



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:25 AM UTC

PDB ID : 4DEP / pdb_00004dep
Title : Structure of the IL-1b signaling complex
Authors : Thomas, C.; Garcia, K.C.
Deposited on : 2012-01-21
Resolution : 3.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

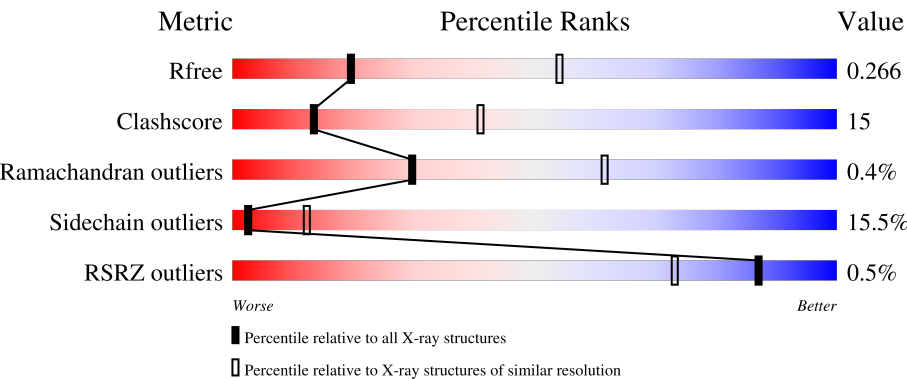
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	158	68%23% . .
1	D	158	66%27% . .
2	B	321	% 58%29%5%8%
2	E	321	57%31%7% . .
3	C	349	% 49%30%. .18%

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Mol	Chain	Length	Quality of chain
3	F	349	% 50% 27% 6% 17%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11679 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 Interleukin-1 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	0	0
			1167	744	194	221	8			
1	D	152	Total	C	N	O	S	0	0	0
			1193	760	197	228	8			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P01584
A	-3	PRO	-	expression tag	UNP P01584
A	-2	LEU	-	expression tag	UNP P01584
A	-1	GLY	-	expression tag	UNP P01584
A	0	SER	-	expression tag	UNP P01584
D	-4	GLY	-	expression tag	UNP P01584
D	-3	PRO	-	expression tag	UNP P01584
D	-2	LEU	-	expression tag	UNP P01584
D	-1	GLY	-	expression tag	UNP P01584
D	0	SER	-	expression tag	UNP P01584

- Molecule 2 is a protein called Interleukin-1 receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	296	Total	C	N	O	S	0	0	0
			2174	1393	370	400	11			
2	E	307	Total	C	N	O	S	0	1	0
			2442	1563	415	451	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLU	-	expression tag	UNP P14778
B	0	PRO	-	expression tag	UNP P14778

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	GLU	-	expression tag	UNP P14778
E	0	PRO	-	expression tag	UNP P14778

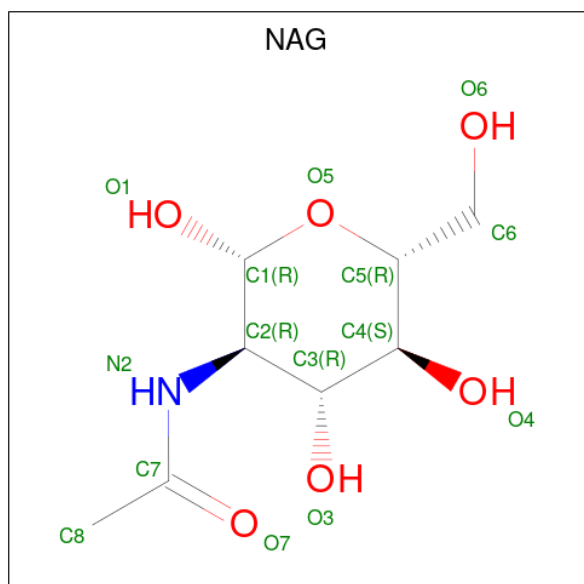
- Molecule 3 is a protein called Interleukin-1 receptor accessory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	287	Total	C	N	O	S	0	1	0
			2260	1451	385	408	16			
3	F	289	Total	C	N	O	S	0	0	0
			2240	1440	376	410	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	GLU	-	expression tag	UNP Q9NPH3
C	0	PRO	-	expression tag	UNP Q9NPH3
F	-1	GLU	-	expression tag	UNP Q9NPH3
F	0	PRO	-	expression tag	UNP Q9NPH3

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

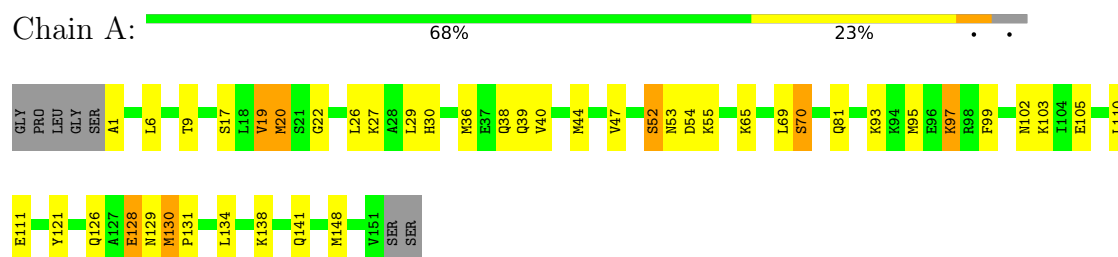
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	O	0	0
			1	1		
5	E	4	Total	O	0	0
			4	4		
5	F	2	Total	O	0	0
			2	2		

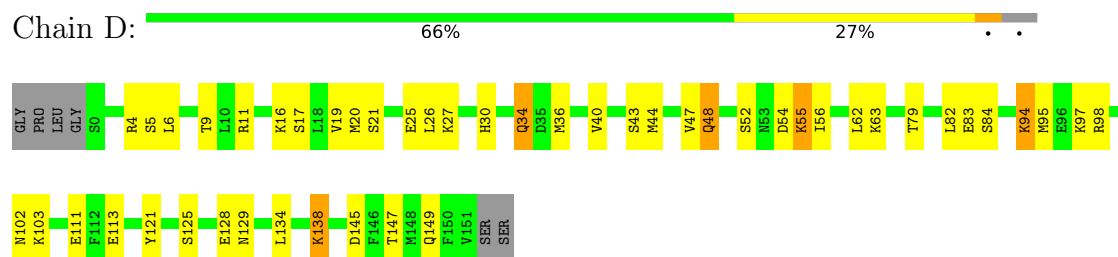
3 Residue-property plots [i](#)

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.

