuraminate lyase

Chain E:



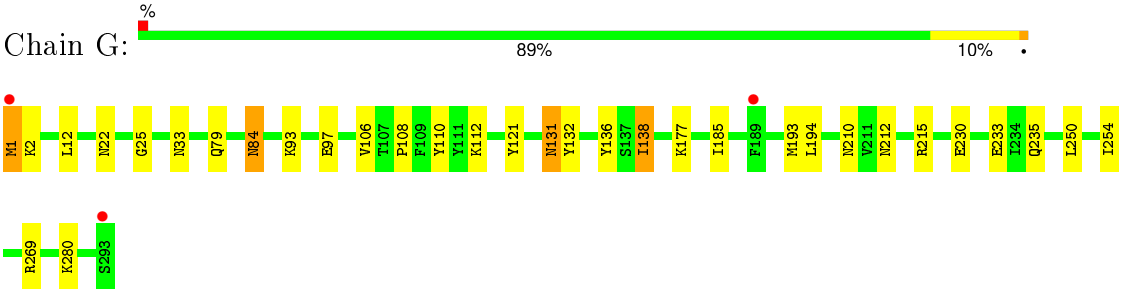
• Molecule 1: N-acetylneuraminate lyase

Chain F:



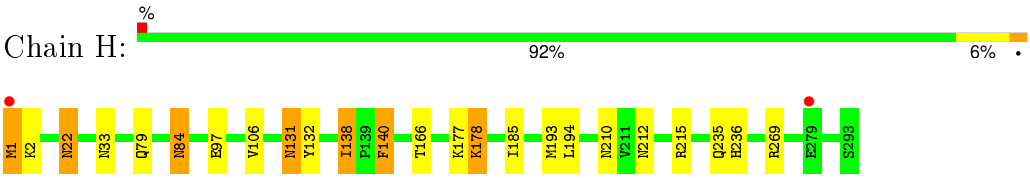
• Molecule 1: N-acetylneuraminate lyase

Chain G:



• Molecule 1: N-acetylneuraminate lyase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.14Å 147.71Å 111.98Å 90.00° 98.51° 90.00°	Depositor
Resolution (Å)	39.26 – 1.75 39.23 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.26-1.75) 99.1 (39.23-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.91 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.175 , 0.208 0.175 , 0.208	Depositor DCC
R_{free} test set	14540 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 47.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 287943 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	21389	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.07% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG6, ME2

