



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 12:01 AM EST

PDB ID : 3VI3
Title : Crystal structure of alpha5beta1 integrin headpiece (ligand-free form)
Authors : Nagae, M.; Nogi, T.; Takagi, J.
Deposited on : unknown
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

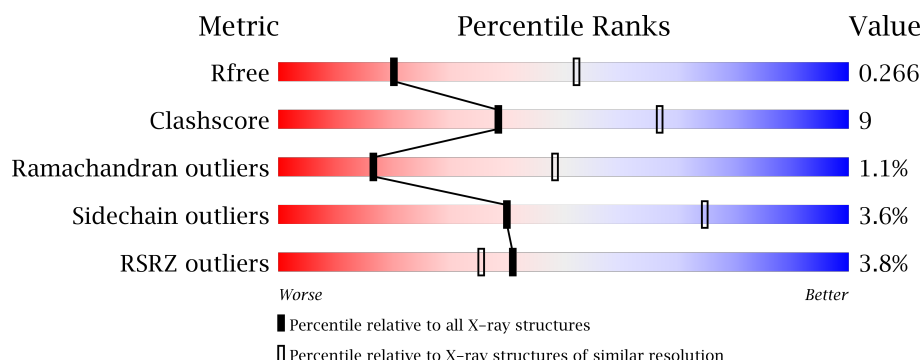
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	632	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• 5%</div> </div> </div>
1	C	632	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• 7%</div> </div> </div>
2	B	454	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>• 6%</div> </div> </div>
2	D	454	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>
3	E	219	<div> <div></div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	L	219	
4	F	218	
4	H	218	

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
9	MG	B	2003	-	-	-	X
9	MG	D	2003	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 22803 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 Integrin alpha-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4567	2892	768	893	14			
1	C	589	Total	C	N	O	S	0	0	0
			4470	2832	748	876	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	624	GLY	-	EXPRESSION TAG	UNP P08648
A	625	GLY	-	EXPRESSION TAG	UNP P08648
A	626	LEU	-	EXPRESSION TAG	UNP P08648
A	627	GLU	-	EXPRESSION TAG	UNP P08648
A	628	ASN	-	EXPRESSION TAG	UNP P08648
A	629	LEU	-	EXPRESSION TAG	UNP P08648
A	630	TYR	-	EXPRESSION TAG	UNP P08648
A	631	PHE	-	EXPRESSION TAG	UNP P08648
A	632	GLN	-	EXPRESSION TAG	UNP P08648
C	624	GLY	-	EXPRESSION TAG	UNP P08648
C	625	GLY	-	EXPRESSION TAG	UNP P08648
C	626	LEU	-	EXPRESSION TAG	UNP P08648
C	627	GLU	-	EXPRESSION TAG	UNP P08648
C	628	ASN	-	EXPRESSION TAG	UNP P08648
C	629	LEU	-	EXPRESSION TAG	UNP P08648
C	630	TYR	-	EXPRESSION TAG	UNP P08648
C	631	PHE	-	EXPRESSION TAG	UNP P08648
C	632	GLN	-	EXPRESSION TAG	UNP P08648

- Molecule 2 is a protein called Integrin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3327	2082	567	654	24			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	432	Total	C	N	O	S	0	0	0
			3367	2106	574	663	24			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	92	HIS	THR	SEE REMARK 999	UNP P05556
B	195	THR	SER	SEE REMARK 999	UNP P05556
B	446	GLY	-	EXPRESSION TAG	UNP P05556
B	447	GLY	-	EXPRESSION TAG	UNP P05556
B	448	LEU	-	EXPRESSION TAG	UNP P05556
B	449	GLU	-	EXPRESSION TAG	UNP P05556
B	450	ASN	-	EXPRESSION TAG	UNP P05556
B	451	LEU	-	EXPRESSION TAG	UNP P05556
B	452	TYR	-	EXPRESSION TAG	UNP P05556
B	453	PHE	-	EXPRESSION TAG	UNP P05556
B	454	GLN	-	EXPRESSION TAG	UNP P05556
D	92	HIS	THR	SEE REMARK 999	UNP P05556
D	195	THR	SER	SEE REMARK 999	UNP P05556
D	446	GLY	-	EXPRESSION TAG	UNP P05556
D	447	GLY	-	EXPRESSION TAG	UNP P05556
D	448	LEU	-	EXPRESSION TAG	UNP P05556
D	449	GLU	-	EXPRESSION TAG	UNP P05556
D	450	ASN	-	EXPRESSION TAG	UNP P05556
D	451	LEU	-	EXPRESSION TAG	UNP P05556
D	452	TYR	-	EXPRESSION TAG	UNP P05556
D	453	PHE	-	EXPRESSION TAG	UNP P05556
D	454	GLN	-	EXPRESSION TAG	UNP P05556

- Molecule 3 is a protein called SG/19 Fab fragment (Light chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			
3	E	219	Total	C	N	O	S	0	0	0
			1701	1066	292	335	8			

- Molecule 4 is a protein called SG/19 Fab fragment (Heavy chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

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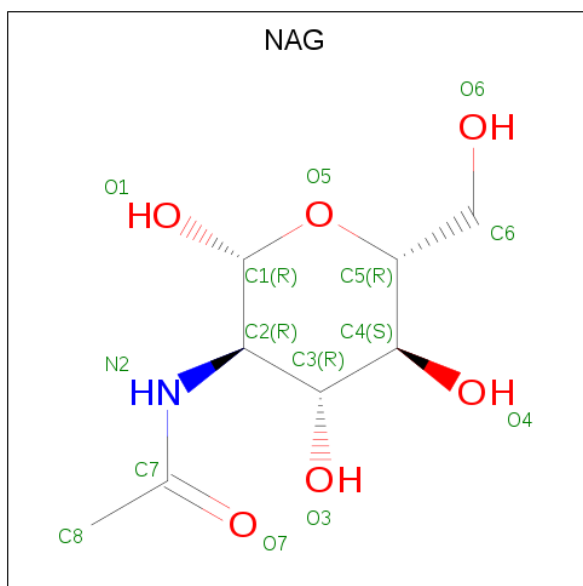
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	218	Total	C	N	O	S	0	0	0
			1651	1051	268	324	8			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		
5	A	4	Total	Ca	0	0
			4	4		
5	D	2	Total	Ca	0	0
			2	2		
5	C	4	Total	Ca	0	0
			4	4		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



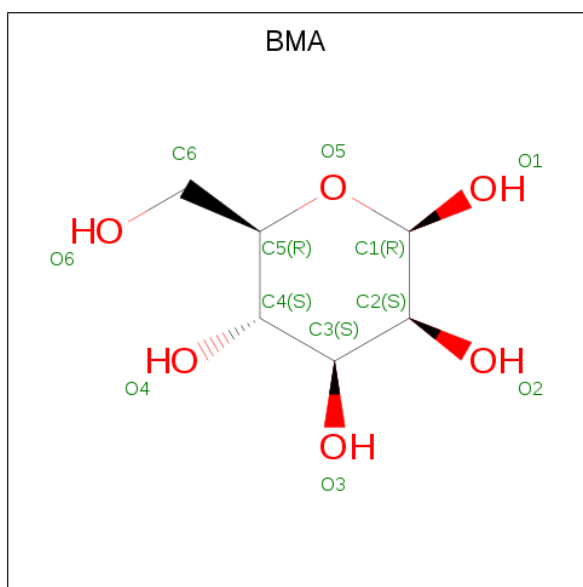
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

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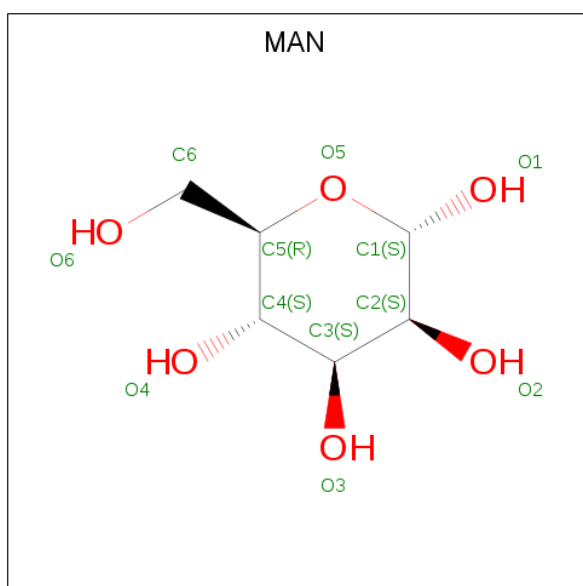
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	A	1	Total	C	O	0	0
			11	6	5		