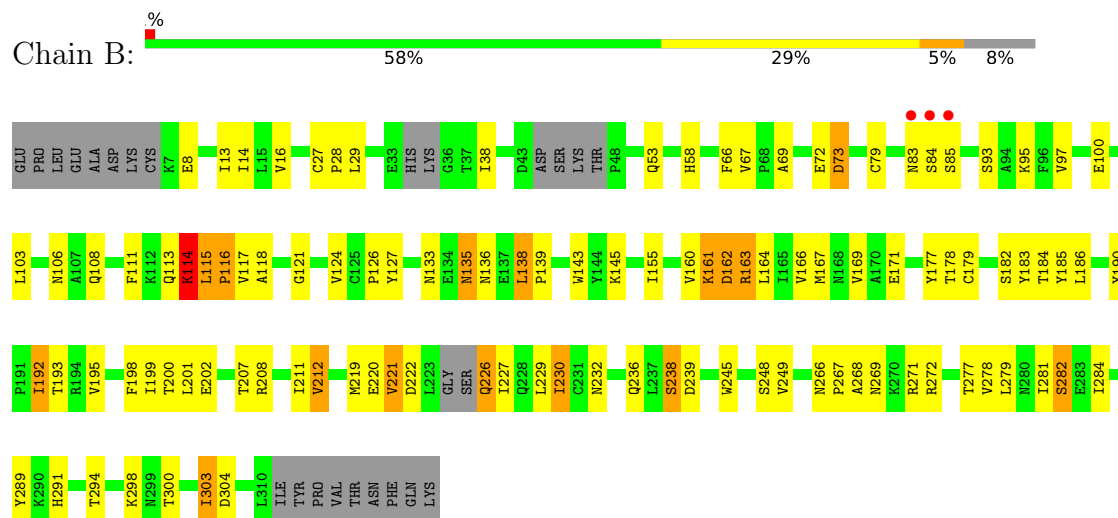
- Molecule 1: Interleukin-1 beta



- Molecule 1: Interleukin-1 beta

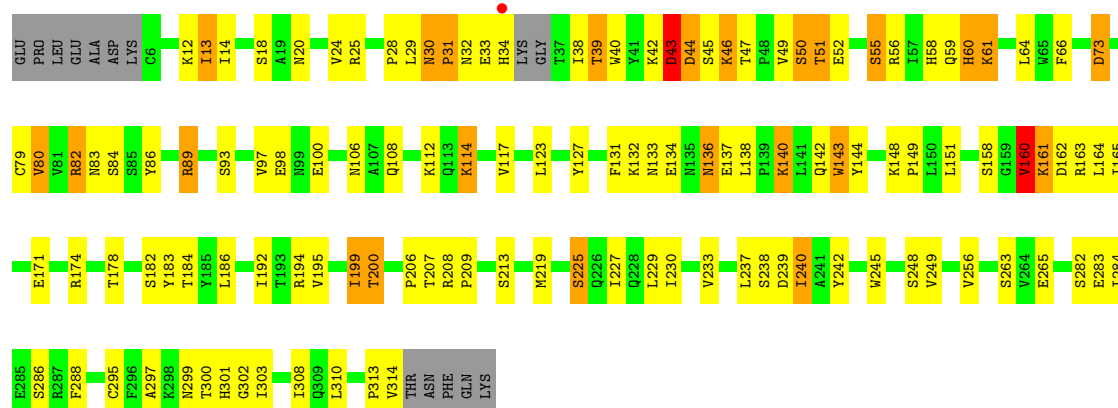


- Molecule 2: Interleukin-1 receptor type 1



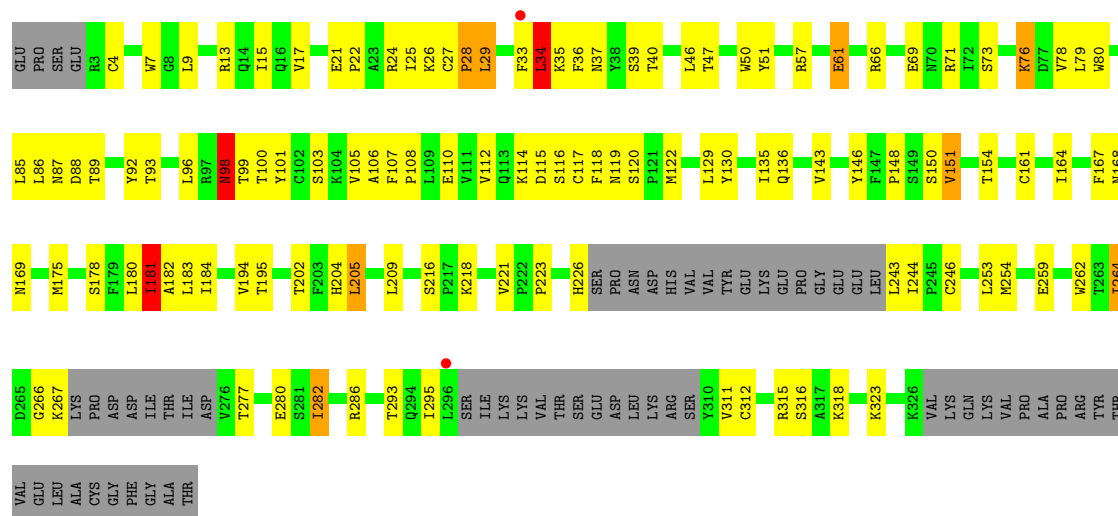
- Molecule 2: Interleukin-1 receptor type 1