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	0.73	0/2353	0.96	8/3171 (0.3%)
1	B	0.83	0/2337	0.86	1/3148 (0.0%)
1	C	0.75	0/2365	0.82	2/3187 (0.1%)
1	D	0.81	0/2365	0.85	1/3186 (0.0%)
1	E	0.69	0/2365	0.80	1/3187 (0.0%)
1	F	0.78	0/2357	0.89	2/3176 (0.1%)
1	G	0.72	0/2353	0.83	2/3171 (0.1%)
1	H	0.79	0/2365	0.84	1/3187 (0.0%)
All	All	0.76	0/18860	0.86	18/25413 (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
1	F	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	269	ARG	NE-CZ-NH1	18.16	129.38	120.30
1	A	269	ARG	NE-CZ-NH2	-17.52	111.54	120.30
1	A	269	ARG	CD-NE-CZ	7.89	134.65	123.60
1	H	269	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	B	269	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	G	250	LEU	CA-CB-CG	6.12	129.37	115.30
1	A	269	ARG	CA-CB-CG	6.03	126.67	113.40
1	A	18	ASP	CB-CG-OD1	5.95	123.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	138[A]	ILE	CB-CA-C	-5.71	100.19	111.60
1	F	138[B]	ILE	CB-CA-C	-5.71	100.19	111.60
1	D	215	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	E	250	LEU	CA-CB-CG	5.61	128.21	115.30
1	G	269	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	269	ARG	CB-CG-CD	5.48	125.86	111.60
1	A	138[A]	ILE	CB-CA-C	-5.45	100.69	111.60
1	A	138[B]	ILE	CB-CA-C	-5.45	100.69	111.60
1	C	138[A]	ILE	CB-CA-C	-5.02	101.56	111.60
1	C	138[B]	ILE	CB-CA-C	-5.02	101.56	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	1	MET	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	2311	0	2339	38	0
1	B	2295	0	2323	33	0
1	C	2322	0	2347	43	0
1	D	2322	0	2346	29	0
1	E	2322	0	2347	26	0
1	F	2314	0	2342	29	0
1	G	2311	0	2339	30	0
1	H	2319	0	2348	20	0
2	B	20	0	32	13	0
2	C	10	0	16	13	0
2	D	10	0	16	4	0
2	E	20	0	32	9	0
2	G	10	0	16	6	0
3	G	18	0	26	2	0
4	A	305	0	0	5	0
4	B	383	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	358	0	0	6	0
4	D	369	0	0	11	0
4	E	316	0	0	6	0
4	F	366	0	0	6	0
4	G	313	0	0	6	0
4	H	375	0	0	4	0
All	All	21389	0	18869	254	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (254) 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:58:GLU:OE2	2:B:302:ME2:H31	1.46	1.14
1:C:140[B]:PHE:CE1	2:C:5001:ME2:H11	1.88	1.09
2:C:5001:ME2:H71	4:D:756:HOH:O	1.56	1.05
1:C:106:VAL:HG23	1:C:138[A]:ILE:HD11	1.40	1.04
1:B:58:GLU:OE2	2:B:302:ME2:C3	2.12	0.97
2:E:301:ME2:H21	4:E:712:HOH:O	1.64	0.96
1:F:248:ASN:HB3	1:F:253:THR:HG21	1.44	0.95
2:B:302:ME2:H21	4:B:666:HOH:O	1.69	0.91
1:F:1:MET:HA	4:F:651:HOH:O	1.70	0.91
1:D:153:GLU:HG2	4:D:723:HOH:O	1.72	0.89
1:C:153:GLU:HG2	4:C:5448:HOH:O	1.72	0.88
1:F:249:GLY:O	1:F:253:THR:HG23	1.74	0.86
1:B:230:GLU:HG3	4:B:579:HOH:O	1.74	0.85
1:E:131:ASN:HD22	1:E:132:TYR:H	1.28	0.82
1:C:131:ASN:HD22	1:C:132:TYR:H	1.26	0.82
1:F:131:ASN:HD22	1:F:132:TYR:H	1.30	0.79
1:C:138[A]:ILE:HD12	1:C:138[A]:ILE:N	1.98	0.79
1:B:82:SER:HB2	4:B:564:HOH:O	1.83	0.79
1:C:138[A]:ILE:HD12	1:C:138[A]:ILE:H	1.48	0.79
1:A:22[A]:ASN:HD22	1:A:25:GLY:H	1.30	0.78
1:B:174:GLU:OE1	1:D:236:HIS:HD2	1.67	0.77
1:E:279:GLU:HG3	4:E:713:HOH:O	1.83	0.77
2:E:302:ME2:H21	4:H:395:HOH:O	1.86	0.75
1:C:140[A]:PHE:O	2:C:5001:ME2:H13	1.87	0.74
1:C:22[A]:ASN:HD22	1:C:25:GLY:H	1.34	0.74
2:D:301:ME2:H41	4:D:767:HOH:O	1.88	0.73
1:B:82:SER:CB	4:B:564:HOH:O	2.36	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22[A]:ASN:HD22	1:G:25:GLY:H	1.35	0.72