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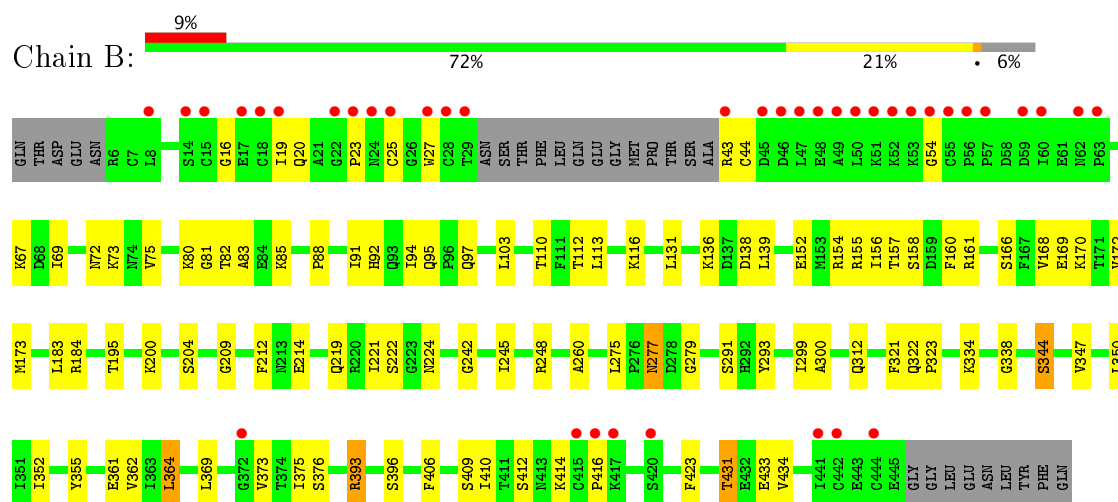
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

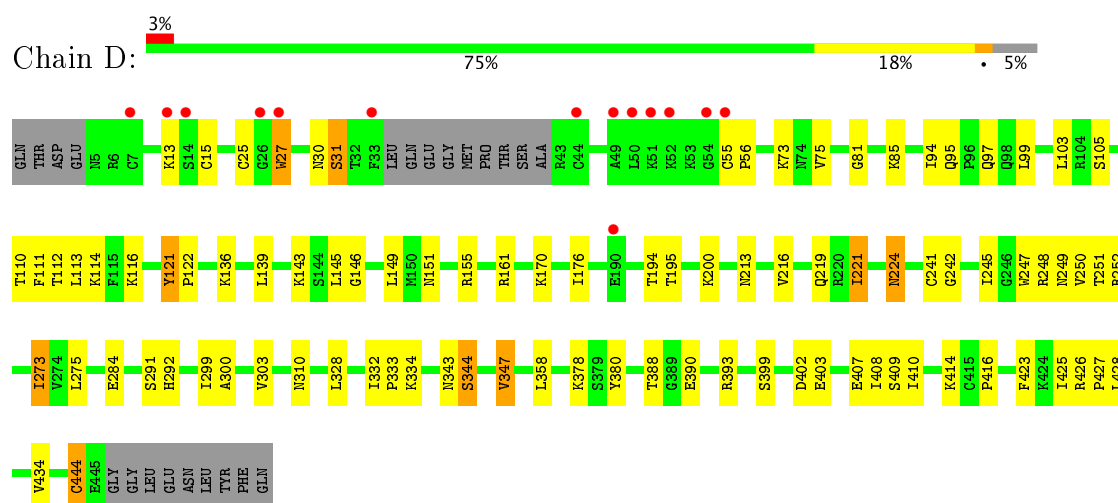
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

LEU
GLN
LEU
GLU
VAL
PHE
GLY
GLU
GLN
GLN
ASN
GLY
GLY
LEU
GLU
ASN
LEU
LEU
PHE
GLN

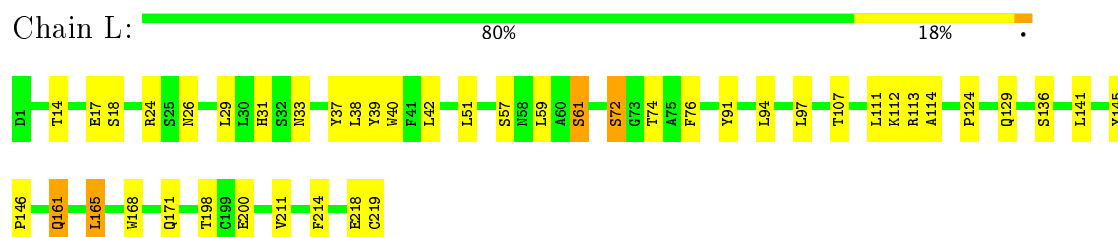
• Molecule 2: Integrin beta-1



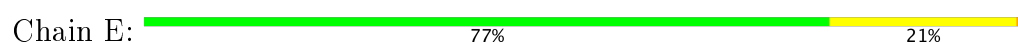
• Molecule 2: Integrin beta-1

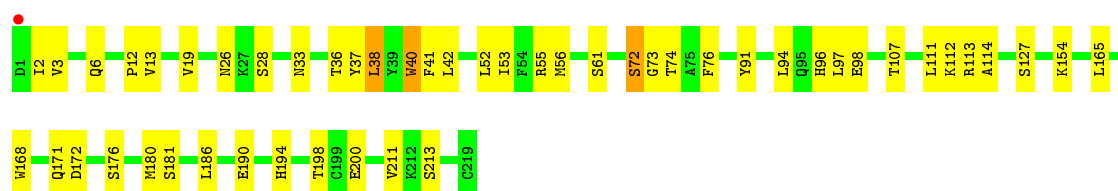


• Molecule 3: SG/19 Fab fragment (Light chain)

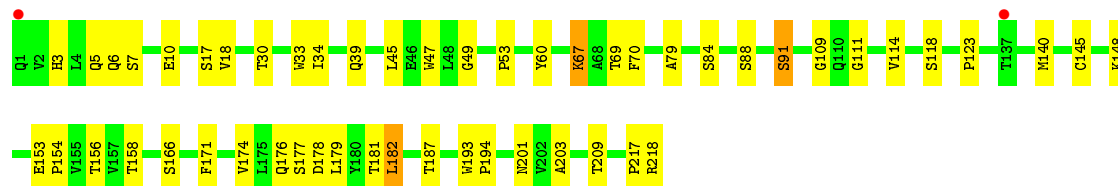
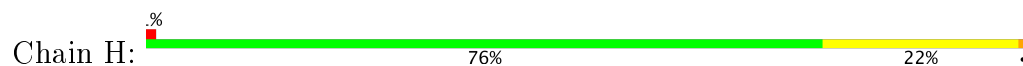


• Molecule 3: SG/19 Fab fragment (Light chain)

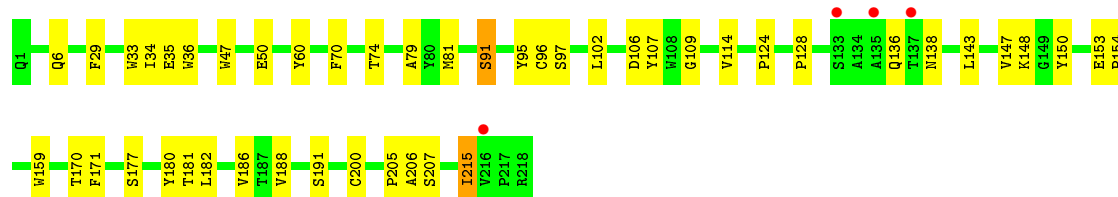
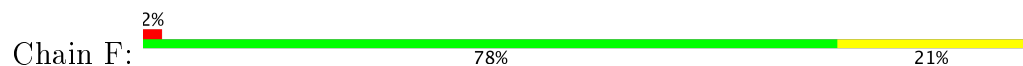




- Molecule 4: SG/19 Fab fragment (Heavy chain)



- Molecule 4: SG/19 Fab fragment (Heavy chain)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.96Å 102.81Å 125.08Å 76.10° 70.19° 71.28°	Depositor
Resolution (Å)	100.00 – 2.90 46.03 – 2.87	Depositor EDS
% Data completeness (in resolution range)	98.9 (100.00-2.90) 93.6 (46.03-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.207 , 0.267 0.206 , 0.266	Depositor DCC
R_{free} test set	4473 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 30.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22803	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, MG, BMA, CA, NAG

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	0.46	4/4684 (0.1%)	0.61	0/6374
1	C	0.47	4/4584 (0.1%)	0.63	0/6240
2	B	0.41	1/3384 (0.0%)	0.58	0/4565
2	D	0.43	1/3425 (0.0%)	0.61	0/4621
3	E	0.49	2/1741 (0.1%)	0.63	0/2364
3	L	0.50	2/1741 (0.1%)	0.63	1/2364 (0.0%)
4	F	0.55	0/1698	0.62	0/2323
4	H	0.55	0/1698	0.64	0/2323
All	All	0.47	14/22955 (0.1%)	0.61	1/31174 (0.0%)

