Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 07:40 PM EDT

PDB ID	:	6HGE
Title	:	Crystal structure of Alpha1-antichymotrypsin variant NewBG-I in the uncleaved S-conformation
Authors	:	Gardill, B.R.; Schmidt, K.; Muller, Y.A.
Deposited on	:	2018-08-23
Resolution	:	2.80 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:

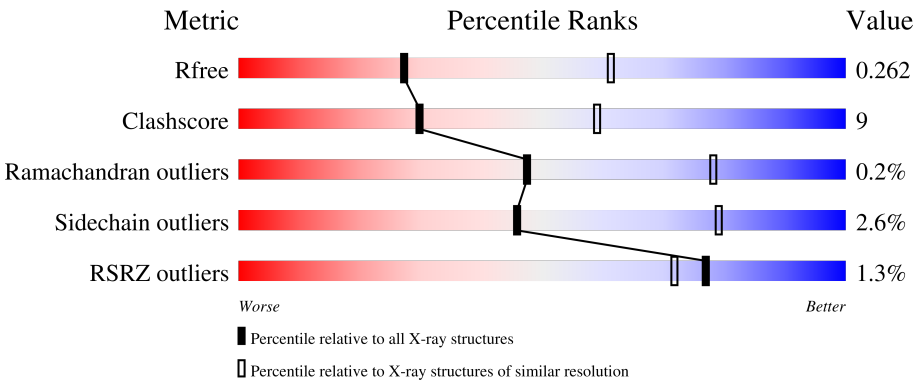
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	409	% 69% 19% 11%
2	B	409	% 70% 18% • 11%
3	C	409	67% 18% 14%
4	D	409	2% 61% 22% • 15%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11577 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 Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2931	1886	483	549	13	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	initiating methionine	UNP P01011
A	-7	LYS	-	expression tag	UNP P01011
A	-6	HIS	-	expression tag	UNP P01011
A	-5	HIS	-	expression tag	UNP P01011
A	-4	HIS	-	expression tag	UNP P01011
A	-3	HIS	-	expression tag	UNP P01011
A	-2	HIS	-	expression tag	UNP P01011
A	-1	HIS	-	expression tag	UNP P01011
A	0	MET	-	expression tag	UNP P01011
A	1	LYS	-	expression tag	UNP P01011
A	2	GLN	-	expression tag	UNP P01011
A	24	ARG	LEU	engineered mutation	UNP P01011
A	242	GLN	GLU	engineered mutation	UNP P01011
A	244	ASN	LYS	engineered mutation	UNP P01011
A	269	SER	LEU	engineered mutation	UNP P01011
A	270	ARG	PRO	engineered mutation	UNP P01011
A	274	ASN	LYS	engineered mutation	UNP P01011
A	277	GLY	ARG	engineered mutation	UNP P01011
A	382	ASP	PRO	engineered mutation	UNP P01011
A	383	HIS	THR	engineered mutation	UNP P01011
A	384	PHE	ASP	engineered mutation	UNP P01011
A	386	TRP	GLN	engineered mutation	UNP P01011
A	387	SER	ASN	engineered mutation	UNP P01011

- Molecule 2 is a protein called Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	364	2941	1894	483	551	13	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	initiating methionine	UNP P01011
B	-7	LYS	-	expression tag	UNP P01011
B	-6	HIS	-	expression tag	UNP P01011
B	-5	HIS	-	expression tag	UNP P01011
B	-4	HIS	-	expression tag	UNP P01011
B	-3	HIS	-	expression tag	UNP P01011
B	-2	HIS	-	expression tag	UNP P01011
B	-1	HIS	-	expression tag	UNP P01011
B	0	MET	-	expression tag	UNP P01011
B	1	LYS	-	expression tag	UNP P01011
B	2	GLN	-	expression tag	UNP P01011
B	24	ARG	LEU	engineered mutation	UNP P01011
B	242	GLN	GLU	engineered mutation	UNP P01011
B	244	ASN	LYS	engineered mutation	UNP P01011
B	269	SER	LEU	engineered mutation	UNP P01011
B	270	ARG	PRO	engineered mutation	UNP P01011
B	274	ASN	LYS	engineered mutation	UNP P01011
B	277	GLY	ARG	engineered mutation	UNP P01011
B	382	ASP	PRO	engineered mutation	UNP P01011
B	383	HIS	THR	engineered mutation	UNP P01011
B	384	PHE	ASP	engineered mutation	UNP P01011
B	386	TRP	GLN	engineered mutation	UNP P01011
B	387	SER	ASN	engineered mutation	UNP P01011

- Molecule 3 is a protein called Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	350	2833	1825	465	530	13	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	MET	-	initiating methionine	UNP P01011
C	-7	LYS	-	expression tag	UNP P01011
C	-6	HIS	-	expression tag	UNP P01011
C	-5	HIS	-	expression tag	UNP P01011

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P01011
C	-3	HIS	-	expression tag	UNP P01011
C	-2	HIS	-	expression tag	UNP P01011
C	-1	HIS	-	expression tag	UNP P01011
C	0	MET	-	expression tag	UNP P01011
C	1	LYS	-	expression tag	UNP P01011
C	2	GLN	-	expression tag	UNP P01011
C	24	ARG	LEU	engineered mutation	UNP P01011
C	242	GLN	GLU	engineered mutation	UNP P01011
C	244	ASN	LYS	engineered mutation	UNP P01011
C	269	SER	LEU	engineered mutation	UNP P01011
C	270	ARG	PRO	engineered mutation	UNP P01011
C	274	ASN	LYS	engineered mutation	UNP P01011
C	277	GLY	ARG	engineered mutation	UNP P01011
C	382	ASP	PRO	engineered mutation	UNP P01011
C	383	HIS	THR	engineered mutation	UNP P01011
C	384	PHE	ASP	engineered mutation	UNP P01011
C	386	TRP	GLN	engineered mutation	UNP P01011
C	387	SER	ASN	engineered mutation	UNP P01011

- Molecule 4 is a protein called Alpha-1-antichymotrypsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	348	2814	1816	459	526	13	0	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-8	MET	-	initiating methionine	UNP P01011
D	-7	LYS	-	expression tag	UNP P01011
D	-6	HIS	-	expression tag	UNP P01011
D	-5	HIS	-	expression tag	UNP P01011
D	-4	HIS	-	expression tag	UNP P01011
D	-3	HIS	-	expression tag	UNP P01011
D	-2	HIS	-	expression tag	UNP P01011
D	-1	HIS	-	expression tag	UNP P01011
D	0	MET	-	expression tag	UNP P01011
D	1	LYS	-	expression tag	UNP P01011
D	2	GLN	-	expression tag	UNP P01011
D	24	ARG	LEU	engineered mutation	UNP P01011
D	242	GLN	GLU	engineered mutation	UNP P01011

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	244	ASN	LYS	engineered mutation	UNP P01011
D	269	SER	LEU	engineered mutation	UNP P01011
D	270	ARG	PRO	engineered mutation	UNP P01011
D	274	ASN	LYS	engineered mutation	UNP P01011
D	277	GLY	ARG	engineered mutation	UNP P01011
D	382	ASP	PRO	engineered mutation	UNP P01011
D	383	HIS	THR	engineered mutation	UNP P01011
D	384	PHE	ASP	engineered mutation	UNP P01011
D	386	TRP	GLN	engineered mutation	UNP P01011
D	387	SER	ASN	engineered mutation	UNP P01011

- Molecule 5 is water.