1:C:140[B]:PHE:CD1	2:C:5001:ME2:H11	2.24	0.71
1:H:236:HIS:HE1	4:H:535:HOH:O	1.72	0.71
1:C:93:LYS:O	1:C:97:GLU:HG2	1.89	0.71
1:G:1:MET:SD	4:G:664:HOH:O	2.48	0.71
1:A:86:GLN:HG2	2:B:302:ME2:H22	1.73	0.71
1:E:93:LYS:NZ	2:E:302:ME2:H42	2.05	0.71
1:A:236:HIS:HE1	4:A:430:HOH:O	1.73	0.71
1:A:131:ASN:HD22	1:A:132:TYR:H	1.36	0.70
1:B:236:HIS:HD2	1:D:174:GLU:OE1	1.74	0.70
1:E:106:VAL:HG23	1:E:138[A]:ILE:HD11	1.73	0.70
1:G:131:ASN:HD22	1:G:132:TYR:H	1.38	0.70
2:D:301:ME2:H32	4:D:769:HOH:O	1.91	0.70
1:H:131:ASN:HD22	1:H:132:TYR:H	1.40	0.69
1:B:131:ASN:HD22	1:B:132:TYR:H	1.39	0.69
1:F:106:VAL:HG23	1:F:138[A]:ILE:HD11	1.74	0.69
1:B:236:HIS:HE1	4:D:556:HOH:O	1.74	0.68
1:C:140[B]:PHE:CZ	2:C:5001:ME2:H11	2.28	0.68
1:A:106:VAL:HG23	1:A:138[A]:ILE:HD11	1.74	0.68
1:A:153:GLU:HG3	4:A:599:HOH:O	1.92	0.68
1:C:236:HIS:HE1	4:C:5317:HOH:O	1.76	0.67
1:B:140:PHE:O	2:B:301:ME2:H73	1.94	0.67
1:A:22[B]:ASN:HD22	1:A:22[B]:ASN:C	1.96	0.67
2:C:5001:ME2:H62	4:C:5384:HOH:O	1.95	0.66
1:E:22[A]:ASN:HD22	1:E:25:GLY:H	1.43	0.66
1:A:174:GLU:OE1	1:C:236:HIS:HD2	1.79	0.65
2:C:5001:ME2:H41	4:D:673:HOH:O	1.97	0.64
1:E:140[B]:PHE:O	2:E:301:ME2:H72	2.00	0.62
1:C:22[A]:ASN:ND2	1:C:25:GLY:H	1.98	0.62
4:B:609:HOH:O	1:D:236:HIS:HE1	1.82	0.62
1:B:229:LYS:HE2	4:D:618:HOH:O	1.98	0.62
1:D:131:ASN:HD22	1:D:132:TYR:H	1.47	0.62
1:D:22[A]:ASN:HD22	1:D:22[A]:ASN:C	2.04	0.61
1:G:138[A]:ILE:HD12	1:G:138[A]:ILE:N	2.16	0.61
1:G:93:LYS:O	1:G:97:GLU:HG3	2.00	0.61
1:E:33:ASN:HD21	1:E:210:ASN:HA	1.64	0.61
1:E:93:LYS:HD3	2:E:302:ME2:H41	1.83	0.60
1:D:22[B]:ASN:HD22	1:D:25:GLY:H	1.50	0.60
1:B:193:MET:HB3	1:B:235:GLN:HE22	1.67	0.60
1:F:236:HIS:HE1	4:F:588:HOH:O	1.84	0.60
1:H:212:ASN:HD21	1:H:215:ARG:HD2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG23	1:A:138[A]:ILE:CD1	2.31	0.60
1:B:33:ASN:HD21	1:B:210:ASN:HA	1.67	0.59
1:C:140[B]:PHE:O	2:C:5001:ME2:H13	2.00	0.59
1:E:131:ASN:HD22	1:E:132:TYR:N	1.98	0.59
1:E:93:LYS:HZ2	2:E:302:ME2:H42	1.65	0.59
1:A:236:HIS:HD2	1:C:174:GLU:OE1	1.85	0.59
1:F:279:GLU:H	1:F:279:GLU:CD	2.06	0.59
1:D:38:LYS:NZ	1:D:38:LYS:HB3	2.18	0.59
1:A:233:GLU:HG3	4:A:601:HOH:O	2.03	0.59
1:F:212:ASN:HD21	1:F:215:ARG:HH11	1.50	0.59
1:G:138[A]:ILE:HD12	1:G:138[A]:ILE:H	1.68	0.58
1:E:173:LEU:HD11	1:E:185:ILE:HG21	1.85	0.58
1:A:84:ASN:OD1	2:B:302:ME2:H11	2.03	0.58
1:C:22[B]:ASN:HD22	1:C:22[B]:ASN:C	2.05	0.58
2:C:5001:ME2:H12	1:D:112:LYS:HE3	1.86	0.58
1:G:112:LYS:HZ1	2:G:301:ME2:H52	1.68	0.58
1:F:33:ASN:HD21	1:F:210:ASN:HA	1.69	0.58
1:E:194:LEU:H	1:E:235:GLN:NE2	2.02	0.57
2:E:301:ME2:C2	4:E:712:HOH:O	2.36	0.57
1:A:22[A]:ASN:ND2	1:A:25:GLY:H	2.00	0.57
1:G:22[A]:ASN:ND2	1:G:25:GLY:H	2.03	0.57
1:H:22[A]:ASN:C	1:H:22[A]:ASN:HD22	2.08	0.57
1:E:140[A]:PHE:O	2:E:301:ME2:H72	2.04	0.57
1:G:22[B]:ASN:HD22	1:G:22[B]:ASN:C	2.05	0.57
1:B:230:GLU:CG	4:B:579:HOH:O	2.43	0.57
1:C:131:ASN:HD22	1:C:132:TYR:N	2.00	0.57
1:F:106:VAL:HG23	1:F:138[A]:ILE:CD1	2.34	0.57
1:D:38:LYS:HE2	1:D:38:LYS:CA	2.35	0.56
2:G:301:ME2:H72	1:H:140:PHE:O	2.06	0.56
1:D:33:ASN:HD21	1:D:210:ASN:HA	1.71	0.56
1:H:178:LYS:NZ	4:H:584:HOH:O	2.35	0.56
3:G:302:PG6:H21	4:G:571:HOH:O	2.04	0.56
1:G:112:LYS:HZ1	2:G:301:ME2:H61	1.71	0.55
1:H:33:ASN:HD21	1:H:210:ASN:HA	1.71	0.55
1:C:138[A]:ILE:HD13	1:C:142:THR:HG23	1.89	0.55
1:C:106:VAL:CG2	1:C:138[A]:ILE:HD11	2.26	0.55