Chain E: 



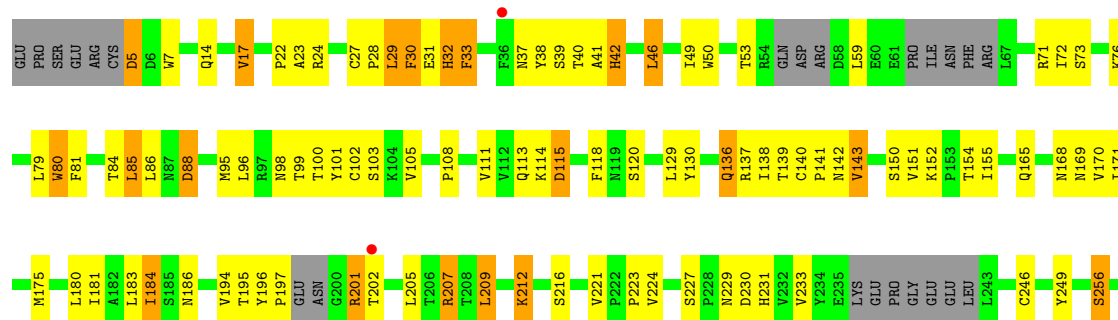
• Molecule 3: Interleukin-1 receptor accessory protein

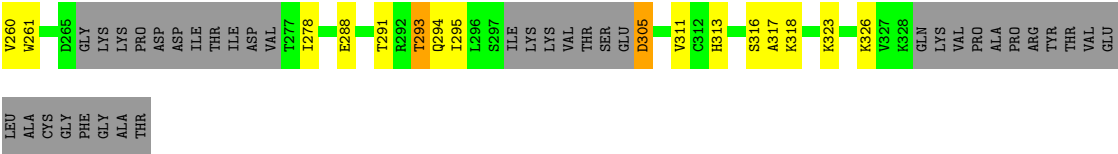
Chain C: 



• Molecule 3: Interleukin-1 receptor accessory protein

Chain F: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.99Å 65.90Å 163.40Å 90.00° 90.35° 90.00°	Depositor
Resolution (Å)	19.70 – 3.10 19.70 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.70-3.10) 98.9 (19.70-3.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 3.09Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.210 , 0.277 0.204 , 0.266	Depositor DCC
R_{free} test set	2055 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.9	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11679	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.90	2/1190 (0.2%)	1.03	6/1609 (0.4%)
1	D	0.75	0/1216	1.00	1/1640 (0.1%)
2	B	1.02	5/2228 (0.2%)	1.13	18/3053 (0.6%)
2	E	1.06	10/2504 (0.4%)	1.11	19/3410 (0.6%)
3	C	0.88	6/2320 (0.3%)	1.06	9/3164 (0.3%)
3	F	0.87	1/2297 (0.0%)	1.12	19/3136 (0.6%)
All	All	0.94	24/11755 (0.2%)	1.09	72/16012 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	E	0	1
3	C	0	2
All	All	0	4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	GLY	C-O	-6.77	1.17	1.23
2	B	115	LEU	C-O	-6.58	1.17	1.24
3	C	29	LEU	C-O	-6.51	1.16	1.24
1	A	52	SER	CA-C	-6.30	1.45	1.52
2	B	166	VAL	C-O	-6.27	1.17	1.24
2	E	137	GLU	C-O	-6.23	1.16	1.24
2	E	43	ASP	C-O	-6.13	1.17	1.24
2	B	161	LYS	CA-C	-5.70	1.48	1.53
3	C	181	ILE	C-O	-5.61	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	143	TRP	CA-C	-5.59	1.45	1.52
2	E	131	PHE	C-O	-5.46	1.17	1.24
3	C	34	LEU	CA-C	-5.45	1.46	1.52
2	E	213	SER	C-O	-5.44	1.17	1.24
3	C	182	ALA	C-O	-5.41	1.17	1.23
2	E	60	HIS	CG-ND1	-5.39	1.32	1.38
3	F	143	VAL	CA-CB	-5.25	1.49	1.54
2	B	115	LEU	CA-C	-5.23	1.46	1.52
3	C	183	LEU	C-O	-5.19	1.17	1.23
2	E	43	ASP	CA-C	-5.19	1.46	1.52
3	C	28	PRO	C-O	-5.17	1.17	1.24
2	E	142	GLN	C-O	-5.10	1.17	1.23
2	E	143	TRP	NE1-CE2	-5.08	1.31	1.37
2	E	60	HIS	CA-C	-5.04	1.46	1.52
1	A	19	VAL	CA-C	-5.01	1.46	1.52