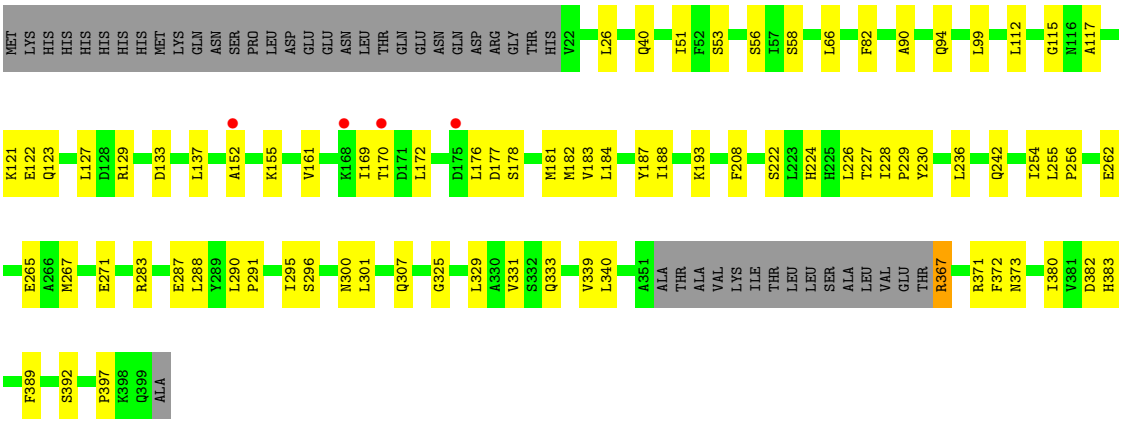
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	21	21	21	0	0
			Total	O		
5	B	21	21	21	0	0
			Total	O		
5	C	12	12	12	0	0
			Total	O		
5	D	4	4	4	0	0

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.

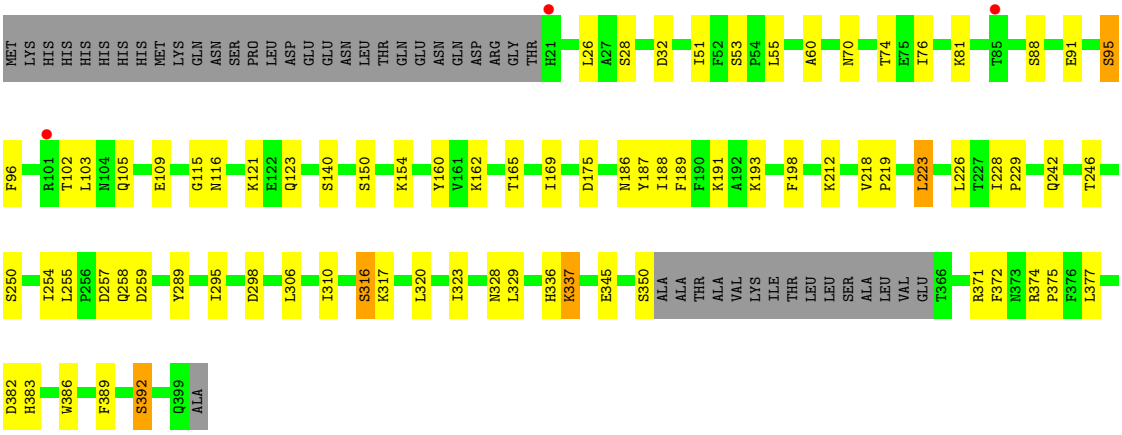
• Molecule 1: Alpha-1-antichymotrypsin

Chain A:



• Molecule 2: Alpha-1-antichymotrypsin

Chain B:



• Molecule 3: Alpha-1-antichymotrypsin

Chain C:

MET LYS HIS HIS HIS HIS HIS HIS MET LYS GLN ASN SER PRO LEU ASP GLU GLU ASN LEU THR GLN GLU ASN GLN ASP ARG GLY THR HIS VAL D23 R24 G25 L26 A27 S28 K39 M49 S53 P54 L55 S56 T59 A60 F63 L64 S65 T71 T72 L73 S88

E91 I92 H93 Q94 S95 H98 T102 D108 Q111 L112 S113 M114 G115 Q123 L127 D133 R136 L137 F147 A152 L156 K162 N163 G164 T165 ARG GLY LYS ILE THR ASP LEU ILE LYS ASP L176 D177 S178 M182 N186 Y187 I188 F189 D202

K212 V216 S222 F231 E235 L255 D259 W276 S279 L280 L288 Y289 L290 P291 I295 D303 E311 E312 D319 L320 S321 T324 S332 A349 SER ALA ALA THR ALA VAL LYS ILE THR LEU LEU SER ALA LEU VAL GLU THR R367 R371

F372 N373 R374 D382 W386 F389 F390 M391 K398 Q399 ALA

- Molecule 4: Alpha-1-antichymotrypsin

Chain D: 2% 61% 22% • 15%

MET LYS HIS HIS HIS HIS HIS HIS MET LYS GLN ASN SER PRO LEU ASP GLU GLU ASN LEU THR GLN GLU ASN GLN ASP ARG GLY THR HIS VAL ASP R24 K39 A45 K48 I51 F52 S53 P54 A60 L61 A62 F63 L66 L80 L84 T85 E86 T87 S88 E89

A90 E91 Q94 R101 S106 S107 D108 E109 L110 Q111 L112 G115 F119 E122 Q123 L124 R129 D133 A134 K135 R136 E141 D146 F147 Q148 D149 S150 A151 K155 L156 D159 G164 T165 ARG GLY LYS ILE THR ASP LEU ILE LYS ASP LEU D177 S178

M182 N186 Y187 I188 F189 W194 P197 R207 L210 S211 K212 V216 S222 L223 P229 D233 E234 E235 L236 T239 G247 N248 A249 L252 F253 I254 L255 Q258 E265 A266 M267 E271 W276 L280 E281 F282 R283 L288 S294 R297