1:G:106:VAL:HG23	1:G:138[A]:ILE:HD11	1.89	0.55
1:F:131:ASN:ND2	1:F:132:TYR:H	2.01	0.54
1:B:58:GLU:OE2	2:B:302:ME2:H32	2.05	0.54
1:F:86:GLN:NE2	4:F:653:HOH:O	2.40	0.54
1:D:38:LYS:HE2	1:D:38:LYS:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:ASN:HD22	1:F:253:THR:CG2	2.20	0.54
2:G:301:ME2:H41	4:H:615:HOH:O	2.07	0.54
1:G:233:GLU:HG2	4:G:668:HOH:O	2.08	0.54
2:D:301:ME2:H11	4:D:755:HOH:O	2.07	0.53
1:E:106:VAL:HG23	1:E:138[A]:ILE:CD1	2.38	0.53
1:C:140[B]:PHE:CZ	2:C:5001:ME2:C1	2.91	0.53
1:F:212:ASN:ND2	1:F:215:ARG:HH11	2.06	0.53
1:F:1:MET:HG2	1:F:2:LYS:H	1.73	0.53
1:C:84:ASN:C	1:C:84:ASN:HD22	2.13	0.53
1:F:138[A]:ILE:HD12	1:F:138[A]:ILE:N	2.23	0.52
1:E:194:LEU:C	1:E:194:LEU:HD23	2.30	0.52
1:A:177:LYS:HG2	1:A:185:ILE:HD12	1.91	0.52
1:B:212:ASN:HD21	1:B:215:ARG:HH11	1.56	0.52
1:E:93:LYS:HG2	2:E:302:ME2:H73	1.91	0.52
1:G:136:TYR:CE2	1:G:138[A]:ILE:HG13	2.45	0.52
1:G:177:LYS:HG2	1:G:185:ILE:HD12	1.92	0.52
1:A:228:LEU:HD11	1:C:228:LEU:HD21	1.92	0.52
1:F:248:ASN:HD22	1:F:253:THR:HG21	1.76	0.51
1:C:86:GLN:NE2	4:C:5367:HOH:O	2.42	0.51
1:A:286:GLU:HG2	4:A:564:HOH:O	2.11	0.51
1:D:22[B]:ASN:ND2	1:D:25:GLY:H	2.08	0.51
1:H:138[A]:ILE:HG23	1:H:166:THR:HB	1.91	0.51
1:G:2:LYS:HG2	4:G:604:HOH:O	2.10	0.51
1:G:106:VAL:HG23	1:G:138[A]:ILE:CD1	2.41	0.51
1:G:212:ASN:HD21	1:G:215:ARG:HH11	1.59	0.51
1:G:131:ASN:HD22	1:G:132:TYR:N	2.08	0.50
1:E:22[A]:ASN:ND2	1:E:25:GLY:H	2.09	0.50
1:C:177:LYS:HG2	1:C:185:ILE:HD12	1.94	0.50
1:C:12:LEU:HD11	1:C:254:ILE:HG21	1.94	0.50
1:F:84:ASN:HD22	1:F:84:ASN:C	2.13	0.50
1:A:212:ASN:HD21	1:A:215:ARG:HH11	1.58	0.50
1:B:84:ASN:C	1:B:84:ASN:HD22	2.15	0.50
1:C:140[B]:PHE:CE1	2:C:5001:ME2:C1	2.79	0.50
1:F:131:ASN:HD22	1:F:132:TYR:N	2.04	0.50
1:G:112:LYS:NZ	2:G:301:ME2:H61	2.26	0.50
1:H:84:ASN:C	1:H:84:ASN:HD22	2.13	0.50
1:G:33:ASN:HD21	1:G:210:ASN:HA	1.76	0.50
1:C:2:LYS:HD2	4:C:5260:HOH:O	2.11	0.50
1:H:131:ASN:ND2	1:H:132:TYR:H	2.09	0.50
1:B:61:GLU:CD	1:B:64:ARG:HH21	2.15	0.50
1:H:194:LEU:H	1:H:235:GLN:NE2	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:127:GLU:HG2	4:F:665:HOH:O	2.11	0.49
1:F:248:ASN:CB	1:F:253:THR:HG21	2.31	0.49
1:A:60:LYS:NZ	4:A:516:HOH:O	2.35	0.49
1:H:138[A]:ILE:HG23	1:H:166:THR:CG2	2.43	0.49
1:D:173[B]:LEU:HD13	1:D:173[B]:LEU:O	2.13	0.49
1:B:55:SER:HB3	2:B:302:ME2:C1	2.42	0.49
1:D:84:ASN:C	1:D:84:ASN:HD22	2.15	0.48
1:A:86:GLN:HB3	2:B:302:ME2:H13	1.95	0.48
1:H:106:VAL:HG23	1:H:138[A]:ILE:HD11	1.94	0.48
1:C:274:LYS:HG2	4:C:5275:HOH:O	2.13	0.48
1:B:194:LEU:HD23	1:B:194:LEU:C	2.33	0.48
1:H:194:LEU:HD23	1:H:194:LEU:C	2.34	0.48
1:D:165:PHE:CD2	1:D:173[B]:LEU:HD23	2.50	0.47
1:A:93:LYS:O	1:A:97:GLU:HG2	2.13	0.47
1:A:22[B]:ASN:ND2	1:A:22[B]:ASN:C	2.67	0.47
2:C:5001:ME2:H22	1:D:112:LYS:NZ	2.28	0.47
1:G:194:LEU:HD23	1:G:194:LEU:C	2.34	0.47
1:F:138[A]:ILE:H	1:F:138[A]:ILE:HD12	1.79	0.47
1:H:193:MET:HB3	1:H:235:GLN:HE22	1.79	0.47
1:D:2:LYS:HD2	4:D:718:HOH:O	2.14	0.47
1:A:84:ASN:HD22	1:A:84:ASN:C	2.17	0.47
1:G:84:ASN:HD22	1:G:84:ASN:C	2.18	0.47
1:F:177:LYS:HG2	1:F:185:ILE:HD12	1.97	0.47
1:F:136:TYR:CE2	1:F:138[A]:ILE:HG13	2.50	0.47
1:F:57:GLU:HG2	4:F:648:HOH:O	2.14	0.47
1:F:108:PRO:HD3	1:F:121:TYR:CE2	2.51	0.46
1:E:5:LYS:NZ	4:E:588:HOH:O	2.34	0.46
1:D:173[A]:LEU:CD1	1:D:185:ILE:HD13	2.45	0.46
1:C:33:ASN:HD21	1:C:210:ASN:HA	1.80	0.46