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	38	TYR	N-CA-C	-9.31	98.52	110.53
2	E	46	LYS	N-CA-C	-8.51	100.79	113.72
3	C	244	ILE	N-CA-C	8.30	116.37	108.15
1	A	70	SER	N-CA-C	8.13	121.84	109.23
2	E	225	SER	N-CA-C	7.90	120.13	110.41
2	E	161	LYS	CB-CA-C	-7.85	107.51	116.54
2	B	8	GLU	N-CA-C	7.84	122.08	110.48
3	C	254	MET	N-CA-C	7.73	119.34	111.07
2	E	61	LYS	N-CA-C	-7.60	94.61	110.80
2	B	221	VAL	N-CA-C	7.55	119.02	107.99
1	A	65	LYS	N-CA-C	-7.26	104.03	114.12
3	F	42	HIS	N-CA-C	-7.24	104.48	113.38
2	E	132	LYS	N-CA-C	-7.22	100.99	110.53
3	C	143	VAL	N-CA-C	-7.00	107.06	113.71
3	F	37	ASN	N-CA-C	6.79	119.57	109.59
2	B	212	VAL	CB-CA-C	-6.50	103.41	111.92
2	B	212	VAL	N-CA-C	6.48	117.48	111.45
3	F	32	HIS	N-CA-C	6.40	119.04	108.48
2	E	30	ASN	N-CA-C	-6.33	100.83	110.01
2	B	13	ILE	N-CA-C	6.28	116.42	106.88
3	F	31	GLU	CA-C-N	6.22	129.11	121.64
3	F	31	GLU	C-N-CA	6.22	129.11	121.64
2	E	117	VAL	CB-CA-C	-6.04	104.69	111.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	80	TRP	N-CA-C	6.03	118.49	110.53
2	B	38	ILE	N-CA-C	5.91	117.27	108.23
2	B	162	ASP	N-CA-C	-5.89	105.96	113.02
2	E	58	HIS	N-CA-C	5.86	116.14	107.88
1	A	52	SER	N-CA-C	-5.84	100.47	109.52
2	B	155	ILE	N-CA-C	-5.84	107.01	111.62
2	B	100	GLU	CA-C-N	5.83	126.17	119.93
2	B	100	GLU	C-N-CA	5.83	126.17	119.93
3	C	254	MET	CA-C-N	-5.76	115.32	123.03
3	C	254	MET	C-N-CA	-5.76	115.32	123.03
2	B	115	LEU	C-N-CD	-5.73	101.51	125.00
2	E	136	ASN	N-CA-C	5.66	119.20	111.39
2	E	233	VAL	N-CA-C	5.62	116.09	107.77
3	F	76	LYS	CB-CA-C	-5.57	110.17	116.63
3	F	76	LYS	N-CA-C	5.55	117.46	108.08
2	B	161	LYS	CB-CA-C	-5.55	110.16	116.54
2	E	160	VAL	CB-CA-C	-5.54	102.25	110.33
3	F	118	PHE	N-CA-C	5.51	121.22	113.56
3	F	33	PHE	N-CA-C	5.45	117.22	111.28
3	F	256	SER	N-CA-C	-5.45	100.14	109.24
2	E	29	LEU	N-CA-C	5.40	117.76	109.07
2	E	242	TYR	N-CA-C	5.38	117.16	109.14
1	A	22	GLY	N-CA-C	-5.36	101.40	112.34
3	C	98	ASN	N-CA-C	-5.36	99.38	110.80
2	B	114	LYS	N-CA-C	5.35	117.32	109.24
2	B	220	GLU	N-CA-C	5.34	118.04	110.50
2	E	100	GLU	CA-C-N	5.33	124.78	119.24
2	E	100	GLU	C-N-CA	5.33	124.78	119.24
3	C	118	PHE	N-CA-C	5.32	119.35	112.86
2	B	281	ILE	N-CA-C	-5.30	102.24	109.55
3	F	88	ASP	N-CA-C	-5.29	106.79	113.20
2	E	44	ASP	CA-C-N	-5.26	113.60	120.44
2	E	44	ASP	C-N-CA	-5.26	113.60	120.44
3	F	28	PRO	N-CA-C	-5.25	107.30	113.86
3	F	33	PHE	N-CA-CB	-5.23	102.43	110.12
3	C	311	VAL	N-CA-C	5.21	115.40	108.11
3	C	76	LYS	CB-CA-C	-5.20	110.59	116.63
3	F	30	PHE	N-CA-C	5.17	117.99	109.76
2	B	230	ILE	N-CA-C	5.15	115.72	108.36
3	F	278	ILE	N-CA-C	5.14	115.49	107.99
2	B	135	ASN	N-CA-C	-5.11	106.89	113.02
1	A	1	ALA	CA-C-N	5.10	124.71	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	ALA	C-N-CA	5.10	124.71	119.56
2	E	240	ILE	N-CA-C	5.09	116.62	108.89
3	F	311	VAL	N-CA-C	5.08	115.29	107.77
2	B	58	HIS	N-CA-C	5.05	115.20	108.38
2	E	86	TYR	N-CA-C	5.05	117.65	109.06
1	D	129	ASN	N-CA-C	5.04	118.39	111.54
3	F	59	LEU	N-CA-C	5.02	115.94	108.86

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	20	MET	Peptide
3	C	15	ILE	Peptide
3	C	264	ILE	Peptide
2	E	313	PRO	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	1167	0	1140	26	0
1	D	1193	0	1178	30	0
2	B	2174	0	1914	71	0
2	E	2442	0	2347	88	0
3	C	2260	0	2143	70	0
3	F	2240	0	2075	73	0
4	B	42	0	39	0	0
4	C	56	0	52	1	0
4	E	56	0	52	1	0
4	F	42	0	39	0	0
5	C	1	0	0	0	0
5	E	4	0	0	0	0
5	F	2	0	0	0	0
All	All	11679	0	10979	334	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 15.