D298 E312 T315 S316 D319 L320 S321 T324 L329 H336 K337 A338 G346 A349 S350 ALA ALA THR ALA VAL LYS ILE THR LEU LEU SER ALA LEU VAL GLU THR ARG T368 I369 V370 R371 F372 N373 I380 F384 F390 M391 S392 T395 N396 P397 K398 Q399

ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	58.00Å 124.71Å 127.50Å 90.00° 90.91° 90.00°	Depositor
Resolution (Å)	34.54 – 2.80 34.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (34.54-2.80) 98.1 (34.54-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.184 , 0.262 0.184 , 0.262	Depositor DCC
R_{free} test set	4388 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.1	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.002 for -h,l,k 0.014 for -h,-l,-k 0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11577	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: MLY

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	0.47	0/2879	0.62	0/3901
2	B	0.49	0/2868	0.62	0/3890
3	C	0.43	0/2780	0.60	0/3767
4	D	0.39	0/2728	0.60	0/3701
All	All	0.45	0/11255	0.61	0/15259

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2931	0	2930	53	0
2	B	2941	0	2934	56	0
3	C	2833	0	2820	47	0
4	D	2814	0	2796	62	0
5	A	21	0	0	0	0
5	B	21	0	0	1	0
5	C	12	0	0	0	0
5	D	4	0	0	0	0
All	All	11577	0	11480	215	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 9.