1:E:220:PHE:O	1:E:224:GLN:HG3	2.15	0.46
1:D:22[A]:ASN:ND2	1:D:25:GLY:H	2.14	0.46
1:D:177:LYS:HG2	1:D:185:ILE:HD12	1.98	0.46
1:C:212:ASN:HD21	1:C:215:ARG:HH11	1.62	0.46
1:B:293:SER:OG	1:B:293:SER:OXT	2.34	0.46
1:G:108:PRO:HD3	1:G:121:TYR:CE2	2.51	0.46
1:G:97:GLU:HG2	4:G:619:HOH:O	2.16	0.45
2:D:301:ME2:C4	4:D:767:HOH:O	2.56	0.45
1:B:1:MET:HE2	4:B:650:HOH:O	2.15	0.45
1:G:12:LEU:HD11	1:G:254:ILE:HG21	1.99	0.45
1:A:132:TYR:CD2	1:A:159:LYS:HE2	2.52	0.45
1:F:173:LEU:HD11	1:F:185:ILE:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLN:CG	2:B:302:ME2:H22	2.42	0.45
1:E:22[B]:ASN:HD22	1:E:22[B]:ASN:C	2.20	0.45
1:C:70:ALA:O	1:C:73:GLU:HG2	2.16	0.45
1:A:194:LEU:H	1:A:235:GLN:NE2	2.14	0.45
1:C:193:MET:HB3	1:C:235:GLN:HE22	1.82	0.45
1:G:193:MET:HB3	1:G:235:GLN:HE22	1.82	0.45
1:A:108:PRO:HD3	1:A:121:TYR:CE2	2.52	0.45
1:F:194:LEU:H	1:F:235:GLN:NE2	2.14	0.44
1:D:193:MET:CE	1:D:209:PHE:CZ	3.00	0.44
1:E:2:LYS:HD2	4:E:631:HOH:O	2.17	0.44
1:A:131:ASN:HD22	1:A:132:TYR:N	2.09	0.44
1:B:194:LEU:H	1:B:235:GLN:NE2	2.15	0.44
1:A:33:ASN:HD21	1:A:210:ASN:HA	1.82	0.44
1:B:274:LYS:HE3	4:B:667:HOH:O	2.17	0.44
1:D:173[B]:LEU:HD21	1:D:185:ILE:HG21	1.99	0.44
1:C:194:LEU:H	1:C:235:GLN:NE2	2.15	0.44
1:A:170:PHE:CD1	1:C:170:PHE:CD1	3.06	0.43
1:A:173:LEU:HD11	1:A:185:ILE:HG21	1.99	0.43
1:D:194:LEU:H	1:D:235:GLN:NE2	2.17	0.43
1:A:8:PHE:CE2	1:A:41:GLY:HA3	2.54	0.43
1:C:131:ASN:ND2	1:C:132:TYR:H	2.06	0.43
1:B:212:ASN:ND2	1:B:215:ARG:HH11	2.17	0.43
1:F:71:LYS:HE2	4:F:497:HOH:O	2.18	0.43
1:E:177:LYS:HG2	1:E:185:ILE:HD12	1.99	0.43
1:G:194:LEU:H	1:G:235:GLN:NE2	2.17	0.43
1:A:212:ASN:HD21	1:A:215:ARG:HD2	1.83	0.43
1:A:131:ASN:ND2	1:A:132:TYR:H	2.11	0.42
1:A:228:LEU:HD21	1:C:228:LEU:HD11	2.00	0.42
1:A:194:LEU:HB2	1:A:235:GLN:HE21	1.85	0.42
1:B:131:ASN:ND2	1:B:132:TYR:H	2.10	0.42
1:E:108:PRO:HD3	1:E:121:TYR:CE2	2.55	0.42
1:A:212:ASN:ND2	1:A:215:ARG:HH11	2.17	0.42
1:D:290:LYS:HG3	4:D:726:HOH:O	2.20	0.42
1:H:194:LEU:HB2	1:H:235:GLN:HE21	1.84	0.42
1:C:212:ASN:ND2	1:C:215:ARG:HH11	2.17	0.42
1:B:82:SER:HB3	4:B:564:HOH:O	2.12	0.42
1:E:193:MET:HB3	1:E:235:GLN:HE22	1.84	0.42
1:B:208:THR:HG21	1:B:242:ILE:HG12	2.01	0.42
1:D:165:PHE:CE2	1:D:173[B]:LEU:HD23	2.55	0.41
1:B:72:ASP:OD2	1:H:97:GLU:HB2	2.19	0.41
1:G:22[B]:ASN:C	1:G:22[B]:ASN:ND2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138[B]:ILE:HG23	1:A:138[B]:ILE:O	2.20	0.41
1:H:177:LYS:HG2	1:H:185:ILE:HD12	2.01	0.41
1:G:280:LYS:HE2	3:G:302:PG6:H82	2.01	0.41
1:D:194:LEU:HB2	1:D:235:GLN:HE21	1.85	0.41
1:H:138[B]:ILE:O	1:H:138[B]:ILE:HG23	2.20	0.41
1:B:12:LEU:HD11	1:B:254:ILE:HG21	2.02	0.41
1:C:22[B]:ASN:ND2	1:C:25:GLY:H	2.18	0.41
1:D:173[B]:LEU:C	1:D:173[B]:LEU:HD13	2.41	0.41
1:B:112:LYS:NZ	2:B:301:ME2:H22	2.36	0.41
1:E:38:LYS:NZ	4:E:491:HOH:O	2.54	0.41
1:C:138[A]:ILE:HD13	1:C:142:THR:CG2	2.51	0.41
1:D:131:ASN:HD22	1:D:132:TYR:N	2.15	0.41
1:G:12:LEU:HD11	1:G:254:ILE:CG2	2.51	0.41
1:C:106:VAL:HG23	1:C:138[A]:ILE:CD1	2.29	0.41
1:A:86:GLN:CB	2:B:302:ME2:H22	2.51	0.40
1:C:140[B]:PHE:CD1	2:C:5001:ME2:C1	2.98	0.40
1:C:138[B]:ILE:O	1:C:138[B]:ILE:HG23	2.22	0.40
1:B:194:LEU:HB2	1:B:235:GLN:HE21	1.87	0.40
1:B:55:SER:HB3	2:B:302:ME2:H12	2.03	0.40
1:E:173:LEU:HD12	1:E:185:ILE:HD13	2.03	0.40
2:G:301:ME2:H22	4:G:662:HOH:O	2.21	0.40
1:H:1:MET:HB2	1:H:2:LYS:H	1.70	0.40