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	C	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	168	TRP	CD2-CE2	5.50	1.48	1.41
1	A	100	TRP	CD2-CE2	5.42	1.47	1.41
1	C	509	TRP	CD2-CE2	5.34	1.47	1.41
1	C	157	TRP	CD2-CE2	5.28	1.47	1.41
3	L	168	TRP	CD2-CE2	5.24	1.47	1.41
1	A	157	TRP	CD2-CE2	5.22	1.47	1.41
3	E	40	TRP	CD2-CE2	5.18	1.47	1.41
3	L	40	TRP	CD2-CE2	5.15	1.47	1.41
1	C	60	TRP	CD2-CE2	5.10	1.47	1.41
2	B	27	TRP	CD2-CE2	5.06	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	27	TRP	CD2-CE2	5.04	1.47	1.41
1	A	121	TRP	CD2-CE2	5.03	1.47	1.41
1	C	121	TRP	CD2-CE2	5.02	1.47	1.41
1	A	406	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	94	LEU	CA-CB-CG	6.05	129.23	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	155	PHE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	4567	0	4363	73	0
1	C	4470	0	4259	81	0
2	B	3327	0	3283	69	0
2	D	3367	0	3317	65	0
3	E	1701	0	1649	38	0
3	L	1701	0	1649	28	0
4	F	1651	0	1610	27	0
4	H	1651	0	1610	28	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
6	A	98	0	89	3	0
6	B	42	0	38	0	0
6	C	112	0	101	0	0
6	D	14	0	13	0	0
7	A	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	11	0	8	0	0
8	A	33	0	29	0	0
8	C	33	0	29	0	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
All	All	22803	0	22055	387	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 (387) 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:94:ILE:HD11	2:B:113:LEU:HD21	1.52	0.91
2:D:110:THR:HG22	2:D:409:SER:CB	2.04	0.88
2:D:73:LYS:H	2:D:97:GLN:HE22	1.22	0.86
1:A:123:THR:HG22	1:A:126:GLU:O	1.76	0.84
1:C:99:GLN:HG3	1:C:116:ALA:HB1	1.59	0.84
4:H:10:GLU:HG2	4:H:18:VAL:HG21	1.58	0.84
1:A:34:SER:HB3	1:A:59:PRO:HA	1.59	0.83
1:C:282:ALA:HB3	2:D:299:ILE:HD12	1.62	0.80
1:C:575:ALA:HB3	1:C:576:PRO:HD3	1.63	0.80
2:D:110:THR:HG22	2:D:409:SER:HB3	1.64	0.80
1:A:512:GLN:HE22	1:A:517:ARG:HB3	1.47	0.80
2:B:85:LYS:HG2	3:E:37:TYR:CZ	2.17	0.80
2:B:338:GLY:HA3	2:B:350:LEU:HD11	1.66	0.78
4:H:67:LYS:HE2	4:H:84:SER:O	1.85	0.77
1:A:303:LEU:HD23	1:A:326:VAL:HG22	1.66	0.77
3:L:111:LEU:H	3:L:171:GLN:HE22	1.31	0.76
1:C:189:GLN:HE22	1:C:222:ALA:H	1.35	0.74
4:F:153:GLU:HG2	4:F:154:PRO:HA	1.69	0.74
1:C:164:CYS:HB2	1:C:185:SER:OG	1.88	0.74
1:C:319:GLN:HB2	1:C:347:GLU:HG3	1.69	0.74
4:H:171:PHE:O	4:H:182:LEU:HD12	1.88	0.74
1:C:461:PHE:HB3	1:C:462:PRO:HD3	1.69	0.72
1:A:310:MET:HG3	2:B:300:ALA:HB2	1.72	0.72
1:A:487:CYS:HB3	1:A:541:GLU:HG2	1.72	0.71
2:B:184:ARG:HA	2:B:195:THR:HG22	1.72	0.71
2:D:73:LYS:N	2:D:97:GLN:HE22	1.89	0.70
3:L:200:GLU:HG2	3:L:211:VAL:HG22	1.73	0.70
2:B:369:LEU:HD11	2:B:375:ILE:HG13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:LEU:HD11	1:C:525:ARG:HD3	1.73	0.70
2:D:73:LYS:H	2:D:97:GLN:NE2	1.90	0.70
2:B:113:LEU:HD11	2:B:434:VAL:HG21	1.74	0.69
4:H:217:PRO:O	4:H:218:ARG:HB2	1.91	0.69
2:B:152:GLU:HG2	2:B:352:ILE:HD11	1.75	0.69
2:B:375:ILE:HG12	2:B:410:ILE:HG12	1.75	0.68
3:L:161:GLN:HG2	3:L:161:GLN:O	1.95	0.67
1:A:282:ALA:HB3	2:B:299:ILE:HD12	1.77	0.67
4:F:171:PHE:O	4:F:182:LEU:HD13	1.95	0.67
3:L:31:HIS:HD2	3:L:33:ASN:H	1.43	0.66
1:A:587:HIS:HD2	1:A:589:GLN:H	1.43	0.66
4:H:10:GLU:CG	4:H:18:VAL:HG21	2.26	0.66
1:A:506:GLN:HG2	1:A:528:THR:HG22	1.79	0.64
3:E:6:GLN:HE21	3:E:107:THR:HG23	1.62	0.64
3:E:198:THR:HG22	3:E:213:SER:CB	2.27	0.64
1:A:293:ASP:O	1:A:367:ASN:HB2	1.98	0.64
2:D:145:LEU:HG	2:D:146:GLY:N	2.12	0.64
2:D:344:SER:O	2:D:347:VAL:HG22	1.98	0.64
1:C:427:GLY:HA3	1:C:580:HIS:CE1	2.34	0.63
2:B:344:SER:O	2:B:347:VAL:HG23	1.98	0.63
1:A:110:SER:HB2	1:A:141:ASN:H	1.64	0.62
1:A:190:GLY:HA3	1:A:231:LEU:HB3	1.82	0.62
1:A:123:THR:HG23	1:A:125:LYS:H	1.64	0.62
1:C:562:PRO:HB3	1:C:599:GLN:HB3	1.82	0.62
3:L:42:LEU:HD13	3:L:91:TYR:CZ	2.34	0.62
3:E:13:VAL:HG21	3:E:19:VAL:CG2	2.31	0.61
1:A:562:PRO:HB3	1:A:599:GLN:HG2	1.83	0.61
2:D:110:THR:HG22	2:D:409:SER:HB2	1.79	0.61
2:B:154:ARG:O	3:E:55:ARG:NH2	2.34	0.61
4:F:6:GLN:HE21	4:F:109:GLY:HA3	1.65	0.61
3:E:3:VAL:HB	3:E:26:ASN:HD22	1.65	0.61
1:C:111:SER:HA	1:C:138:SER:O	2.01	0.60
2:B:155:ARG:HH21	3:E:61:SER:N	2.00	0.60
1:C:487:CYS:HB3	1:C:541:GLU:HB3	1.84	0.60
2:B:170:LYS:HE3	2:B:291:SER:O	2.02	0.59
2:D:241:CYS:HB2	2:D:245:ILE:CD1	2.33	0.59
2:D:170:LYS:HE3	2:D:291:SER:O	2.02	0.59
1:C:193:LEU:HD23	1:C:218:GLN:HG2	1.84	0.59
1:C:427:GLY:HA3	1:C:580:HIS:HE1	1.67	0.59
3:E:113:ARG:HG2	3:E:114:ALA:N	2.17	0.59
4:H:177:SER:O	4:H:179:LEU:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:ILE:CD1	2:B:113:LEU:HD21	2.29	0.59
2:D:176:ILE:HG22	2:D:224:ASN:HB2	1.85	0.59
3:E:97:LEU:HG	3:E:98:GLU:HG2	1.84	0.58
2:B:131:LEU:HD12	2:B:166:SER:HB2	1.84	0.58
1:C:382:GLY:HA3	1:C:415:PHE:O	2.04	0.58
3:E:3:VAL:H	3:E:26:ASN:ND2	2.01	0.58
4:H:158:THR:HB	4:H:201:ASN:HB2	1.85	0.58
4:H:34:ILE:HD13	4:H:79:ALA:HB2	1.84	0.58
1:C:323:ARG:NH1	1:C:343:THR:OG1	2.36	0.58
1:C:424:ASP:OD2	1:C:428:ASN:O	2.22	0.58
2:D:81:GLY:HA2	4:H:33:TRP:CZ2	2.38	0.58
1:C:351:PHE:HA	1:C:373:ALA:HB2	1.86	0.57
1:C:425:LEU:CD2	1:C:445:VAL:HG11	2.34	0.57
2:B:131:LEU:HD12	2:B:166:SER:CB	2.33	0.57
2:D:273:ILE:HD12	2:D:292:HIS:O	2.04	0.57
2:D:247:TRP:HB3	2:D:252:ARG:NE	2.20	0.57
1:C:137:LEU:HD21	1:C:197:GLN:HG2	1.86	0.57
4:H:123:PRO:HB3	4:H:209:THR:HG21	1.86	0.57
1:A:193:LEU:HD23	1:A:218:GLN:HG2	1.87	0.57
3:L:17:GLU:HG2	3:L:18:SER:N	2.19	0.57
3:L:129:GLN:HE22	3:L:136:SER:HB2	1.70	0.56
1:A:107:ALA:CB	1:A:112:ILE:HG22	2.35	0.56
1:A:262:VAL:HG21	1:A:304:VAL:HG21	1.87	0.56
4:F:34:ILE:HD13	4:F:79:ALA:HB2	1.88	0.56
3:E:42:LEU:HD13	3:E:91:TYR:CZ	2.40	0.56
2:D:155:ARG:NH1	3:L:61:SER:HB3	2.20	0.56
2:B:16:GLY:HA2	2:B:19:ILE:HD12	1.86	0.56
2:D:161:ARG:HH12	2:D:248:ARG:HD3	1.70	0.56
1:A:350:ARG:O	1:A:373:ALA:HA	2.06	0.56
1:A:462:PRO:HD2	1:A:482:ILE:HG23	1.88	0.56
1:A:449:ARG:HE	1:A:585:ALA:HB2	1.71	0.55
1:C:502:THR:HG22	1:C:532:THR:HG22	1.87	0.55
1:C:506:GLN:HB2	1:C:566:ALA:HB3	1.88	0.55
1:C:465:PHE:CD1	1:C:550:LEU:HB2	2.42	0.55
1:C:9:ALA:HB3	1:C:445:VAL:HB	1.88	0.55
1:A:319:GLN:HB2	1:A:347:GLU:HG3	1.89	0.55
3:E:198:THR:HG22	3:E:213:SER:HB2	1.89	0.55
4:F:6:GLN:HE22	4:F:95:TYR:HA	1.71	0.55
2:B:85:LYS:HG2	3:E:37:TYR:OH	2.07	0.55
4:H:6:GLN:HE21	4:H:109:GLY:HA3	1.71	0.55
3:E:33:ASN:ND2	3:E:37:TYR:OH	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:148:LYS:HB3	4:H:181:THR:HG23	1.89	0.54