All (215) 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)
2:B:198:PHE:CD2	2:B:223:LEU:HD22	2.05	0.91
1:A:26:LEU:HD23	1:A:99:LEU:HD12	1.63	0.80
2:B:51:ILE:HG13	2:B:392:SER:HB2	1.65	0.77
4:D:229:PRO:HB2	4:D:280:LEU:HD23	1.67	0.75
3:C:127:LEU:HD13	3:C:324:THR:C	2.08	0.73
3:C:26:LEU:HD22	3:C:95:SER:HB3	1.71	0.71
3:C:23:ASP:HB3	3:C:24:ARG:HH11	1.55	0.70
2:B:162:MLY:HG2	2:B:169:ILE:HD11	1.75	0.69
1:A:367:ARG:HG2	1:A:367:ARG:HH21	1.58	0.68
2:B:198:PHE:CE2	2:B:223:LEU:CD2	2.77	0.67
4:D:124:LEU:HD23	4:D:324:THR:HG21	1.78	0.66
4:D:188:ILE:HG22	4:D:338:ALA:HA	1.77	0.66
2:B:198:PHE:CD2	2:B:223:LEU:CD2	2.78	0.65
4:D:380:ILE:HD13	4:D:390:PHE:HB2	1.77	0.64
2:B:198:PHE:CE2	2:B:223:LEU:HD22	2.33	0.63
2:B:26:LEU:HD22	2:B:95:SER:HB3	1.80	0.61
1:A:229:PRO:HB2	1:A:242:GLN:HB3	1.82	0.61
2:B:60:ALA:HA	2:B:116:ASN:HD21	1.65	0.61
4:D:236:LEU:HD21	4:D:267:MET:HG3	1.82	0.60
4:D:276:TRP:O	4:D:280:LEU:HD12	2.01	0.60
1:A:254:ILE:O	1:A:256:PRO:HD3	2.00	0.60
2:B:116:ASN:O	2:B:140:SER:HB2	2.02	0.60
1:A:51:ILE:HG13	1:A:392:SER:HB2	1.83	0.59
2:B:154:MLY:HE3	2:B:175:ASP:HA	1.83	0.59
4:D:177:ASP:OD1	4:D:178:SER:N	2.36	0.59
2:B:320:LEU:HD12	2:B:329:LEU:HD12	1.84	0.58
3:C:177:ASP:OD1	3:C:178:SER:N	2.32	0.58
1:A:112:LEU:HD11	1:A:188:ILE:HD11	1.85	0.58
2:B:250:SER:OG	2:B:383:HIS:NE2	2.37	0.58
3:C:55:LEU:O	3:C:59:THR:HG23	2.04	0.58
4:D:210:LEU:HD21	4:D:396:ASN:HB2	1.86	0.58
1:A:123:GLN:OE1	1:A:123:GLN:N	2.32	0.57
1:A:227:THR:HA	1:A:283:ARG:O	2.05	0.57
3:C:93:HIS:HB3	3:C:137:LEU:HD13	1.86	0.57
1:A:53:SER:HB3	1:A:56:SER:HB3	1.86	0.57
4:D:248:ASN:HB3	4:D:384:PHE:CZ	2.40	0.57
2:B:162:MLY:HG2	2:B:169:ILE:CD1	2.35	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:ALA:O	3:C:156:LEU:HG	2.04	0.56
4:D:155:LYS:O	4:D:159:ASP:N	2.33	0.56
1:A:367:ARG:HH21	1:A:367:ARG:CG	2.18	0.56
4:D:186:ASN:OD1	4:D:336:HIS:HA	2.05	0.56
4:D:61:LEU:HB2	4:D:80:LEU:HD21	1.87	0.56
4:D:115:GLY:O	4:D:186:ASN:HA	2.06	0.56
3:C:133:ASP:OD2	3:C:136:ARG:NH1	2.38	0.55
2:B:165:THR:HG23	2:B:189:PHE:CD2	2.41	0.55
1:A:300:ASN:HD21	1:A:333:GLN:NE2	2.05	0.55
1:A:382:ASP:HB2	1:A:389:PHE:CZ	2.42	0.55
3:C:255:LEU:HB2	3:C:372:PHE:CE2	2.42	0.54
3:C:127:LEU:CD1	3:C:324:THR:C	2.74	0.54
1:A:229:PRO:HB3	2:B:316:SER:HB2	1.90	0.53
4:D:282:PHE:O	4:D:283:ARG:HD2	2.08	0.53
4:D:66:LEU:HD21	4:D:133:ASP:HB3	1.90	0.53
2:B:123:GLN:OE1	2:B:123:GLN:N	2.38	0.53
2:B:115:GLY:HA3	2:B:187:TYR:CZ	2.44	0.53
1:A:255:LEU:HB2	1:A:372:PHE:CE2	2.44	0.52
4:D:106:SER:O	4:D:108:ASP:N	2.36	0.52
4:D:283:ARG:HA	4:D:283:ARG:HH21	1.74	0.52
2:B:55:LEU:HD21	2:B:103:LEU:HD21	1.90	0.52
2:B:382:ASP:HB2	2:B:389:PHE:CZ	2.45	0.52
3:C:113:SER:HB3	3:C:189:PHE:HB2	1.91	0.52
1:A:183:VAL:HG22	1:A:333:GLN:HB2	1.91	0.51
2:B:345:GLU:HB2	2:B:350:SER:HB2	1.92	0.51
4:D:253:PHE:HB3	4:D:372:PHE:CZ	2.46	0.51
1:A:236:LEU:HD22	1:A:267:MET:HG3	1.91	0.51
4:D:155:LYS:HG2	4:D:159:ASP:OD2	2.10	0.51
4:D:51:ILE:HG22	4:D:297:ARG:HB2	1.92	0.51
3:C:382:ASP:HB2	3:C:389:PHE:CZ	2.45	0.51
3:C:23:ASP:HB3	3:C:24:ARG:NH1	2.24	0.51
2:B:53:SER:HB2	2:B:188:ILE:HG21	1.93	0.51
1:A:224:HIS:ND1	1:A:287:GLU:HG2	2.26	0.51
1:A:90:ALA:O	1:A:94:GLN:HG2	2.11	0.50
3:C:49:ASN:HB3	3:C:295:ILE:HD11	1.94	0.50
3:C:127:LEU:CD1	3:C:324:THR:O	2.61	0.49
3:C:235:GLU:N	3:C:235:GLU:OE1	2.45	0.49
4:D:164:GLY:HA3	4:D:189:PHE:CD2	2.47	0.49
3:C:88:SER:OG	3:C:91:GLU:OE1	2.27	0.49
4:D:235:GLU:HG3	4:D:236:LEU:HD12	1.93	0.49
4:D:51:ILE:HG23	4:D:338:ALA:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:SER:OG	4:D:91:GLU:HB2	2.12	0.49
1:A:152:ALA:O	1:A:155:LYS:HB3	2.13	0.49
2:B:51:ILE:HD12	2:B:295:ILE:HG23	1.95	0.49
2:B:320:LEU:HB3	2:B:323:ILE:HD12	1.93	0.49
1:A:290:LEU:HD12	1:A:291:PRO:HD2	1.95	0.49
1:A:226:LEU:HG	1:A:228:ILE:HG23	1.95	0.49
2:B:229:PRO:HB2	2:B:242:GLN:HB3	1.95	0.49
2:B:298:ASP:OD1	2:B:337:MLY:HB3	2.13	0.49
1:A:340:LEU:HD21	1:A:380:ILE:HD11	1.94	0.49
3:C:115:GLY:O	3:C:186:ASN:HA	2.12	0.49
4:D:368:THR:HG22	4:D:369:ILE:H	1.78	0.49
3:C:53:SER:HB3	3:C:56:SER:HB3	1.95	0.48
4:D:235:GLU:HG3	4:D:236:LEU:CD1	2.43	0.48
4:D:233:ASP:OD1	4:D:235:GLU:HB3	2.13	0.48
1:A:230:TYR:CD2	1:A:283:ARG:HD2	2.48	0.48
2:B:328:ASN:HB2	5:B:512:HOH:O	2.13	0.48
4:D:254:ILE:HG12	4:D:276:TRP:CZ3	2.49	0.48
2:B:193:MLY:O	2:B:246:THR:HG23	2.13	0.48
3:C:182:MET:O	3:C:332:SER:HB2	2.13	0.48
1:A:115:GLY:HA3	1:A:187:TYR:CZ	2.48	0.48
2:B:115:GLY:HA3	2:B:187:TYR:CE2	2.49	0.48
4:D:164:GLY:HA3	4:D:189:PHE:CE2	2.49	0.48
4:D:222:SER:HA	4:D:288:LEU:O	2.14	0.48
1:A:271:GLU:OE2	4:D:207:ARG:HD2	2.14	0.48
3:C:212:LYS:HD2	3:C:259:ASP:OD1	2.14	0.48
2:B:257:ASP:HA	2:B:374:ARG:HH11	1.79	0.47
3:C:98:HIS:O	3:C:102:THR:HG23	2.13	0.47
1:A:367:ARG:CG	1:A:367:ARG:NH2	2.76	0.47
3:C:56:SER:OG	3:C:186:ASN:OD1	2.31	0.47
3:C:123:GLN:OE1	3:C:123:GLN:N	2.36	0.47
4:D:229:PRO:HB2	4:D:280:LEU:CD2	2.39	0.47
2:B:165:THR:HG23	2:B:189:PHE:CG	2.50	0.47
2:B:289:TYR:HB2	2:B:371:ARG:HA	1.97	0.47
3:C:255:LEU:HD11	3:C:374:ARG:HG3	1.96	0.47