There are no symmetry-related clashes.

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	293/293 (100%)	291 (99%)	1 (0%)	1 (0%)	46 25
1	B	291/293 (99%)	287 (99%)	4 (1%)	0	100 100
1	C	294/293 (100%)	292 (99%)	1 (0%)	1 (0%)	46 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	294/293 (100%)	291 (99%)	2 (1%)	1 (0%)	46 25
1	E	294/293 (100%)	292 (99%)	2 (1%)	0	100 100
1	F	293/293 (100%)	290 (99%)	3 (1%)	0	100 100
1	G	293/293 (100%)	291 (99%)	1 (0%)	1 (0%)	46 25
1	H	294/293 (100%)	292 (99%)	2 (1%)	0	100 100
All	All	2346/2344 (100%)	2326 (99%)	16 (1%)	4 (0%)	52 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	110	TYR
1	A	110	TYR
1	C	110	TYR
1	D	110	TYR

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	244/242 (101%)	235 (96%)	9 (4%)	41 16
1	B	242/242 (100%)	236 (98%)	6 (2%)	55 30
1	C	245/242 (101%)	237 (97%)	8 (3%)	45 19
1	D	245/242 (101%)	235 (96%)	10 (4%)	37 13
1	E	245/242 (101%)	236 (96%)	9 (4%)	41 16
1	F	244/242 (101%)	234 (96%)	10 (4%)	37 13
1	G	244/242 (101%)	237 (97%)	7 (3%)	50 24
1	H	245/242 (101%)	235 (96%)	10 (4%)	37 13
All	All	1954/1936 (101%)	1885 (96%)	69 (4%)	47 17