All (334) 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)
3:C:33:PHE:C	3:C:34:LEU:HD23	1.49	1.36
3:F:84:THR:O	3:F:85:LEU:HD23	1.19	1.29
3:F:84:THR:C	3:F:85:LEU:HD23	1.58	1.26
2:E:82:ARG:HG3	2:E:82:ARG:HH11	1.09	1.16
2:B:266:ASN:OD1	2:B:267:PRO:HD2	1.44	1.15
2:B:221:VAL:CB	2:B:289:TYR:HE2	1.61	1.12
3:F:84:THR:O	3:F:85:LEU:CD2	2.05	1.05
2:B:138:LEU:H	2:B:138:LEU:HD12	0.88	1.02
2:B:138:LEU:HD12	2:B:138:LEU:N	1.72	1.01
2:B:138:LEU:H	2:B:138:LEU:CD1	1.74	1.01
3:C:34:LEU:HD23	3:C:34:LEU:N	1.58	0.97
3:C:33:PHE:O	3:C:34:LEU:HD23	1.65	0.96
2:E:82:ARG:HH11	2:E:82:ARG:CG	1.80	0.95
3:C:98:ASN:OD1	4:C:401:NAG:O5	1.81	0.93
2:B:221:VAL:CB	2:B:289:TYR:CE2	2.52	0.91
3:C:33:PHE:CE2	3:C:105:VAL:HG21	2.04	0.91
2:B:266:ASN:OD1	2:B:267:PRO:CD	2.20	0.90
3:C:116:SER:CB	2:E:59:GLN:HE22	1.85	0.90
2:B:162:ASP:OD1	2:B:163:ARG:NH1	2.09	0.85
2:E:82:ARG:HG3	2:E:82:ARG:NH1	1.90	0.85
3:C:34:LEU:N	3:C:34:LEU:CD2	2.34	0.83
3:C:33:PHE:C	3:C:34:LEU:CD2	2.44	0.81
3:F:143:VAL:CG1	3:F:143:VAL:O	2.29	0.80
3:C:46:LEU:HB3	3:C:96:LEU:HD22	1.64	0.80
2:B:267:PRO:HD2	2:B:268:ALA:H	1.47	0.79
3:F:71:ARG:HG2	3:F:72:ILE:HG13	1.63	0.79
3:C:266:GLY:O	3:C:267:LYS:CB	2.30	0.79
3:C:26:LYS:O	3:C:28:PRO:HD3	1.84	0.77
3:C:116:SER:HB3	2:E:59:GLN:HE22	1.51	0.76
1:D:128:GLU:HG2	2:E:127:TYR:CE1	2.21	0.75
3:F:98:ASN:HB2	3:F:101:TYR:HB3	1.68	0.75
2:E:42:LYS:O	2:E:43:ASP:C	2.30	0.74
3:F:212:LYS:HE3	3:F:288:GLU:HG3	1.70	0.74
1:A:128:GLU:HG2	2:B:127:TYR:CE1	2.23	0.74
3:C:71:ARG:NH2	3:C:88:ASP:OD2	2.21	0.73
2:E:45:SER:C	2:E:47:THR:H	1.96	0.73
2:E:56:ARG:NH2	2:E:73:ASP:OD1	2.21	0.73
3:F:143:VAL:O	3:F:143:VAL:HG12	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:115:ASP:OD1	3:C:116:SER:N	2.22	0.72
2:E:60:HIS:O	2:E:61:LYS:C	2.30	0.70
2:B:163:ARG:HH11	2:B:163:ARG:HG2	1.57	0.70
1:D:21:SER:OG	1:D:25:GLU:HG2	1.92	0.70
3:F:229:ASN:HB3	3:F:231:HIS:H	1.56	0.69
2:E:42:LYS:CG	2:E:43:ASP:H	2.05	0.69
2:E:45:SER:O	2:E:46:LYS:HB2	1.91	0.69
3:C:57:ARG:NH1	3:C:61:GLU:OE1	2.24	0.69
3:C:33:PHE:HE2	3:C:105:VAL:HG21	1.58	0.68
2:E:174:ARG:HH21	2:E:200:THR:HG22	1.58	0.68
3:F:260:VAL:O	3:F:294:GLN:NE2	2.27	0.68
1:A:19:VAL:HG12	1:A:38:GLN:O	1.93	0.68
3:F:139:THR:O	3:F:141:PRO:HD3	1.94	0.67
3:F:33:PHE:CE2	3:F:105:VAL:HG21	2.30	0.67
3:F:39:SER:C	3:F:41:ALA:H	2.02	0.67
3:C:46:LEU:CD2	3:C:98:ASN:OD1	2.43	0.67
3:C:116:SER:CB	2:E:59:GLN:NE2	2.58	0.66
1:D:54:ASP:HB2	2:E:300:THR:HG23	1.77	0.66
2:E:44:ASP:O	2:E:45:SER:C	2.36	0.66
2:E:34:HIS:HB3	2:E:83:ASN:CB	2.25	0.66
2:E:123:LEU:HD12	2:E:164:LEU:HD23	1.76	0.66
3:F:33:PHE:CZ	3:F:105:VAL:HG21	2.31	0.66
1:A:55:LYS:HD2	1:A:102:ASN:HB3	1.78	0.66
3:F:71:ARG:NH2	3:F:85:LEU:HG	2.10	0.66
2:B:226:GLN:HA	2:B:282:SER:HA	1.78	0.66
3:C:21:GLU:OE1	3:C:204[B]:HIS:ND1	2.28	0.65
2:E:30:ASN:OD1	2:E:31:PRO:HD2	1.96	0.65
2:E:45:SER:O	2:E:46:LYS:CB	2.43	0.65
3:F:223:PRO:HG3	3:F:316:SER:HB3	1.78	0.65
2:E:127:TYR:O	2:E:194:ARG:NH2	2.25	0.65
3:C:46:LEU:HD23	3:C:98:ASN:OD1	1.97	0.65
3:F:39:SER:O	3:F:41:ALA:N	2.29	0.65
3:F:130:TYR:O	3:F:136:GLN:NE2	2.30	0.64
2:B:298:LYS:HB2	2:B:303:ILE:HG13	1.78	0.64
2:B:171:GLU:HA	2:B:200:THR:HG21	1.78	0.64