1:C:351:PHE:O	1:C:372:GLY:O	2.24	0.54
4:H:91:SER:HA	4:H:114:VAL:O	2.08	0.54
4:H:153:GLU:HG3	4:H:154:PRO:HA	1.89	0.54
4:F:47:TRP:HZ2	4:F:50:GLU:HG2	1.73	0.54
1:A:27:ARG:HG3	1:A:33:VAL:HG13	1.90	0.54
3:E:2:ILE:HD11	3:E:98:GLU:HG3	1.90	0.53
3:E:6:GLN:NE2	3:E:107:THR:HG23	2.22	0.53
2:D:85:LYS:HB2	3:L:31:HIS:CE1	2.43	0.53
1:A:454:ALA:HA	1:A:489:ASN:O	2.08	0.53
1:C:518:ARG:HB3	1:C:563:ILE:HG12	1.89	0.53
3:E:38:LEU:HD13	3:E:76:PHE:CD2	2.43	0.53
2:D:143:LYS:O	2:D:213:ASN:ND2	2.41	0.53
4:F:124:PRO:HB2	4:F:147:VAL:HG13	1.89	0.53
4:H:6:GLN:NE2	4:H:109:GLY:HA3	2.24	0.53
3:E:13:VAL:HG21	3:E:19:VAL:HG21	1.91	0.53
2:D:112:THR:HG22	2:D:407:GLU:HG3	1.89	0.52
1:A:474:LEU:HG	1:A:475:GLU:H	1.74	0.52
2:D:75:VAL:HG13	2:D:95:GLN:HG3	1.92	0.52
2:B:152:GLU:CD	2:B:155:ARG:NH1	2.63	0.52
2:B:82:THR:HG22	3:E:96:HIS:CE1	2.45	0.52
1:C:465:PHE:HB3	1:C:550:LEU:HD22	1.92	0.52
3:E:198:THR:HG22	3:E:213:SER:OG	2.09	0.52
1:A:536:GLN:HB3	1:A:539:ALA:HB2	1.92	0.52
2:D:410:ILE:HD11	2:D:423:PHE:HZ	1.75	0.52
2:D:247:TRP:HB3	2:D:252:ARG:HE	1.75	0.52
2:B:131:LEU:HD21	2:B:139:LEU:HD13	1.92	0.52
1:C:294:VAL:HG11	1:C:394:LEU:HB2	1.92	0.51
3:E:13:VAL:HG21	3:E:19:VAL:HG22	1.92	0.51
1:C:189:GLN:NE2	1:C:222:ALA:H	2.06	0.51
1:C:358:LEU:HB2	1:C:368:ASP:O	2.10	0.51
1:A:461:PHE:HB3	1:A:462:PRO:HD3	1.93	0.51
1:A:107:ALA:HB2	1:A:112:ILE:HG22	1.91	0.51
1:C:285:PHE:H	1:C:306:ALA:HA	1.75	0.51
2:B:168:VAL:HG21	2:B:222:SER:HB3	1.93	0.51
2:B:312:GLN:HG2	2:B:334:LYS:HG3	1.91	0.51
1:C:575:ALA:CB	1:C:576:PRO:HD3	2.39	0.51
3:E:2:ILE:CD1	3:E:98:GLU:HG3	2.41	0.51
2:B:334:LYS:NZ	2:B:361:GLU:O	2.43	0.51
3:E:111:LEU:H	3:E:171:GLN:HE22	1.57	0.51
4:H:6:GLN:NE2	4:H:111:GLY:H	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:VAL:HG13	1:A:567:LEU:CD1	2.41	0.50
2:B:136:LYS:HG3	2:B:221:ILE:HG21	1.94	0.50
1:C:123:THR:HG22	1:C:124:GLU:H	1.76	0.50
4:H:177:SER:C	4:H:179:LEU:H	2.15	0.50
2:B:275:LEU:HD23	2:B:293:TYR:CE2	2.46	0.50
1:C:249:VAL:HG22	1:C:264:ILE:HG12	1.93	0.50
2:D:414:LYS:O	2:D:416:PRO:HD3	2.10	0.50
4:F:171:PHE:O	4:F:182:LEU:CD1	2.58	0.50
3:L:29:LEU:HA	3:L:97:LEU:HD22	1.94	0.50
1:A:262:VAL:HG21	1:A:304:VAL:CG2	2.42	0.50
2:B:161:ARG:HH11	2:B:248:ARG:HE	1.60	0.50
2:D:155:ARG:HH12	3:L:61:SER:HB3	1.77	0.50
1:A:309:LEU:HD22	1:A:323:ARG:HB2	1.93	0.50
1:A:349:GLY:HA2	1:A:375:PHE:HB2	1.94	0.50
2:B:209:GLY:O	2:B:212:PHE:HB3	2.12	0.50
2:D:145:LEU:HG	2:D:146:GLY:H	1.77	0.50
2:B:155:ARG:O	4:F:102:LEU:HD11	2.11	0.50
2:B:364:LEU:O	2:B:393:ARG:HD3	2.11	0.50
1:C:255:GLY:H	1:C:260:GLY:HA2	1.77	0.49
1:A:575:ALA:N	1:A:576:PRO:HD3	2.26	0.49
1:C:108:HIS:CE1	1:C:174:LYS:O	2.65	0.49
1:C:12:SER:HB3	1:C:442:LYS:HG2	1.93	0.49
1:C:263:THR:HG22	1:C:275:ASN:OD1	2.11	0.49
4:H:193:TRP:CD1	4:H:194:PRO:HA	2.47	0.49
2:D:85:LYS:HG2	3:L:37:TYR:CZ	2.47	0.49
2:D:99:LEU:HD11	2:D:111:PHE:CG	2.47	0.49
2:D:410:ILE:CD1	2:D:423:PHE:HZ	2.25	0.49
1:C:173:THR:OG1	1:C:177:ARG:HB3	2.13	0.49
4:F:159:TRP:CZ3	4:F:200:CYS:HB3	2.47	0.49
2:B:113:LEU:HD22	2:B:364:LEU:HD21	1.93	0.49
2:B:113:LEU:CD1	2:B:434:VAL:HG21	2.41	0.49
2:D:248:ARG:C	2:D:250:VAL:H	2.15	0.49
4:F:70:PHE:CE1	4:F:81:MET:HE2	2.47	0.49
3:L:113:ARG:HG2	3:L:114:ALA:N	2.27	0.49
2:D:121:TYR:CD2	2:D:122:PRO:HD2	2.48	0.49
2:B:375:ILE:HG22	2:B:376:SER:N	2.27	0.48
4:F:91:SER:HA	4:F:114:VAL:O	2.11	0.48
1:C:411:THR:HB	1:C:412:PRO:HD2	1.94	0.48
3:E:40:TRP:HB2	3:E:53:ILE:HB	1.96	0.48
3:L:165:LEU:HD11	4:H:174:VAL:HB	1.95	0.48
3:E:190:GLU:O	3:E:194:HIS:HD2	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:145:LEU:HD11	2:D:149:LEU:HB2	1.96	0.48
2:D:85:LYS:HG2	3:L:37:TYR:CE2	2.49	0.48
1:A:113:LEU:HD11	1:A:135:CYS:HB3	1.96	0.47
1:C:430:TYR:CE1	1:C:450:PRO:HA	2.47	0.47
2:B:81:GLY:HA2	4:F:33:TRP:CZ2	2.48	0.47
1:C:323:ARG:HD2	1:C:325:TYR:CZ	2.50	0.47
4:F:148:LYS:HB3	4:F:181:THR:HG23	1.96	0.47
2:B:172:VAL:HG12	2:B:173:MET:O	2.14	0.47
1:C:282:ALA:HB3	2:D:299:ILE:CD1	2.38	0.47
2:D:399:SER:O	2:D:402:ASP:HB2	2.13	0.47
3:L:38:LEU:HD13	3:L:76:PHE:CD2	2.49	0.47
1:C:99:GLN:HG3	1:C:116:ALA:CB	2.40	0.47
2:B:88:PRO:HA	2:B:91:ILE:HD12	1.95	0.47
1:A:512:GLN:NE2	1:A:517:ARG:HB3	2.22	0.47
4:F:29:PHE:CE1	4:F:34:ILE:HD11	2.49	0.47
1:A:460:ILE:HG23	1:A:482:ILE:CG2	2.45	0.47
2:B:75:VAL:CG1	2:B:116:LYS:HD3	2.45	0.47
4:F:170:THR:HG22	4:F:182:LEU:HD11	1.96	0.47
3:L:14:THR:HG23	3:L:112:LYS:HB3	1.96	0.47
1:A:511:LYS:C	1:A:513:LYS:H	2.18	0.47
3:L:24:ARG:HA	3:L:74:THR:O	2.15	0.47
1:C:498:SER:HB3	1:C:536:GLN:HE21	1.80	0.46
2:D:380:TYR:HE2	2:D:407:GLU:HB2	1.80	0.46
1:C:19:PHE:CE1	1:C:37:VAL:HG11	2.50	0.46
1:C:77:SER:HB2	1:C:94:GLU:HG3	1.97	0.46
1:A:356:THR:CG2	1:A:419:LEU:HB3	2.46	0.46
2:B:375:ILE:HD11	2:B:423:PHE:CE1	2.49	0.46
3:L:17:GLU:HG2	3:L:18:SER:H	1.77	0.46
2:B:69:ILE:HG21	2:B:72:ASN:HD22	1.81	0.46
2:B:169:GLU:HG3	2:B:170:LYS:N	2.30	0.46
4:F:128:PRO:HB3	4:F:215:ILE:HG22	1.98	0.46
1:A:153:SER:OG	1:A:161:GLN:NE2	2.48	0.46
1:A:269:ASP:O	1:A:270:ILE:C	2.54	0.46
2:B:157:THR:CG2	2:B:160:PHE:HB2	2.46	0.46
1:C:310:MET:HG3	2:D:300:ALA:HB2	1.97	0.46
1:C:462:PRO:HD2	1:C:482:ILE:HG23	1.98	0.46
3:E:113:ARG:HG2	3:E:114:ALA:H	1.81	0.46
4:H:3:HIS:NE2	4:H:5:GLN:HG2	2.31	0.46
1:A:465:PHE:CE1	1:A:550:LEU:HB2	2.50	0.46
1:C:323:ARG:HD3	1:C:341:THR:HB	1.98	0.46
1:C:382:GLY:HA3	1:C:415:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:GLN:O	1:C:164:CYS:HB3	2.16	0.45
1:C:303:LEU:HG	1:C:326:VAL:HG22	1.99	0.45
2:B:152:GLU:HA	2:B:155:ARG:NH1	2.30	0.45
4:F:205:PRO:C	4:F:207:SER:H	2.19	0.45
2:B:338:GLY:CA	2:B:350:LEU:HD11	2.42	0.45
1:C:57:LEU:HB2	1:C:70:ILE:HD11	1.97	0.45
4:H:30:THR:HA	4:H:53:PRO:HB2	1.98	0.45
2:D:161:ARG:NH1	2:D:248:ARG:HD3	2.31	0.45
2:D:94:ILE:HD12	2:D:434:VAL:HG23	1.97	0.45
3:L:31:HIS:CD2	3:L:33:ASN:H	2.29	0.45
1:A:460:ILE:HG23	1:A:482:ILE:HG21	1.99	0.45
1:A:508:ASP:O	1:A:512:GLN:HG2	2.16	0.45
2:B:376:SER:HB3	2:B:409:SER:HB3	1.98	0.45
1:C:453:SER:H	1:C:492:GLY:HA3	1.81	0.45
2:B:138:ASP:OD2	2:B:344:SER:HB2	2.16	0.45
2:D:221:ILE:HG13	2:D:221:ILE:H	1.31	0.45
2:D:30:ASN:O	2:D:31:SER:HB3	2.16	0.45
1:A:164:CYS:HB2	1:A:185:SER:OG	2.17	0.45
2:B:112:THR:HA	2:B:406:PHE:O	2.17	0.45
1:A:412:PRO:HG2	2:B:275:LEU:HD11	1.98	0.45
2:D:200:LYS:NZ	2:D:219:GLN:HE22	2.15	0.45