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	79	GLN
1	A	84	ASN
1	A	86	GLN
1	A	131	ASN
1	A	138[A]	ILE
1	A	138[B]	ILE
1	A	190	ASP
1	A	269	ARG
1	B	1	MET
1	B	36	LYS
1	B	79	GLN
1	B	84	ASN
1	B	131	ASN
1	B	250	LEU
1	C	1	MET
1	C	79	GLN
1	C	84	ASN
1	C	131	ASN
1	C	138[A]	ILE
1	C	138[B]	ILE
1	C	227	LYS
1	C	230	GLU
1	D	22[A]	ASN
1	D	22[B]	ASN
1	D	24	LYS
1	D	38	LYS
1	D	79	GLN
1	D	84	ASN
1	D	131	ASN
1	D	178	LYS
1	D	233	GLU
1	D	261	ASP
1	E	1	MET
1	E	22[A]	ASN
1	E	22[B]	ASN
1	E	79	GLN
1	E	131	ASN
1	E	138[A]	ILE
1	E	138[B]	ILE
1	E	149	GLU
1	E	250	LEU
1	F	1	MET

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Mol	Chain	Res	Type
1	F	79	GLN
1	F	84	ASN
1	F	131	ASN
1	F	138[A]	ILE
1	F	138[B]	ILE
1	F	149	GLU
1	F	156	LYS
1	F	253	THR
1	F	261	ASP
1	G	1	MET
1	G	79	GLN
1	G	84	ASN
1	G	131	ASN
1	G	138[A]	ILE
1	G	138[B]	ILE
1	G	230	GLU
1	H	1	MET
1	H	22[A]	ASN
1	H	22[B]	ASN
1	H	79	GLN
1	H	84	ASN
1	H	131	ASN
1	H	138[A]	ILE
1	H	138[B]	ILE
1	H	140	PHE
1	H	178	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	86	GLN
1	A	131	ASN
1	A	212	ASN
1	A	235	GLN
1	A	236	HIS
1	B	33	ASN
1	B	84	ASN
1	B	86	GLN
1	B	131	ASN
1	B	212	ASN
1	B	235	GLN

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Mol	Chain	Res	Type
1	B	236	HIS
1	C	33	ASN
1	C	84	ASN
1	C	131	ASN
1	C	212	ASN
1	C	235	GLN
1	C	236	HIS
1	D	33	ASN
1	D	84	ASN
1	D	120	HIS
1	D	131	ASN
1	D	235	GLN
1	D	236	HIS
1	E	33	ASN
1	E	131	ASN
1	E	212	ASN
1	E	235	GLN
1	F	33	ASN
1	F	84	ASN
1	F	86	GLN
1	F	131	ASN
1	F	212	ASN
1	F	235	GLN
1	F	236	HIS
1	F	248	ASN
1	G	33	ASN
1	G	84	ASN
1	G	131	ASN
1	G	212	ASN
1	G	224	GLN
1	G	235	GLN
1	H	33	ASN
1	H	84	ASN
1	H	131	ASN
1	H	212	ASN
1	H	235	GLN
1	H	236	HIS