1:D:36:MET:HE3	2:E:112:LYS:HB2	1.79	0.64
2:B:133:ASN:O	2:B:136:ASN:N	2.30	0.63
3:C:89:THR:HG23	3:C:110:GLU:HA	1.80	0.63
3:F:197:PRO:HA	3:F:201:ARG:O	2.00	0.62
2:B:267:PRO:CD	2:B:268:ALA:H	2.12	0.62
3:C:37:ASN:OD1	3:C:39:SER:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:ASN:O	2:B:85:SER:N	2.32	0.62
2:E:45:SER:C	2:E:47:THR:N	2.54	0.62
1:A:27:LYS:HA	1:A:131:PRO:HA	1.83	0.61
3:F:140:CYS:HB3	3:F:175:MET:HE3	1.83	0.61
2:E:44:ASP:O	2:E:46:LYS:HG2	2.01	0.61
3:F:7:TRP:HB3	3:F:33:PHE:CE1	2.36	0.61
1:D:147:THR:HG22	1:D:149:GLN:HE22	1.65	0.60
3:F:169:ASN:ND2	3:F:186:ASN:OD1	2.34	0.60
2:B:73:ASP:OD1	2:B:73:ASP:N	2.30	0.60
3:F:39:SER:C	3:F:41:ALA:N	2.58	0.60
2:E:42:LYS:CG	2:E:43:ASP:N	2.64	0.60
1:A:126:GLN:NE2	1:A:141:GLN:O	2.34	0.60
2:B:66:PHE:HB3	2:B:69:ALA:HB2	1.84	0.60
3:F:169:ASN:HB3	3:F:170:VAL:HG23	1.83	0.60
2:E:42:LYS:HG2	2:E:43:ASP:H	1.66	0.59
1:D:121:TYR:CE2	1:D:138:LYS:HD2	2.37	0.59
3:C:98:ASN:HB2	3:C:101:TYR:HB3	1.84	0.59
1:D:83:GLU:OE1	1:D:98:ARG:NE	2.35	0.59
2:B:163:ARG:NH2	3:C:168:ASN:O	2.36	0.58
4:E:401:NAG:O7	4:E:401:NAG:H3	2.02	0.58
2:E:49:VAL:HG22	2:E:50:SER:H	1.69	0.58
3:F:84:THR:C	3:F:85:LEU:CD2	2.54	0.58
2:B:245:TRP:NE1	2:B:291:HIS:O	2.27	0.58
3:C:9:LEU:HD21	3:C:108:PRO:HG3	1.86	0.57
3:C:130:TYR:O	3:C:136:GLN:NE2	2.36	0.57
3:C:33:PHE:O	3:C:34:LEU:CD2	2.46	0.57
1:D:121:TYR:CZ	1:D:138:LYS:HD2	2.40	0.57
3:F:224:VAL:HB	3:F:249:TYR:HB2	1.86	0.57
3:C:71:ARG:HH22	3:C:88:ASP:CG	2.12	0.57
1:A:128:GLU:HG2	2:B:127:TYR:CZ	2.39	0.56
3:F:49:ILE:HB	3:F:95:MET:HB3	1.86	0.56
2:B:117:VAL:HA	2:B:169:VAL:HB	1.87	0.56
1:D:4:ARG:HD2	2:E:263:SER:HB3	1.88	0.56
1:D:147:THR:HG22	1:D:149:GLN:NE2	2.21	0.56
2:E:162:ASP:OD1	2:E:163:ARG:HD3	2.05	0.56
1:A:95:MET:HE3	1:A:99:PHE:HB3	1.87	0.55
3:F:143:VAL:HG11	3:F:175:MET:HE2	1.88	0.55
3:C:33:PHE:CZ	3:C:105:VAL:HG21	2.41	0.55
3:F:230:ASP:HA	3:F:326:LYS:HD2	1.89	0.55
3:F:27:CYS:SG	3:F:29:LEU:HB2	2.47	0.55
2:E:163:ARG:NH2	3:F:168:ASN:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:LYS:HE2	2:E:238:SER:O	2.08	0.54
1:A:110:LEU:HD11	1:A:148:MET:HB2	1.89	0.54
2:B:117:VAL:HG13	2:B:201:LEU:O	2.07	0.54
3:C:223:PRO:HG3	3:C:316:SER:HB3	1.89	0.54
1:D:25:GLU:OE2	2:E:30:ASN:ND2	2.41	0.54
2:B:67:VAL:HG11	2:B:185:TYR:HD2	1.73	0.54
1:A:105:GLU:HG3	1:A:110:LEU:HG	1.89	0.54
2:B:212:VAL:HB	2:B:232:ASN:HB3	1.89	0.54
3:C:181:ILE:HG22	3:C:181:ILE:O	2.08	0.54
2:E:143:TRP:HA	2:E:178:THR:O	2.07	0.54
2:B:53:GLN:NE2	2:B:186:LEU:HD21	2.22	0.53
2:B:83:ASN:O	2:B:84:SER:CB	2.56	0.53
2:B:117:VAL:O	2:B:118:ALA:HB3	2.06	0.53
1:D:83:GLU:CD	1:D:98:ARG:HE	2.16	0.53
1:D:21:SER:HB3	1:D:27:LYS:HD2	1.90	0.53
2:B:163:ARG:NH1	2:B:163:ARG:CG	2.71	0.53
3:C:115:ASP:HB3	3:C:119:ASN:H	1.72	0.53
2:E:206:PRO:HB3	2:E:301:HIS:CE1	2.44	0.53
2:E:225:SER:O	2:E:284:ILE:HG12	2.08	0.53
2:B:229:LEU:HD23	2:B:279:LEU:HD23	1.90	0.53
3:C:259:GLU:OE1	3:C:315:ARG:NH1	2.42	0.53
1:D:56:ILE:HD13	2:E:240:ILE:HG23	1.91	0.53
1:D:6:LEU:HD11	1:D:44:MET:HE2	1.92	0.52
1:D:128:GLU:HG2	2:E:127:TYR:CZ	2.44	0.52
3:F:22:PRO:HG2	3:F:196:TYR:OH	2.08	0.52
3:F:316:SER:C	3:F:318:LYS:H	2.18	0.52
3:C:46:LEU:HD13	3:C:96:LEU:HD13	1.91	0.52