1:A:241:SER:CB	6:A:2008:NAG:H82	2.47	0.45
1:A:99:GLN:HG3	1:A:116:ALA:HB1	1.99	0.45
2:B:277:ASN:HD22	2:B:279:GLY:H	1.65	0.45
2:D:408:ILE:HD13	2:D:425:ILE:HD13	1.99	0.45
2:B:200:LYS:NZ	2:B:219:GLN:HE22	2.15	0.44
1:C:119:TYR:OH	1:C:152:ARG:NH1	2.49	0.44
4:H:17:SER:HB2	4:H:84:SER:HA	1.99	0.44
1:A:335:GLU:HA	1:A:336:PRO:HD3	1.80	0.44
1:A:16:GLY:N	1:A:441:ASP:OD1	2.48	0.44
2:B:110:THR:HG22	2:B:409:SER:OG	2.18	0.44
1:C:224:SER:HA	1:C:227:ASP:OD2	2.17	0.44
1:C:284:TYR:HB3	1:C:287:TYR:HB2	1.99	0.44
2:D:143:LYS:HA	2:D:216:VAL:HG13	1.98	0.44
3:L:218:GLU:O	3:L:219:CYS:SG	2.76	0.44
2:B:312:GLN:HG2	2:B:334:LYS:CG	2.46	0.44
4:F:136:GLN:HG3	4:F:138:ASN:O	2.18	0.44
2:B:431:THR:O	2:B:433:GLU:HG3	2.17	0.44
1:C:361:LEU:HB3	1:C:368:ASP:OD1	2.18	0.44
2:D:252:ARG:HH11	2:D:310:ASN:H	1.66	0.44
1:A:428:ASN:ND2	1:A:430:TYR:HB2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:GLU:HG3	1:A:530:THR:HG22	1.98	0.44
2:B:158:SER:HA	3:E:55:ARG:NH1	2.33	0.44
2:D:94:ILE:HA	2:D:114:LYS:O	2.17	0.44
3:E:165:LEU:HA	3:E:165:LEU:HD12	1.90	0.44
1:A:460:ILE:HD11	1:A:565:ILE:HG13	1.99	0.44
2:B:83:ALA:HA	2:B:85:LYS:HZ3	1.83	0.44
4:H:140:MET:HB3	4:H:187:THR:HG22	2.00	0.44
1:A:503:VAL:HG13	1:A:567:LEU:HD11	2.00	0.43
2:B:25:CYS:HB3	2:B:44:CYS:SG	2.58	0.43
1:C:382:GLY:CA	1:C:415:PHE:HB3	2.48	0.43
3:L:111:LEU:H	3:L:171:GLN:NE2	2.08	0.43
1:A:474:LEU:HD12	1:A:525:ARG:HD3	2.00	0.43
2:D:103:LEU:HD21	2:D:410:ILE:HG22	2.00	0.43
2:D:344:SER:O	2:D:347:VAL:CG2	2.66	0.43
1:C:3:LEU:HD22	1:C:446:TYR:HB3	1.99	0.43
3:E:171:GLN:OE1	3:E:176:SER:HB2	2.18	0.43
3:L:39:TYR:HD1	3:L:51:LEU:HD11	1.82	0.43
2:D:334:LYS:HG3	2:D:428:LEU:HB3	2.00	0.43
3:E:72:SER:OG	3:E:73:GLY:N	2.52	0.43
1:A:195:ALA:HB2	1:A:216:GLN:HG3	2.00	0.43
1:A:235:VAL:HA	1:A:249:VAL:O	2.19	0.43
1:C:358:LEU:HD11	1:C:370:ALA:HB2	2.00	0.43
1:C:99:GLN:HB2	1:C:119:TYR:HA	2.00	0.43
2:D:194:THR:HG22	2:D:195:THR:O	2.18	0.43
2:D:334:LYS:NZ	2:D:358:LEU:O	2.51	0.43
3:E:154:LYS:HB2	3:E:198:THR:OG1	2.19	0.43
4:H:60:TYR:CE2	4:H:70:PHE:CD2	3.06	0.43
2:B:72:ASN:OD1	2:B:95:GLN:HG3	2.19	0.43
1:C:157:TRP:CG	1:C:158:ALA:N	2.85	0.43
4:F:60:TYR:CE2	4:F:70:PHE:CD2	3.07	0.43
4:F:35:GLU:O	4:F:96:CYS:HA	2.19	0.43
4:F:97:SER:HB2	4:F:107:TYR:O	2.18	0.43
1:A:1:PHE:HA	1:A:400:GLN:HB2	2.00	0.43
2:D:390:GLU:H	2:D:390:GLU:CD	2.22	0.43
1:A:241:SER:HB2	6:A:2008:NAG:C8	2.48	0.43
1:A:578:ASP:CG	1:A:579:SER:H	2.23	0.43
1:A:580:HIS:O	1:A:582:LEU:N	2.52	0.43
2:B:73:LYS:HD3	2:B:92:HIS:CD2	2.53	0.43
1:C:258:THR:OG1	1:C:281:MET:HG3	2.18	0.43
4:F:143:LEU:HB3	4:F:215:ILE:HD12	2.00	0.43
1:C:24:GLU:HB3	1:C:36:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:217:PRO:O	4:H:218:ARG:CB	2.65	0.42
1:A:453:SER:HB3	1:A:587:HIS:HB2	2.01	0.42
2:D:378:LYS:HG2	2:D:388:THR:HG22	2.00	0.42
2:D:75:VAL:HG22	2:D:95:GLN:HE21	1.84	0.42
1:C:130:ASP:OD1	1:C:162:GLY:HA3	2.19	0.42
2:D:95:GLN:HB2	2:D:114:LYS:HB2	2.01	0.42
3:L:145:TYR:CG	3:L:146:PRO:HA	2.55	0.42
1:A:85:SER:O	1:A:87:SER:N	2.52	0.42
1:A:95:TYR:OH	1:A:122:ARG:HB2	2.19	0.42
1:C:264:ILE:HD11	1:C:302:LEU:HD22	2.00	0.42
3:E:42:LEU:HB2	3:E:52:LEU:HD11	2.01	0.42
3:E:200:GLU:HG2	3:E:211:VAL:HG22	2.00	0.42
4:H:156:THR:OG1	4:H:203:ALA:HB3	2.19	0.42
1:C:19:PHE:CZ	1:C:37:VAL:HG11	2.55	0.42
3:E:180:MET:HG2	3:E:181:SER:N	2.35	0.42
1:A:474:LEU:CG	1:A:475:GLU:H	2.33	0.42
2:D:151:ASN:HD21	3:L:59:LEU:H	1.66	0.42
2:D:332:ILE:HA	2:D:333:PRO:HD3	1.86	0.42
3:L:124:PRO:HB3	3:L:214:PHE:CZ	2.55	0.42
2:D:299:ILE:O	2:D:303:VAL:HG23	2.19	0.42
3:E:12:PRO:HB2	3:E:112:LYS:HG3	2.01	0.42
3:E:172:ASP:O	3:E:176:SER:HA	2.19	0.42
1:C:356:THR:HG22	1:C:370:ALA:HB3	2.02	0.42
1:C:23:VAL:HG23	1:C:420:ARG:HB2	2.02	0.42
3:E:41:PHE:HE2	3:E:94:LEU:HB3	1.84	0.42
1:C:577:VAL:HG22	1:C:583:ARG:HE	1.85	0.41
1:C:569:PHE:HB2	1:C:592:SER:HB2	2.02	0.41
3:E:190:GLU:O	3:E:194:HIS:CD2	2.73	0.41
4:F:186:VAL:HG22	4:F:188:VAL:HG23	2.02	0.41
2:B:156:ILE:HG21	2:B:355:TYR:CE2	2.56	0.41
1:A:241:SER:HB2	6:A:2008:NAG:H82	2.03	0.41
1:C:108:HIS:HE1	1:C:174:LYS:O	2.03	0.41
2:B:260:ALA:HA	2:B:321:PHE:CE2	2.55	0.41
4:F:124:PRO:HA	4:F:150:TYR:HB3	2.02	0.41
4:F:36:TRP:CZ3	4:F:96:CYS:HB3	2.54	0.41
1:A:150:PRO:HB3	1:A:216:GLN:OE1	2.20	0.41
1:C:293:ASP:O	1:C:367:ASN:HB2	2.21	0.41
2:B:375:ILE:CG2	2:B:376:SER:N	2.83	0.41
1:C:507:LEU:HD23	1:C:565:ILE:HD13	2.02	0.41
2:D:15:CYS:HB3	2:D:444:CYS:HB2	1.97	0.41
1:A:123:THR:CG2	1:A:126:GLU:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:PRO:HD3	1:A:399:SER:HB3	2.01	0.41
1:C:323:ARG:HH11	1:C:323:ARG:HG3	1.86	0.41
2:B:20:GLN:O	2:B:414:LYS:HE2	2.20	0.41
1:C:131:PRO:O	1:C:164:CYS:O	2.39	0.41
2:D:426:ARG:HA	2:D:427:PRO:HD3	1.99	0.41
1:A:495:VAL:HG12	1:A:496:ALA:H	1.85	0.41
1:A:479:VAL:HG12	1:A:552:ASN:HB2	2.02	0.41
2:D:55:CYS:HA	2:D:56:PRO:HD3	1.86	0.41
3:L:141:LEU:N	3:L:141:LEU:HD12	2.36	0.41
2:B:103:LEU:HD21	2:B:412:SER:HB3	2.03	0.41
2:B:277:ASN:ND2	2:B:279:GLY:H	2.18	0.41
2:D:328:LEU:HG	2:D:332:ILE:HD12	2.03	0.41
3:L:14:THR:O	3:L:17:GLU:HB3	2.21	0.41
1:A:46:GLN:HA	1:A:47:PRO:HD2	1.91	0.41
1:C:40:PRO:HA	1:C:101:PHE:O	2.20	0.41
2:D:116:LYS:HB2	2:D:403:GLU:HG2	2.02	0.41
2:D:343:ASN:O	2:D:344:SER:HB2	2.21	0.41
4:H:39:GLN:HB2	4:H:45:LEU:HD23	2.02	0.41
4:H:47:TRP:CH2	4:H:49:GLY:HA2	2.56	0.40
1:A:397:LYS:HA	1:A:398:PRO:HD3	1.82	0.40
1:A:404:PRO:HD3	1:A:415:PHE:CG	2.56	0.40
2:B:204:SER:HB2	2:B:245:ILE:O	2.21	0.40
2:B:322:GLN:N	2:B:323:PRO:HD2	2.37	0.40
1:C:356:THR:CG2	1:C:370:ALA:HB3	2.51	0.40
2:D:161:ARG:HH12	2:D:248:ARG:CD	2.33	0.40
1:A:577:VAL:HG13	1:A:581:GLY:HA2	2.04	0.40
1:C:340:LEU:HG	1:C:341:THR:N	2.36	0.40
2:B:67:LYS:HD3	2:B:110:THR:O	2.21	0.40
4:F:150:TYR:CE1	4:F:180:TYR:HB2	2.57	0.40
2:B:369:LEU:HD13	2:B:373:VAL:HG12	2.04	0.40
2:B:43:ARG:HH11	2:B:43:ARG:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	599/632 (95%)	538 (90%)	53 (9%)	8 (1%)	14	43
1	C	583/632 (92%)	515 (88%)	59 (10%)	9 (2%)	12	39
2	B	423/454 (93%)	380 (90%)	39 (9%)	4 (1%)	20	54
2	D	428/454 (94%)	381 (89%)	42 (10%)	5 (1%)	15	46
3	E	217/219 (99%)	210 (97%)	6 (3%)	1 (0%)	32	68
3	L	217/219 (99%)	204 (94%)	11 (5%)	2 (1%)	20	54
4	F	216/218 (99%)	192 (89%)	23 (11%)	1 (0%)	32	68
4	H	216/218 (99%)	198 (92%)	16 (7%)	2 (1%)	20	54
All	All	2899/3046 (95%)	2618 (90%)	249 (9%)	32 (1%)	17	48