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ME2	B	301	-	9,9,9	0.64	0	8,8,8	0.74	0
2	ME2	B	302	-	9,9,9	0.65	0	8,8,8	0.64	0
2	ME2	C	5001	-	9,9,9	0.55	0	8,8,8	0.50	0
2	ME2	D	301	-	9,9,9	1.01	0	8,8,8	1.04	0
2	ME2	E	301	-	9,9,9	0.50	0	8,8,8	0.73	0
2	ME2	E	302	-	9,9,9	0.74	0	8,8,8	1.76	3 (37%)
2	ME2	G	301	-	9,9,9	0.44	0	8,8,8	0.42	0
3	PG6	G	302	-	17,17,17	1.01	0	16,16,16	1.16	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ME2	B	301	-	-	0/7/7/7	0/0/0/0
2	ME2	B	302	-	-	0/7/7/7	0/0/0/0
2	ME2	C	5001	-	-	0/7/7/7	0/0/0/0
2	ME2	D	301	-	-	0/7/7/7	0/0/0/0
2	ME2	E	301	-	-	0/7/7/7	0/0/0/0
2	ME2	E	302	-	-	0/7/7/7	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ME2	G	301	-	-	0/7/7/7	0/0/0/0
3	PG6	G	302	-	-	0/15/15/15	0/0/0/0

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	302	ME2	O3-C5-C4	-3.03	96.91	110.36
3	G	302	PG6	O4-C7-C6	2.13	119.83	110.36
3	G	302	PG6	O5-C9-C8	2.19	120.09	110.36
3	G	302	PG6	O4-C8-C9	2.38	120.96	110.36
2	E	302	ME2	C6-O3-C5	2.50	122.36	112.80
2	E	302	ME2	O2-C4-C5	2.76	122.62	110.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	ME2	2	0
2	B	302	ME2	11	0
2	C	5001	ME2	13	0
2	D	301	ME2	4	0
2	E	301	ME2	4	0
2	E	302	ME2	5	0
2	G	301	ME2	6	0
3	G	302	PG6	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

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, 95^{th} 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	293/293 (100%)	-0.19	4 (1%)	78	84	10, 16, 26, 57	0
1	B	293/293 (100%)	-0.28	2 (0%)	89	92	8, 12, 22, 63	0
1	C	293/293 (100%)	-0.16	2 (0%)	89	92	9, 14, 26, 54	0
1	D	293/293 (100%)	-0.20	2 (0%)	89	92	8, 12, 21, 50	0
1	E	293/293 (100%)	-0.09	3 (1%)	84	89	10, 17, 29, 60	0
1	F	293/293 (100%)	-0.22	1 (0%)	94	95	8, 13, 22, 50	0
1	G	293/293 (100%)	-0.21	3 (1%)	84	89	10, 15, 27, 62	0
1	H	293/293 (100%)	-0.17	2 (0%)	89	92	8, 13, 23, 50	0
All	All	2344/2344 (100%)	-0.19	19 (0%)	87	91	8, 14, 25, 63	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	MET	6.3
1	A	1	MET	6.3
1	C	1	MET	6.0
1	E	1	MET	5.4
1	G	1	MET	5.2
1	D	1	MET	5.0
1	E	293	SER	4.0
1	F	1	MET	3.3
1	A	293	SER	3.1
1	C	293	SER	2.8
1	G	293	SER	2.6
1	H	1	MET	2.5
1	H	279	GLU	2.3
1	G	189	PHE	2.2
1	E	140[A]	PHE	2.2
1	D	127	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	279	GLU	2.1
1	A	140	PHE	2.0
1	A	286	GLU	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 carbohydrates 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. 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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	PG6	G	302	18/18	0.70	0.22	14.29	33,38,46,48	0
2	ME2	D	301	10/10	0.59	0.25	10.00	25,34,37,38	0
2	ME2	B	302	10/10	0.79	0.19	3.66	22,27,28,32	0
2	ME2	E	302	10/10	0.82	0.19	2.91	27,29,32,32	0
2	ME2	B	301	10/10	0.84	0.15	1.96	28,31,33,35	0
2	ME2	E	301	10/10	0.90	0.14	1.19	28,31,34,37	0
2	ME2	G	301	10/10	0.88	0.12	1.14	30,31,34,36	0
2	ME2	C	5001	10/10	0.85	0.14	1.10	22,30,31,35	0

6.5 Other polymers (i)

There are no such residues in this entry.