2:B:258:GLN:O	2:B:259:ASP:HB2	2.15	0.47
3:C:216:VAL:HG13	3:C:398:LYS:HE3	1.97	0.47
4:D:135:LYS:HD2	4:D:141:GLU:HG2	1.97	0.47
3:C:276:TRP:O	3:C:280:LEU:HG	2.15	0.47
4:D:319:ASP:OD1	4:D:321:SER:HB3	2.14	0.47
1:A:40:GLN:NE2	1:A:307:GLN:OE1	2.37	0.46
1:A:383:HIS:CE1	2:B:317:MLY:HG3	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:112:LEU:HD11	4:D:188:ILE:HD11	1.96	0.46
4:D:255:LEU:HB2	4:D:372:PHE:CE2	2.49	0.46
3:C:289:TYR:HB2	3:C:371:ARG:HG3	1.98	0.46
2:B:102:THR:O	2:B:105:GLN:HG2	2.16	0.46
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.62	0.46
1:A:169:ILE:HD12	1:A:170:THR:O	2.15	0.46
4:D:52:PHE:O	4:D:54:PRO:HD3	2.14	0.46
1:A:117:ALA:O	1:A:184:LEU:HD12	2.16	0.46
1:A:182:MET:CE	1:A:331:VAL:HG22	2.46	0.46
2:B:109:GLU:HG2	2:B:246:THR:OG1	2.15	0.46
2:B:226:LEU:CD2	2:B:228:ILE:CG2	2.94	0.46
4:D:312:GLU:O	4:D:315:THR:HB	2.16	0.46
3:C:216:VAL:CG1	3:C:398:LYS:HE3	2.45	0.46
4:D:210:LEU:HD23	4:D:395:THR:O	2.15	0.46
2:B:383:HIS:HD1	2:B:386:TRP:HZ3	1.64	0.45
1:A:181:MET:HE2	1:A:329:LEU:HA	1.97	0.45
2:B:218:VAL:CG2	2:B:219:PRO:HD2	2.47	0.45
4:D:107:SER:HA	4:D:110:LEU:O	2.16	0.45
4:D:188:ILE:CG2	4:D:338:ALA:HA	2.45	0.45
4:D:115:GLY:HA3	4:D:187:TYR:CE2	2.50	0.45
4:D:197:PRO:O	4:D:223:LEU:HD21	2.17	0.45
1:A:182:MET:HE3	1:A:331:VAL:HG22	1.97	0.45
3:C:202:ASP:HB3	3:C:222:SER:OG	2.17	0.45
1:A:51:ILE:HD12	1:A:295:ILE:HG23	1.99	0.45
2:B:162:MLY:HH22	2:B:162:MLY:HD3	1.77	0.45
1:A:127:LEU:H	1:A:127:LEU:HD12	1.81	0.45
1:A:127:LEU:HD11	1:A:325:GLY:N	2.31	0.45
2:B:88:SER:O	2:B:91:GLU:N	2.47	0.45
4:D:298:ASP:OD1	4:D:337:MLY:HE3	2.17	0.45
4:D:371:ARG:HD2	4:D:373:ASN:ND2	2.32	0.45
4:D:119:PHE:O	4:D:182:MET:HA	2.17	0.45
4:D:194:TRP:CD1	4:D:346:GLY:HA2	2.52	0.45
1:A:122:GLU:HG2	1:A:123:GLN:OE1	2.16	0.45
4:D:216:VAL:HG13	4:D:398:MLY:HD3	1.99	0.44
2:B:186:ASN:O	2:B:336:HIS:HA	2.16	0.44
4:D:39:MLY:HH13	4:D:265:GLU:O	2.16	0.44
3:C:39:MLY:HH22	3:C:39:MLY:HD2	1.85	0.44
2:B:76:ILE:HA	2:B:310:ILE:HG12	1.98	0.44
2:B:186:ASN:OD1	2:B:336:HIS:ND1	2.51	0.44
4:D:122:GLU:OE2	4:D:146:ASP:HB2	2.18	0.44
1:A:115:GLY:HA3	1:A:187:TYR:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:367:ARG:HD2	3:C:367:ARG:HA	1.70	0.44
4:D:45:ALA:O	4:D:48:MLY:HB3	2.18	0.44
4:D:212:MLY:HB3	4:D:212:MLY:HE2	1.56	0.44
2:B:70:ASN:O	2:B:74:THR:HG23	2.18	0.44
2:B:175:ASP:OD2	2:B:175:ASP:N	2.50	0.44
1:A:53:SER:HB2	1:A:188:ILE:HG21	2.00	0.43
3:C:162:MLY:C	3:C:164:GLY:H	2.31	0.43
2:B:255:LEU:HB2	2:B:372:PHE:CE2	2.53	0.43
4:D:320:LEU:HD12	4:D:329:LEU:HG	1.99	0.43
1:A:371:ARG:HD3	1:A:373:ASN:ND2	2.34	0.43
3:C:114:MET:CG	3:C:188:ILE:HG13	2.48	0.43
1:A:133:ASP:O	1:A:137:LEU:HB2	2.18	0.43
3:C:231:PHE:CD1	3:C:279:SER:HB3	2.53	0.43
1:A:296:SER:HB2	1:A:339:VAL:HG22	2.01	0.43
2:B:121:MLY:HH22	2:B:121:MLY:HD3	1.79	0.43
1:A:208:PHE:CE2	1:A:397:PRO:HD3	2.55	0.42
3:C:71:THR:HB	3:C:312:GLU:OE2	2.20	0.42
1:A:161:VAL:HG21	1:A:172:LEU:HD23	2.01	0.42
2:B:254:ILE:HB	2:B:377:LEU:HB2	2.02	0.42
3:C:147:PHE:O	3:C:178:SER:HA	2.19	0.42
2:B:32:ASP:HB3	2:B:81:MLY:HG3	2.00	0.42
2:B:374:ARG:HB2	2:B:375:PRO:HD2	2.01	0.42
3:C:53:SER:HB2	3:C:188:ILE:HG21	2.01	0.41
4:D:52:PHE:CE1	4:D:54:PRO:HG3	2.55	0.41
4:D:283:ARG:HA	4:D:283:ARG:NH2	2.35	0.41
1:A:262:GLU:HA	1:A:265:GLU:HB2	2.02	0.41
4:D:248:ASN:HB3	4:D:384:PHE:CE2	2.55	0.41
4:D:280:LEU:HD12	4:D:280:LEU:H	1.85	0.41
2:B:226:LEU:CD2	2:B:228:ILE:HG23	2.51	0.41
3:C:290:LEU:HD12	3:C:291:PRO:HD2	2.02	0.41
3:C:60:ALA:O	3:C:63:PHE:HB3	2.20	0.41
1:A:187:TYR:CD1	1:A:187:TYR:C	2.94	0.41
3:C:177:ASP:CG	3:C:178:SER:N	2.74	0.41
3:C:319:ASP:OD1	3:C:321:SER:HB3	2.20	0.41
1:A:222:SER:HA	1:A:288:LEU:O	2.20	0.41
2:B:169:ILE:C	2:B:169:ILE:HD12	2.41	0.41
3:C:65:SER:HB2	3:C:73:LEU:HD12	2.03	0.41
3:C:112:LEU:HD23	3:C:112:LEU:HA	1.90	0.41
3:C:114:MET:HG2	3:C:188:ILE:HG13	2.02	0.41
3:C:386:TRP:N	3:C:386:TRP:CD1	2.88	0.41
4:D:247:GLY:O	4:D:249:ALA:N	2.52	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:ND2	1:A:333:GLN:NE2	2.68	0.41
2:B:88:SER:H	2:B:91:GLU:HB2	1.86	0.41
3:C:303:ASP:OD2	3:C:303:ASP:N	2.54	0.41
4:D:90:ALA:O	4:D:94:GLN:HG2	2.21	0.41
4:D:252:LEU:HD12	4:D:252:LEU:HA	1.72	0.41
1:A:193:MLY:HH22	1:A:193:MLY:HD3	1.83	0.40
1:A:301:LEU:HD23	1:A:301:LEU:HA	1.95	0.40
4:D:239:THR:O	4:D:254:ILE:HA	2.20	0.40
1:A:177:ASP:OD2	1:A:178:SER:N	2.54	0.40
4:D:60:ALA:O	4:D:63:PHE:HB3	2.21	0.40
1:A:26:LEU:HD12	1:A:82:PHE:HE2	1.85	0.40
2:B:212:LYS:HB3	2:B:212:LYS:HE2	1.66	0.40
2:B:228:ILE:HB	2:B:229:PRO:HD2	2.03	0.40
2:B:116:ASN:N	2:B:160:TYR:OH	2.54	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	349/409 (85%)	328 (94%)	21 (6%)	0	100	100
2	B	348/409 (85%)	332 (95%)	16 (5%)	0	100	100
3	C	334/409 (82%)	317 (95%)	17 (5%)	0	100	100
4	D	329/409 (80%)	313 (95%)	13 (4%)	3 (1%)	17	46
All	All	1360/1636 (83%)	1290 (95%)	67 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	107	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	349	ALA
4	D	316	SER