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	86	SER
2	B	416	PRO
1	C	256	ASN
1	C	285	PHE
1	C	575	ALA
2	D	31	SER
2	D	105	SER
4	H	178	ASP
3	E	72	SER
1	A	350	ARG
1	A	476	GLY
1	A	576	PRO
1	A	581	GLY
2	B	242	GLY
1	C	51	GLN
2	D	242	GLY
1	A	64	PRO
2	D	249	ASN
3	L	26	ASN
3	L	72	SER
4	F	206	ALA
1	A	243	ASP
1	A	270	ILE
2	B	54	GLY

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Mol	Chain	Res	Type
1	C	31	ASP
1	C	64	PRO
2	D	13	LYS
4	H	176	GLN
1	C	351	PHE
2	B	23	PRO
1	C	270	ILE
1	C	495	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	486/513 (95%)	464 (96%)	22 (4%)	32	66
1	C	476/513 (93%)	465 (98%)	11 (2%)	56	85
2	B	379/402 (94%)	367 (97%)	12 (3%)	44	78
2	D	384/402 (96%)	368 (96%)	16 (4%)	34	69
3	E	194/194 (100%)	187 (96%)	7 (4%)	40	75
3	L	194/194 (100%)	187 (96%)	7 (4%)	40	75
4	F	186/186 (100%)	180 (97%)	6 (3%)	44	78
4	H	186/186 (100%)	177 (95%)	9 (5%)	30	64
All	All	2485/2590 (96%)	2395 (96%)	90 (4%)	40	75