1:D:47:VAL:HG11	1:D:95:MET:HG3	1.92	0.52
2:E:239:ASP:CB	2:E:299:ASN:HB3	2.38	0.52
3:F:14:GLN:HB3	3:F:108:PRO:HG2	1.91	0.52
2:E:82:ARG:CG	2:E:82:ARG:NH1	2.51	0.52
3:F:17:VAL:HG21	3:F:23:ALA:HB2	1.91	0.52
3:C:180:LEU:N	3:C:180:LEU:HD12	2.25	0.51
1:D:34:GLN:NE2	2:E:108:GLN:O	2.42	0.51
1:A:6:LEU:HD11	1:A:44:MET:HE2	1.93	0.51
2:E:31:PRO:O	2:E:32:ASN:OD1	2.29	0.51
2:B:163:ARG:NH1	2:B:163:ARG:HG2	2.25	0.51
3:F:169:ASN:HD22	3:F:186:ASN:HD21	1.57	0.51
3:F:71:ARG:NH2	3:F:88:ASP:OD2	2.44	0.51
2:E:133:ASN:O	2:E:134:GLU:C	2.51	0.51
3:C:98:ASN:HB3	3:C:100:THR:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:PRO:HG2	3:C:151:VAL:HG12	1.93	0.50
3:F:169:ASN:HD22	3:F:186:ASN:ND2	2.09	0.50
3:C:33:PHE:CE2	3:C:105:VAL:CG2	2.89	0.50
2:E:160:VAL:O	2:E:161:LYS:HB2	2.10	0.50
2:B:143:TRP:CE3	2:B:164:LEU:HD22	2.47	0.50
2:E:158:SER:HB2	2:E:165:ILE:HB	1.93	0.50
2:E:133:ASN:C	2:E:133:ASN:OD1	2.55	0.50
3:F:49:ILE:O	3:F:95:MET:N	2.45	0.50
3:F:154:THR:HB	3:F:195:THR:OG1	2.12	0.50
1:A:30:HIS:ND1	2:B:126:PRO:HB3	2.27	0.49
2:E:51:THR:O	2:E:51:THR:OG1	2.30	0.49
2:B:124:VAL:HG22	2:B:163:ARG:HD3	1.94	0.49
2:B:160:VAL:O	2:B:161:LYS:C	2.53	0.49
2:E:14:ILE:HG12	2:E:93:SER:HB2	1.94	0.49
1:A:47:VAL:HG11	1:A:95:MET:HG3	1.93	0.49
2:B:14:ILE:HG22	2:B:14:ILE:O	2.11	0.49
2:E:143:TRP:CE2	2:E:164:LEU:HB2	2.47	0.49
2:B:97:VAL:HG21	2:B:106:ASN:HD22	1.76	0.49
3:F:141:PRO:HG3	3:F:209:LEU:HD23	1.93	0.49
3:F:142:ASN:O	3:F:207:ARG:NH1	2.45	0.49
3:C:93:THR:OG1	3:C:106:ALA:HB2	2.11	0.49
2:E:56:ARG:HH21	2:E:73:ASP:CG	2.21	0.49
3:C:36:PHE:HB2	3:C:40:THR:OG1	2.13	0.49
2:E:237:LEU:HD11	2:E:265:GLU:HG3	1.95	0.49
3:C:7:TRP:CD2	3:C:33:PHE:CD1	3.01	0.49
2:B:114:LYS:O	2:B:115:LEU:HD23	2.12	0.49
2:B:163:ARG:HH11	2:B:163:ARG:CG	2.19	0.48
2:B:183:TYR:HB2	2:B:192:ILE:HD11	1.94	0.48
2:E:30:ASN:OD1	2:E:31:PRO:CD	2.61	0.48
2:E:160:VAL:O	2:E:161:LYS:C	2.49	0.48
3:F:115:ASP:N	3:F:115:ASP:OD1	2.46	0.48
2:E:183:TYR:HB2	2:E:192:ILE:HD11	1.95	0.48
3:C:29:LEU:HA	3:C:33:PHE:HB2	1.95	0.48
2:B:135:ASN:O	2:B:136:ASN:CB	2.61	0.48
3:F:230:ASP:OD2	3:F:323:LYS:HD3	2.13	0.48
2:B:138:LEU:HB3	2:B:139:PRO:HD2	1.95	0.48
2:B:222:ASP:O	2:B:289:TYR:OH	2.30	0.48
2:E:40:TRP:CE2	2:E:79:CYS:HB3	2.48	0.48
2:B:143:TRP:CH2	2:B:179:CYS:HB3	2.49	0.48
2:B:115:LEU:HA	2:B:116:PRO:HD3	1.49	0.47
3:F:50:TRP:CZ2	3:F:79:LEU:HB2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LYS:HD2	1:A:110:LEU:CD2	2.44	0.47
1:A:111:GLU:OE1	1:A:138:LYS:NZ	2.35	0.47
1:D:48:GLN:HB3	1:D:94:LYS:HE2	1.97	0.47
1:D:26:LEU:HD21	1:D:62:LEU:HD21	1.97	0.47
2:E:13:ILE:HD12	2:E:13:ILE:O	2.13	0.47
3:C:21:GLU:HG2	3:C:204[B]:HIS:CE1	2.49	0.47
3:C:116:SER:HB3	2:E:59:GLN:NE2	2.22	0.47
3:C:209:LEU:O	3:C:209:LEU:HD12	2.14	0.47
3:C:282:ILE:H	3:C:282:ILE:HG13	1.58	0.47
2:B:113:GLN:C	2:B:114:LYS:HG2	2.39	0.47
2:B:226:GLN:N	2:B:282:SER:O	2.48	0.47
2:B:111:PHE:CD2	2:B:126:PRO:HG2	2.50	0.47
2:E:133:ASN:O	2:E:134:GLU:O	2.32	0.47
2:B:267:PRO:CD	2:B:268:ALA:N	2.76	0.46
2:E:160:VAL:HG21	3:F:180:LEU:HD21	1.97	0.46
3:F:143:VAL:O	3:F:143:VAL:HG13	2.11	0.46
3:F:46:LEU:HD21	3:F:101:TYR:HD2	1.79	0.46
3:C:246:CYS:HB2	3:C:262:TRP:CZ2	2.51	0.46