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	313/354 (88%)	308 (98%)	5 (2%)	62	88
2	B	312/352 (89%)	303 (97%)	9 (3%)	42	76
3	C	302/354 (85%)	295 (98%)	7 (2%)	50	82
4	D	296/351 (84%)	285 (96%)	11 (4%)	34	68
All	All	1223/1411 (87%)	1191 (97%)	32 (3%)	46	79

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	SER
1	A	66	LEU
1	A	129	ARG
1	A	176	LEU
1	A	367	ARG
2	B	28	SER
2	B	95	SER
2	B	96	PHE
2	B	150	SER
2	B	191	LYS
2	B	223	LEU
2	B	306	LEU
2	B	316	SER
2	B	392	SER
3	C	28	SER
3	C	111	GLN
3	C	288	LEU
3	C	311	GLU
3	C	321	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	391	MET
3	C	399	GLN
4	D	101	ARG
4	D	108	ASP
4	D	129	ARG
4	D	136	ARG
4	D	178	SER
4	D	258	GLN
4	D	271	GLU
4	D	288	LEU
4	D	294	SER
4	D	321	SER
4	D	392	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	333	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)

45 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	$\#\|Z\| > 2$
3	MLY	C	121	3	9,10,11	0.77	0	6,11,13	0.49	0
1	MLY	A	193	1	9,10,11	0.71	0	6,11,13	0.42	0
2	MLY	B	44	2	9,10,11	0.72	0	6,11,13	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MLY	D	337	4	9,10,11	1.00	1 (11%)	6,11,13	0.58	0
2	MLY	B	121	2	9,10,11	0.61	0	6,11,13	0.55	0
4	MLY	D	317	4	9,10,11	0.99	0	6,11,13	0.49	0
2	MLY	B	155	2	9,10,11	0.54	0	6,11,13	0.48	0
4	MLY	D	214	4	9,10,11	0.57	0	6,11,13	0.53	0
4	MLY	D	212	4	9,10,11	0.58	0	6,11,13	0.55	0
3	MLY	C	292	3	9,10,11	0.57	0	6,11,13	0.53	0
1	MLY	A	81	1	9,10,11	0.79	0	6,11,13	0.48	0
4	MLY	D	48	4	9,10,11	0.52	0	6,11,13	0.62	0
3	MLY	C	162	3	9,10,11	0.58	0	6,11,13	0.47	0
4	MLY	D	121	4	9,10,11	0.67	0	6,11,13	0.52	0
1	MLY	A	398	1	9,10,11	0.99	0	6,11,13	0.59	0
4	MLY	D	39	4	9,10,11	0.62	0	6,11,13	0.45	0
1	MLY	A	317	1	9,10,11	0.55	0	6,11,13	0.43	0
2	MLY	B	135	2	9,10,11	0.51	0	6,11,13	0.57	0
4	MLY	D	213	4	9,10,11	0.76	0	6,11,13	0.52	0
1	MLY	A	191	1	9,10,11	0.70	0	6,11,13	0.50	0
4	MLY	D	292	4	9,10,11	0.51	0	6,11,13	0.57	0
1	MLY	A	292	1	9,10,11	0.51	0	6,11,13	0.85	0
3	MLY	C	155	3	9,10,11	0.72	0	6,11,13	0.36	0
2	MLY	B	292	2	9,10,11	0.71	0	6,11,13	0.12	0
1	MLY	A	44	1	9,10,11	0.64	0	6,11,13	0.75	0
2	MLY	B	154	2	9,10,11	0.50	0	6,11,13	0.59	0
1	MLY	A	121	1	9,10,11	0.67	0	6,11,13	1.15	1 (16%)
3	MLY	C	260	3	9,10,11	0.76	0	6,11,13	0.82	0
1	MLY	A	212	1	9,10,11	0.55	0	6,11,13	0.43	0
3	MLY	C	48	3	9,10,11	0.87	0	6,11,13	0.51	0
4	MLY	D	81	4	9,10,11	0.59	0	6,11,13	0.38	0
3	MLY	C	317	3	9,10,11	0.48	0	6,11,13	0.83	0
3	MLY	C	81	3	9,10,11	0.72	0	6,11,13	0.75	0
2	MLY	B	193	2	9,10,11	0.44	0	6,11,13	0.61	0
1	MLY	A	39	1	9,10,11	0.73	0	6,11,13	0.28	0
2	MLY	B	317	2	9,10,11	0.83	0	6,11,13	0.28	0
2	MLY	B	162	2	9,10,11	0.56	0	6,11,13	0.56	0
3	MLY	C	39	3	9,10,11	0.59	0	6,11,13	0.38	0
3	MLY	C	44	3	9,10,11	0.75	0	6,11,13	0.81	0
2	MLY	B	260	2	9,10,11	0.79	0	6,11,13	0.37	0
2	MLY	B	337	2	9,10,11	0.56	0	6,11,13	1.09	1 (16%)
4	MLY	D	398	4	9,10,11	0.58	0	6,11,13	1.19	1 (16%)
2	MLY	B	81	2	9,10,11	0.66	0	6,11,13	0.39	0
4	MLY	D	260	4	9,10,11	0.63	0	6,11,13	0.57	0
4	MLY	D	162	4	9,10,11	0.70	0	6,11,13	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLY	C	121	3	-	4/8/9/11	-
1	MLY	A	193	1	-	2/8/9/11	-
2	MLY	B	44	2	-	0/8/9/11	-
4	MLY	D	337	4	-	3/8/9/11	-
2	MLY	B	121	2	-	6/8/9/11	-
4	MLY	D	317	4	-	4/8/9/11	-
2	MLY	B	155	2	-	3/8/9/11	-
4	MLY	D	214	4	-	1/8/9/11	-
4	MLY	D	212	4	-	4/8/9/11	-
3	MLY	C	292	3	-	1/8/9/11	-
1	MLY	A	81	1	-	5/8/9/11	-
4	MLY	D	48	4	-	3/8/9/11	-
3	MLY	C	162	3	-	0/8/9/11	-
4	MLY	D	121	4	-	2/8/9/11	-
1	MLY	A	398	1	-	4/8/9/11	-
4	MLY	D	39	4	-	4/8/9/11	-
1	MLY	A	317	1	-	2/8/9/11	-
2	MLY	B	135	2	-	1/8/9/11	-
4	MLY	D	213	4	-	4/8/9/11	-
1	MLY	A	191	1	-	7/8/9/11	-
4	MLY	D	292	4	-	1/8/9/11	-
1	MLY	A	292	1	-	5/8/9/11	-
3	MLY	C	155	3	-	0/8/9/11	-
2	MLY	B	292	2	-	4/8/9/11	-
1	MLY	A	44	1	-	1/8/9/11	-
2	MLY	B	154	2	-	1/8/9/11	-
1	MLY	A	121	1	-	1/8/9/11	-
3	MLY	C	260	3	-	4/8/9/11	-
1	MLY	A	212	1	-	2/8/9/11	-
3	MLY	C	48	3	-	5/8/9/11	-
4	MLY	D	81	4	-	1/8/9/11	-
3	MLY	C	317	3	-	3/8/9/11	-
3	MLY	C	81	3	-	3/8/9/11	-
2	MLY	B	193	2	-	1/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MLY	A	39	1	-	2/8/9/11	-
2	MLY	B	317	2	-	3/8/9/11	-
2	MLY	B	162	2	-	6/8/9/11	-
3	MLY	C	39	3	-	1/8/9/11	-
3	MLY	C	44	3	-	0/8/9/11	-
2	MLY	B	260	2	-	5/8/9/11	-
2	MLY	B	337	2	-	5/8/9/11	-
4	MLY	D	398	4	-	3/8/9/11	-
2	MLY	B	81	2	-	3/8/9/11	-
4	MLY	D	260	4	-	2/8/9/11	-
4	MLY	D	162	4	-	2/8/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	337	MLY	CE-NZ	2.06	1.53	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	337	MLY	CD-CE-NZ	-2.53	106.95	113.79
4	D	398	MLY	CD-CE-NZ	-2.42	107.22	113.79
1	A	121	MLY	CD-CE-NZ	-2.16	107.94	113.79