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	33	VAL
1	A	77	SER
1	A	118	LEU
1	A	121	TRP
1	A	122	ARG
1	A	164	CYS

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Mol	Chain	Res	Type
1	A	180	LEU
1	A	193	LEU
1	A	270	ILE
1	A	283	SER
1	A	309	LEU
1	A	312	ARG
1	A	328	LEU
1	A	340	LEU
1	A	413	ASP
1	A	459	THR
1	A	471	SER
1	A	474	LEU
1	A	488	LEU
1	A	502	THR
1	A	588	TYR
2	B	80	LYS
2	B	97	GLN
2	B	183	LEU
2	B	214	GLU
2	B	224	ASN
2	B	277	ASN
2	B	344	SER
2	B	362	VAL
2	B	364	LEU
2	B	393	ARG
2	B	396	SER
2	B	431	THR
1	C	113	LEU
1	C	121	TRP
1	C	139	THR
1	C	144	ARG
1	C	164	CYS
1	C	243	ASP
1	C	284	TYR
1	C	432	ASP
1	C	459	THR
1	C	475	GLU
1	C	479	VAL
2	D	25	CYS
2	D	27	TRP
2	D	113	LEU
2	D	121	TYR

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Mol	Chain	Res	Type
2	D	136	LYS
2	D	139	LEU
2	D	221	ILE
2	D	224	ASN
2	D	251	THR
2	D	273	ILE
2	D	275	LEU
2	D	284	GLU
2	D	344	SER
2	D	347	VAL
2	D	393	ARG
2	D	444	CYS
3	L	57	SER
3	L	61	SER
3	L	72	SER
3	L	107	THR
3	L	161	GLN
3	L	165	LEU
3	L	198	THR
4	H	7	SER
4	H	67	LYS
4	H	69	THR
4	H	88	SER
4	H	91	SER
4	H	118	SER
4	H	145	CYS
4	H	166	SER
4	H	182	LEU
3	E	28	SER
3	E	36	THR
3	E	38	LEU
3	E	56	MET
3	E	74	THR
3	E	127	SER
3	E	186	LEU
4	F	74	THR
4	F	91	SER
4	F	106	ASP
4	F	177	SER
4	F	191	SER
4	F	215	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	161	GLN
1	A	165	GLN
1	A	218	GLN
1	A	329	GLN
1	A	400	GLN
1	A	512	GLN
1	A	587	HIS
2	B	11	ASN
2	B	92	HIS
2	B	219	GLN
2	B	277	ASN
2	B	301	HIS
2	B	312	GLN
1	C	108	HIS
1	C	161	GLN
1	C	165	GLN
1	C	189	GLN
1	C	197	GLN
1	C	400	GLN
1	C	489	ASN
1	C	512	GLN
1	C	536	GLN
1	C	580	HIS
2	D	20	GLN
2	D	92	HIS
2	D	95	GLN
2	D	97	GLN
2	D	151	ASN
2	D	213	ASN
2	D	219	GLN
2	D	309	ASN
2	D	312	GLN
2	D	383	ASN
3	L	31	HIS
3	L	129	GLN
3	L	171	GLN
4	H	5	GLN
4	H	6	GLN
3	E	26	ASN
3	E	33	ASN
3	E	129	GLN

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Mol	Chain	Res	Type
3	E	171	GLN
3	E	194	HIS
4	F	6	GLN
4	F	169	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 41 ligands modelled in this entry, 14 are monoatomic - leaving 27 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	NAG	A	2005	1	14,14,15	0.56	0	15,19,21	0.93	0
6	NAG	A	2006	1	14,14,15	0.48	0	15,19,21	1.02	1 (6%)
6	NAG	A	2007	1	14,14,15	0.46	0	15,19,21	0.98	0
6	NAG	A	2008	1	14,14,15	0.37	0	15,19,21	1.97	2 (13%)
6	NAG	A	2009	1,6	14,14,15	0.78	0	15,19,21	1.25	1 (6%)
6	NAG	A	2010	7,6	14,14,15	0.61	0	15,19,21	2.55	5 (33%)
7	BMA	A	2011	8,6	11,11,12	0.41	0	13,15,17	0.63	0
8	MAN	A	2012	7	11,11,12	0.62	0	13,15,17	0.66	0
8	MAN	A	2013	8,7	11,11,12	0.61	0	13,15,17	0.98	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	A	2014	8	11,11,12	0.65	0	13,15,17	1.12	1 (7%)
6	NAG	A	2015	1	14,14,15	0.43	0	15,19,21	1.91	1 (6%)
6	NAG	B	2004	2	14,14,15	0.53	0	15,19,21	1.24	1 (6%)
6	NAG	B	2005	2,6	14,14,15	0.55	0	15,19,21	0.76	0
6	NAG	B	2006	6	14,14,15	0.52	0	15,19,21	0.75	0
6	NAG	C	2005	1,6	14,14,15	0.58	0	15,19,21	1.19	1 (6%)
6	NAG	C	2006	6	14,14,15	0.51	0	15,19,21	0.98	1 (6%)
6	NAG	C	2007	1	14,14,15	0.50	0	15,19,21	1.08	1 (6%)
6	NAG	C	2008	1	14,14,15	0.52	0	15,19,21	1.20	1 (6%)
6	NAG	C	2009	1	14,14,15	0.60	0	15,19,21	0.98	0
6	NAG	C	2010	1,6	14,14,15	0.63	0	15,19,21	1.36	3 (20%)
6	NAG	C	2011	7,6	14,14,15	0.52	0	15,19,21	2.92	4 (26%)
7	BMA	C	2012	8,6	11,11,12	0.44	0	13,15,17	1.24	2 (15%)
8	MAN	C	2013	7	11,11,12	0.71	0	13,15,17	1.23	3 (23%)
8	MAN	C	2014	8,7	11,11,12	0.70	0	13,15,17	1.48	2 (15%)
8	MAN	C	2015	8	11,11,12	0.57	0	13,15,17	1.25	2 (15%)
6	NAG	C	2016	1	14,14,15	0.43	0	15,19,21	1.35	1 (6%)
6	NAG	D	2004	2	14,14,15	0.48	0	15,19,21	1.20	1 (6%)

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	NAG	A	2005	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2006	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2007	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2009	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2010	7,6	-	0/6/23/26	0/1/1/1
7	BMA	A	2011	8,6	-	0/2/19/22	0/1/1/1
8	MAN	A	2012	7	-	0/2/19/22	0/1/1/1
8	MAN	A	2013	8,7	-	0/2/19/22	0/1/1/1
8	MAN	A	2014	8	-	0/2/19/22	0/1/1/1
6	NAG	A	2015	1	-	0/6/23/26	0/1/1/1
6	NAG	B	2004	2	-	0/6/23/26	0/1/1/1
6	NAG	B	2005	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	2006	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	2005	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	2006	6	-	0/6/23/26	0/1/1/1
6	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2009	1	-	0/6/23/26	0/1/1/1
6	NAG	C	2010	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	2011	7,6	-	0/6/23/26	0/1/1/1
7	BMA	C	2012	8,6	-	0/2/19/22	0/1/1/1
8	MAN	C	2013	7	-	0/2/19/22	0/1/1/1
8	MAN	C	2014	8,7	-	0/2/19/22	0/1/1/1
8	MAN	C	2015	8	-	0/2/19/22	0/1/1/1
6	NAG	C	2016	1	-	0/6/23/26	0/1/1/1
6	NAG	D	2004	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2011	NAG	C4-C3-C2	-5.89	102.39	111.02
6	A	2010	NAG	C4-C3-C2	-5.81	102.50	111.02
6	A	2010	NAG	O5-C1-C2	-3.90	106.05	111.47
6	A	2009	NAG	O5-C1-C2	-2.95	107.36	111.47
7	C	2012	BMA	C1-C2-C3	-2.51	106.47	109.65
7	C	2012	BMA	O5-C1-C2	-2.37	107.07	110.79
6	A	2008	NAG	C6-C5-C4	-2.19	107.88	113.00
6	C	2011	NAG	C3-C4-C5	2.03	113.80	110.22
8	C	2015	MAN	C3-C4-C5	2.05	113.83	110.22
6	A	2006	NAG	C1-O5-C5	2.05	115.00	112.17
8	C	2013	MAN	C2-C3-C4	2.07	114.48	110.88
6	C	2010	NAG	C4-C3-C2	2.07	114.05	111.02
6	A	2010	NAG	C1-O5-C5	2.09	115.04	112.17
6	A	2010	NAG	O3-C3-C2	2.11	113.91	109.39
8	C	2013	MAN	C1-C2-C3	2.12	112.34	109.65
8	A	2014	MAN	C1-O5-C5	2.13	115.11	112.17
6	C	2005	NAG	C1-O5-C5	2.18	115.17	112.17
6	C	2006	NAG	C1-O5-C5	2.25	115.27	112.17
6	C	2010	NAG	C3-C4-C5	2.35	114.35	110.22
8	C	2013	MAN	C3-C4-C5	2.41	114.47	110.22
8	C	2014	MAN	C2-C3-C4	2.58	115.37	110.88
8	A	2013	MAN	C1-O5-C5	2.70	115.89	112.17
6	C	2010	NAG	C1-O5-C5	2.81	116.05	112.17
6	C	2007	NAG	C1-O5-C5	3.19	116.56	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	2015	MAN	C1-O5-C5	3.55	117.06	112.17
6	D	2004	NAG	C1-O5-C5	3.67	117.23	112.17
6	B	2004	NAG	C1-O5-C5	3.78	117.38	112.17
8	C	2014	MAN	C1-C2-C3	3.78	114.45	109.65
6	C	2008	NAG	C1-O5-C5	3.96	117.62	112.17
6	C	2016	NAG	C1-O5-C5	4.22	117.98	112.17
6	C	2011	NAG	C2-N2-C7	5.73	131.31	122.94
6	A	2010	NAG	C2-N2-C7	5.86	131.50	122.94
6	A	2015	NAG	C1-O5-C5	6.21	120.73	112.17
6	A	2008	NAG	C1-O5-C5	6.31	120.86	112.17
6	C	2011	NAG	C1-O5-C5	6.78	121.51	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2008	NAG	3	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, 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	601/632 (95%)	-0.11	14 (2%) 61 57	44, 68, 119, 155	0
1	C	589/632 (93%)	0.10	38 (6%) 20 15	40, 67, 140, 189	0
2	B	427/454 (94%)	0.11	39 (9%) 10 7	43, 66, 161, 185	0
2	D	432/454 (95%)	-0.15	14 (3%) 48 42	40, 59, 136, 158	0
3	E	219/219 (100%)	-0.40	1 (0%) 90 90	47, 64, 84, 97	0
3	L	219/219 (100%)	-0.45	0 100 100	40, 57, 77, 91	0
4	F	218/218 (100%)	-0.37	4 (1%) 69 66	44, 67, 101, 117	0
4	H	218/218 (100%)	-0.45	2 (0%) 84 83	38, 60, 99, 117	0
All	All	2923/3046 (95%)	-0.13	112 (3%) 41 35	38, 64, 127, 189	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	28	CYS	11.2
1	C	465	PHE	6.8
2	B	60	ILE	6.8
2	B	54	GLY	6.8
1	C	509	TRP	6.7
1	C	598	ALA	6.6
1	C	561	SER	5.9
2	B	19	ILE	5.7
2	B	55	CYS	5.7
1	C	588	TYR	5.7
1	C	62	ALA	5.5
1	C	576	PRO	5.4
1	C	519	ALA	5.4
2	B	52	LYS	5.3
1	A	64	PRO	5.2
1	C	464	MET	5.2

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Mol	Chain	Res	Type	RSRZ
2	D	54	GLY	5.1
1	C	563	ILE	5.0
1	C	560	LEU	4.9
1	C	508	ASP	4.8
2	D	33	PHE	4.7
1	C	467	PRO	4.6
1	A	30	THR	4.5
2	B	416	PRO	4.4
1	C	462	PRO	4.4
1	C	599	GLN	4.3
2	B	27	TRP	4.1
1	C	562	PRO	4.1
2	D	51	LYS	3.9
2	D	14	SER	3.9
1	C	512	GLN	3.8
4	H	137	THR	3.7
2	B	49	ALA	3.7
2	B	29	THR	3.7
1	A	461	PHE	3.5
2	B	46	ASP	3.5
2	B	25	CYS	3.4
2	B	15	CYS	3.4
4	F	137	THR	3.3
2	B	8	LEU	3.3
2	B	62	ASN	3.3
1	A	86	SER	3.2
2	D	13	LYS	3.2
1	C	566	ALA	3.2
1	C	31	ASP	3.1
2	B	47	LEU	3.1
1	C	570	SER	3.0
2	B	56	PRO	3.0
3	E	1	ASP	3.0
2	D	55	CYS	3.0
1	C	565	ILE	3.0
1	C	600	ILE	2.9
2	D	26	GLY	2.9
2	B	50	LEU	2.9
4	F	216	VAL	2.9
1	A	90	GLU	2.8
1	C	29	GLY	2.8
2	B	417	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	57	PRO	2.8
2	B	17	GLU	2.8
2	B	24	ASN	2.8
2	D	49	ALA	2.8
2	D	190	GLU	2.7
2	B	63	PRO	2.7
2	B	372	GLY	2.6
1	A	580	HIS	2.6
1	C	491	SER	2.6
2	B	22	GLY	2.6
1	A	517	ARG	2.6
1	A	554	SER	2.6
2	D	27	TRP	2.6
2	D	44	CYS	2.5
1	C	466	ASN	2.5
2	B	441	ILE	2.5
2	B	48	GLU	2.5
2	B	53	LYS	2.5
2	B	442	CYS	2.4
2	D	50	LEU	2.4
1	C	590	SER	2.4
1	A	65	THR	2.4
1	C	463	ALA	2.4
1	A	205	TYR	2.4
2	B	14	SER	2.3
2	D	7	CYS	2.3
1	A	579	SER	2.3
2	B	23	PRO	2.3
2	B	420	SER	2.3
2	B	43	ARG	2.3
1	C	461	PHE	2.3
1	C	569	PHE	2.3
2	B	51	LYS	2.3
2	B	415	CYS	2.2
2	B	444	CYS	2.2
1	C	30	THR	2.2
4	H	1	GLN	2.1
4	F	135	ALA	2.1
1	C	468	GLU	2.1
1	C	492	GLY	2.1
2	D	52	LYS	2.1
2	B	45	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	589	GLN	2.1
1	A	575	ALA	2.1
1	A	464	MET	2.1
1	C	63	SER	2.1
1	C	507	LEU	2.1
1	C	86	SER	2.0
2	B	18	CYS	2.0
1	C	552	ASN	2.0
2	B	59	ASP	2.0
1	A	29	GLY	2.0
1	C	454	ALA	2.0
4	F	133	SER	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, 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	LLDF	B-factors(Å ²)	Q<0.9
9	MG	D	2003	1/1	0.96	0.34	8.47	57,57,57,57	0
9	MG	B	2003	1/1	0.87	0.27	4.15	62,62,62,62	0
6	NAG	A	2008	14/15	0.92	0.21	1.38	62,68,71,72	0
6	NAG	C	2009	14/15	0.93	0.17	1.12	64,70,74,75	0
6	NAG	A	2015	14/15	0.86	0.22	0.29	82,93,103,112	0
6	NAG	C	2005	14/15	0.90	0.16	0.24	74,82,90,100	0
6	NAG	A	2005	14/15	0.88	0.16	-0.05	73,78,86,86	0
5	CA	A	2001	1/1	0.95	0.12	-0.21	69,69,69,69	0
6	NAG	C	2016	14/15	0.89	0.19	-0.76	100,110,118,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	A	2009	14/15	0.95	0.13	-0.82	53,56,65,66	0
5	CA	C	2001	1/1	0.96	0.12	-0.83	63,63,63,63	0
5	CA	C	2004	1/1	0.96	0.11	-0.83	81,81,81,81	0
5	CA	C	2003	1/1	0.96	0.09	-0.88	84,84,84,84	0
5	CA	A	2004	1/1	0.83	0.11	-1.08	88,88,88,88	0
5	CA	C	2002	1/1	0.97	0.11	-1.44	75,75,75,75	0
5	CA	A	2003	1/1	0.98	0.09	-1.50	78,78,78,78	0
5	CA	A	2002	1/1	0.89	0.07	-1.73	84,84,84,84	0
5	CA	D	2002	1/1	0.98	0.10	-1.98	54,54,54,54	0
5	CA	B	2001	1/1	0.91	0.06	-2.73	69,69,69,69	0
5	CA	D	2001	1/1	0.93	0.08	-2.79	65,65,65,65	0
6	NAG	C	2010	14/15	0.98	0.09	-2.84	50,54,59,59	0
5	CA	B	2002	1/1	0.98	0.07	-4.16	62,62,62,62	0
8	MAN	A	2012	11/12	0.84	0.16	-	88,100,105,105	0
6	NAG	D	2004	14/15	0.92	0.10	-	68,71,73,73	0
6	NAG	C	2006	14/15	0.81	0.31	-	108,116,118,121	0
6	NAG	B	2006	14/15	0.84	0.27	-	97,105,111,113	0
8	MAN	C	2014	11/12	0.84	0.14	-	80,85,91,94	0
6	NAG	C	2011	14/15	0.96	0.12	-	55,59,64,71	0
6	NAG	A	2010	14/15	0.92	0.15	-	58,63,70,71	0
8	MAN	A	2013	11/12	0.84	0.18	-	98,101,108,108	0
6	NAG	A	2007	14/15	0.87	0.19	-	92,99,101,104	0
6	NAG	A	2006	14/15	0.84	0.12	-	92,104,108,108	0
7	BMA	A	2011	11/12	0.94	0.09	-	75,83,90,92	0
8	MAN	C	2013	11/12	0.79	0.14	-	69,84,89,90	0
6	NAG	C	2008	14/15	0.84	0.17	-	97,101,105,105	0
8	MAN	C	2015	11/12	0.89	0.16	-	77,85,95,96	0
6	NAG	B	2005	14/15	0.94	0.13	-	74,81,87,92	0
6	NAG	B	2004	14/15	0.95	0.15	-	66,71,77,78	0
7	BMA	C	2012	11/12	0.94	0.10	-	66,73,76,77	0
6	NAG	C	2007	14/15	0.80	0.17	-	87,102,110,111	0
8	MAN	A	2014	11/12	0.91	0.09	-	78,85,91,92	0

6.5 Other polymers [i](#)

There are no such residues in this entry.