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	81	MLY	C-CA-CB-CG
1	A	191	MLY	N-CA-CB-CG
1	A	191	MLY	C-CA-CB-CG
1	A	292	MLY	C-CA-CB-CG
1	A	398	MLY	N-CA-CB-CG
1	A	398	MLY	C-CA-CB-CG
2	B	81	MLY	N-CA-CB-CG
2	B	81	MLY	C-CA-CB-CG
2	B	121	MLY	C-CA-CB-CG
2	B	154	MLY	O-C-CA-CB
2	B	162	MLY	N-CA-CB-CG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	162	MLY	C-CA-CB-CG
2	B	162	MLY	O-C-CA-CB
2	B	260	MLY	C-CA-CB-CG
2	B	260	MLY	O-C-CA-CB
2	B	292	MLY	N-CA-CB-CG
2	B	292	MLY	C-CA-CB-CG
2	B	317	MLY	C-CA-CB-CG
2	B	317	MLY	O-C-CA-CB
2	B	337	MLY	N-CA-CB-CG
3	C	260	MLY	N-CA-CB-CG
3	C	260	MLY	C-CA-CB-CG
4	D	162	MLY	O-C-CA-CB
4	D	212	MLY	N-CA-CB-CG
4	D	212	MLY	C-CA-CB-CG
4	D	214	MLY	C-CA-CB-CG
4	D	260	MLY	C-CA-CB-CG
4	D	317	MLY	C-CA-CB-CG
4	D	317	MLY	O-C-CA-CB
4	D	398	MLY	C-CA-CB-CG
1	A	81	MLY	CD-CE-NZ-CH1
1	A	81	MLY	CD-CE-NZ-CH2
1	A	191	MLY	CD-CE-NZ-CH1
1	A	191	MLY	CD-CE-NZ-CH2
1	A	292	MLY	CD-CE-NZ-CH2
2	B	155	MLY	CD-CE-NZ-CH1
2	B	155	MLY	CD-CE-NZ-CH2
2	B	260	MLY	CD-CE-NZ-CH1
2	B	260	MLY	CD-CE-NZ-CH2
3	C	260	MLY	CD-CE-NZ-CH1
4	D	39	MLY	CD-CE-NZ-CH1
4	D	39	MLY	CD-CE-NZ-CH2
4	D	48	MLY	CD-CE-NZ-CH1
4	D	48	MLY	CD-CE-NZ-CH2
4	D	317	MLY	CD-CE-NZ-CH1
4	D	317	MLY	CD-CE-NZ-CH2
1	A	398	MLY	CG-CD-CE-NZ
2	B	81	MLY	CG-CD-CE-NZ
3	C	39	MLY	CG-CD-CE-NZ
3	C	317	MLY	CG-CD-CE-NZ
4	D	48	MLY	CG-CD-CE-NZ
1	A	81	MLY	CG-CD-CE-NZ
4	D	39	MLY	CG-CD-CE-NZ

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	D	337	MLY	CG-CD-CE-NZ
1	A	292	MLY	CD-CE-NZ-CH1
2	B	121	MLY	CD-CE-NZ-CH2
3	C	121	MLY	CD-CE-NZ-CH1
3	C	260	MLY	CD-CE-NZ-CH2
4	D	121	MLY	CG-CD-CE-NZ
1	A	39	MLY	CD-CE-NZ-CH2
1	A	193	MLY	CD-CE-NZ-CH2
2	B	317	MLY	CD-CE-NZ-CH2
3	C	48	MLY	CD-CE-NZ-CH2
3	C	81	MLY	CD-CE-NZ-CH2
4	D	212	MLY	CD-CE-NZ-CH2
1	A	292	MLY	CG-CD-CE-NZ
1	A	191	MLY	CA-CB-CG-CD
3	C	48	MLY	CD-CE-NZ-CH1
3	C	81	MLY	CD-CE-NZ-CH1
3	C	317	MLY	CD-CE-NZ-CH2
2	B	292	MLY	CA-CB-CG-CD
2	B	337	MLY	CA-CB-CG-CD
3	C	292	MLY	CA-CB-CG-CD
2	B	292	MLY	CE-CD-CG-CB
1	A	191	MLY	CE-CD-CG-CB
1	A	398	MLY	CA-CB-CG-CD
4	D	213	MLY	CE-CD-CG-CB
3	C	317	MLY	CD-CE-NZ-CH1
1	A	39	MLY	CG-CD-CE-NZ
2	B	337	MLY	CG-CD-CE-NZ
2	B	162	MLY	CE-CD-CG-CB
4	D	213	MLY	CG-CD-CE-NZ
2	B	193	MLY	CE-CD-CG-CB
3	C	48	MLY	CE-CD-CG-CB
1	A	212	MLY	CG-CD-CE-NZ
3	C	81	MLY	CE-CD-CG-CB
2	B	162	MLY	CA-CB-CG-CD
2	B	337	MLY	C-CA-CB-CG
4	D	398	MLY	CG-CD-CE-NZ
1	A	44	MLY	CD-CE-NZ-CH1
3	C	121	MLY	CG-CD-CE-NZ
4	D	337	MLY	CE-CD-CG-CB
4	D	212	MLY	CE-CD-CG-CB
4	D	292	MLY	CE-CD-CG-CB
4	D	162	MLY	CE-CD-CG-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	121	MLY	CG-CD-CE-NZ
1	A	121	MLY	CG-CD-CE-NZ
4	D	81	MLY	CA-CB-CG-CD
2	B	121	MLY	CE-CD-CG-CB
3	C	48	MLY	CA-CB-CG-CD
1	A	317	MLY	CD-CE-NZ-CH2
3	C	121	MLY	CA-CB-CG-CD
4	D	39	MLY	CA-CB-CG-CD
1	A	292	MLY	N-CA-CB-CG
2	B	121	MLY	N-CA-CB-CG
2	B	260	MLY	N-CA-CB-CG
4	D	398	MLY	N-CA-CB-CG
3	C	48	MLY	CG-CD-CE-NZ
2	B	121	MLY	CD-CE-NZ-CH1
2	B	155	MLY	CG-CD-CE-NZ
4	D	121	MLY	CD-CE-NZ-CH2
4	D	213	MLY	CD-CE-NZ-CH2
4	D	337	MLY	CD-CE-NZ-CH2
1	A	317	MLY	CD-CE-NZ-CH1
1	A	191	MLY	CG-CD-CE-NZ
2	B	162	MLY	CG-CD-CE-NZ
2	B	337	MLY	CE-CD-CG-CB
4	D	213	MLY	CA-CB-CG-CD
1	A	193	MLY	CG-CD-CE-NZ
1	A	81	MLY	N-CA-CB-CG
1	A	212	MLY	N-CA-CB-CG
3	C	121	MLY	N-CA-CB-CG
4	D	260	MLY	N-CA-CB-CG
2	B	135	MLY	CE-CD-CG-CB

There are no ring outliers.

15 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	193	MLY	1	0
4	D	337	MLY	1	0
2	B	121	MLY	1	0
4	D	212	MLY	1	0
4	D	48	MLY	1	0
3	C	162	MLY	1	0
4	D	39	MLY	1	0
2	B	154	MLY	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	193	MLY	1	0
2	B	317	MLY	1	0
2	B	162	MLY	3	0
3	C	39	MLY	1	0
2	B	337	MLY	1	0
4	D	398	MLY	1	0
2	B	81	MLY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	353/409 (86%)	-0.41	4 (1%)	80	75	18, 36, 75, 92	0
2	B	352/409 (86%)	-0.46	3 (0%)	84	80	21, 34, 65, 91	0
3	C	340/409 (83%)	-0.44	1 (0%)	94	93	24, 39, 64, 87	0
4	D	335/409 (81%)	-0.04	10 (2%)	50	40	43, 59, 90, 106	0
All	All	1380/1636 (84%)	-0.34	18 (1%)	77	72	18, 43, 77, 106	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	151	ALA	4.6
1	A	152	ALA	3.7
4	D	85	THR	3.1
4	D	349	ALA	2.9
4	D	350	SER	2.9
4	D	148	GLN	2.8
4	D	84	LEU	2.7
4	D	156	LEU	2.6
2	B	85	THR	2.6
1	A	175	ASP	2.5
4	D	150	SER	2.3
4	D	87	THR	2.3
3	C	108	ASP	2.3
1	A	168	LYS	2.2
2	B	21	HIS	2.2
4	D	86	GLU	2.2
2	B	101	ARG	2.1
1	A	170	THR	2.1

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
4	MLY	D	162	11/12	0.77	0.26	79,86,97,97	0
4	MLY	D	337	11/12	0.83	0.22	52,62,85,88	0
1	MLY	A	398	11/12	0.84	0.28	46,60,70,70	0
4	MLY	D	292	11/12	0.89	0.28	51,57,72,74	0
2	MLY	B	260	11/12	0.89	0.25	38,45,57,58	0
1	MLY	A	212	11/12	0.90	0.30	43,57,71,76	0
4	MLY	D	260	11/12	0.90	0.24	64,73,78,79	0
3	MLY	C	162	11/12	0.90	0.27	61,68,73,78	0
4	MLY	D	317	11/12	0.90	0.23	49,54,68,76	0
4	MLY	D	121	11/12	0.90	0.23	56,62,68,71	0
1	MLY	A	317	11/12	0.91	0.18	45,50,82,87	0
4	MLY	D	39	11/12	0.91	0.18	48,57,61,64	0
4	MLY	D	212	11/12	0.91	0.21	49,61,72,76	0
4	MLY	D	213	11/12	0.91	0.30	51,62,74,75	0
4	MLY	D	398	11/12	0.91	0.21	46,49,55,56	0
4	MLY	D	48	11/12	0.92	0.17	52,61,65,65	0
3	MLY	C	48	11/12	0.92	0.21	39,48,67,71	0
1	MLY	A	191	11/12	0.93	0.21	29,36,57,60	0
3	MLY	C	121	11/12	0.93	0.16	35,38,45,48	0
1	MLY	A	193	11/12	0.93	0.21	26,32,59,61	0
2	MLY	B	81	11/12	0.93	0.17	25,31,34,36	0
2	MLY	B	162	11/12	0.93	0.18	49,52,61,64	0
1	MLY	A	39	11/12	0.93	0.17	23,30,37,37	0
3	MLY	C	39	11/12	0.93	0.17	30,40,49,56	0
1	MLY	A	121	11/12	0.94	0.12	50,55,63,68	0
3	MLY	C	292	11/12	0.94	0.27	35,38,49,50	0
2	MLY	B	317	11/12	0.94	0.19	22,28,55,56	0
2	MLY	B	155	11/12	0.94	0.15	36,41,46,48	0
4	MLY	D	81	11/12	0.94	0.21	44,53,58,59	0
1	MLY	A	81	11/12	0.94	0.17	24,29,36,45	0
2	MLY	B	193	11/12	0.94	0.24	29,36,60,63	0
4	MLY	D	214	11/12	0.95	0.30	47,54,59,61	0
3	MLY	C	260	11/12	0.95	0.16	42,46,53,59	0
3	MLY	C	44	11/12	0.95	0.14	25,32,40,42	0
3	MLY	C	317	11/12	0.95	0.15	28,32,57,58	0
3	MLY	C	155	11/12	0.95	0.26	55,61,68,70	0
3	MLY	C	81	11/12	0.95	0.16	27,30,50,53	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MLY	B	135	11/12	0.96	0.18	35,42,51,52	0
2	MLY	B	337	11/12	0.96	0.14	23,28,39,40	0
2	MLY	B	154	11/12	0.96	0.17	34,38,57,60	0
1	MLY	A	292	11/12	0.96	0.15	26,28,38,41	0
2	MLY	B	292	11/12	0.96	0.23	29,36,47,51	0
1	MLY	A	44	11/12	0.97	0.14	30,35,40,44	0
2	MLY	B	44	11/12	0.98	0.11	22,29,34,38	0
2	MLY	B	121	11/12	0.98	0.14	29,33,38,40	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.