2:E:30:ASN:O	2:E:32:ASN:N	2.36	0.46
3:F:71:ARG:HH21	3:F:85:LEU:HG	1.79	0.46
3:C:29:LEU:HD23	3:C:33:PHE:CD2	2.51	0.46
1:A:29:LEU:HD12	2:B:127:TYR:OH	2.15	0.46
3:C:85:LEU:N	3:C:88:ASP:OD2	2.31	0.46
3:C:168:ASN:OD1	3:C:169:ASN:N	2.48	0.46
3:F:246:CYS:O	3:F:293:THR:HA	2.15	0.46
2:B:115:LEU:HB2	2:B:198:PHE:CE1	2.51	0.46
3:C:46:LEU:HD21	3:C:98:ASN:OD1	2.15	0.45
2:E:133:ASN:O	2:E:136:ASN:N	2.49	0.45
3:F:227:SER:O	3:F:246:CYS:HA	2.16	0.45
1:D:30:HIS:N	1:D:128:GLU:OE2	2.49	0.45
2:B:16:VAL:HG22	2:B:95:LYS:HB3	1.98	0.45
2:E:20:ASN:ND2	2:E:98:GLU:OE2	2.49	0.45
2:E:209:PRO:HB2	2:E:297:ALA:HB1	1.98	0.45
2:E:52:GLU:O	2:E:55:SER:HB2	2.16	0.45
1:D:16:LYS:HE3	1:D:125:SER:O	2.17	0.45
1:D:26:LEU:HD22	1:D:40:VAL:HG21	1.99	0.45
2:E:49:VAL:HG22	2:E:50:SER:N	2.31	0.45
2:E:245:TRP:CZ2	2:E:288:PHE:HA	2.52	0.45
1:D:113:GLU:HG3	1:D:121:TYR:CE1	2.51	0.45
3:F:183:LEU:HA	3:F:183:LEU:HD23	1.76	0.45
2:B:83:ASN:C	2:B:85:SER:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:GLN:HB2	2:B:239:ASP:OD1	2.17	0.44
2:E:208:ARG:HG2	2:E:302:GLY:HA3	1.99	0.44
3:F:7:TRP:CD2	3:F:33:PHE:HD1	2.36	0.44
1:D:55:LYS:HD2	1:D:102:ASN:HB3	1.98	0.44
3:F:85:LEU:HD23	3:F:85:LEU:N	2.09	0.44
3:F:184:ILE:HD13	3:F:184:ILE:HA	1.62	0.44
1:A:36:MET:O	1:A:39:GLN:HG3	2.18	0.44
2:B:269:ASN:O	2:B:271:ARG:N	2.51	0.44
3:C:22:PRO:HD2	3:C:205:LEU:HD13	2.00	0.44
3:C:253:LEU:HD22	3:C:318:LYS:HG3	1.98	0.44
2:B:28:PRO:HD2	2:B:79:CYS:SG	2.58	0.44
1:D:20:MET:HE2	1:D:20:MET:HB2	1.64	0.44
2:B:183:TYR:O	2:B:190:TYR:N	2.42	0.44
3:F:305:ASP:N	3:F:305:ASP:OD1	2.50	0.44
2:E:45:SER:CB	2:E:47:THR:H	2.31	0.44
1:A:105:GLU:OE1	2:B:238:SER:HB2	2.18	0.44
3:C:120:SER:C	3:C:122:MET:H	2.26	0.44
3:F:17:VAL:O	3:F:111:VAL:HA	2.18	0.43
1:D:9:THR:HB	1:D:149:GLN:HB2	2.00	0.43
3:F:141:PRO:O	3:F:207:ARG:HD3	2.18	0.43
2:B:138:LEU:CB	2:B:139:PRO:HD2	2.48	0.43
3:F:261:TRP:CZ2	3:F:313:HIS:HB3	2.53	0.43
2:E:239:ASP:HB2	2:E:299:ASN:HB3	2.00	0.43
3:F:80:TRP:C	3:F:81:PHE:CD1	2.97	0.43
2:E:39:THR:O	2:E:79:CYS:HA	2.18	0.43
3:F:169:ASN:HD22	3:F:186:ASN:CG	2.26	0.43
3:C:146:TYR:CG	3:C:205:LEU:HD21	2.53	0.42
1:A:20:MET:HE2	1:A:20:MET:HB2	1.62	0.42
1:A:54:ASP:OD2	3:C:286:ARG:NH1	2.49	0.42
2:B:115:LEU:HB2	2:B:198:PHE:HE1	1.84	0.42
3:C:26:LYS:O	3:C:28:PRO:CD	2.63	0.42
3:C:50:TRP:CH2	3:C:79:LEU:HB2	2.54	0.42
2:E:227:ILE:HD11	2:E:310:LEU:HD11	2.01	0.42
2:E:60:HIS:C	2:E:61:LYS:O	2.53	0.42
3:F:7:TRP:CG	3:F:33:PHE:CD1	3.07	0.42
3:F:140:CYS:CB	3:F:175:MET:HE3	2.49	0.42
3:F:139:THR:O	3:F:141:PRO:CD	2.65	0.42
3:C:116:SER:HB2	2:E:59:GLN:NE2	2.34	0.42
3:C:92:TYR:HB2	3:C:107:PHE:CZ	2.55	0.42
2:E:40:TRP:CD2	2:E:79:CYS:HB3	2.55	0.42
2:B:145:LYS:HD2	2:B:177:TYR:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ILE:HG23	3:C:167:PHE:CD2	2.55	0.42
2:E:60:HIS:ND1	2:E:61:LYS:N	2.68	0.42
2:E:171:GLU:O	2:E:174:ARG:HG3	2.19	0.42
3:C:246:CYS:HB2	3:C:262:TRP:CE2	2.55	0.42
3:F:30:PHE:C	3:F:32:HIS:H	2.27	0.42
3:F:256:SER:HA	3:F:317:ALA:HB2	2.00	0.42
1:A:130:MET:HG3	1:A:131:PRO:HD2	2.00	0.42
3:C:7:TRP:HB3	3:C:33:PHE:CE1	2.55	0.41
2:E:24:VAL:O	2:E:25:ARG:HD3	2.20	0.41
2:E:140:LYS:HB2	2:E:140:LYS:HE3	1.54	0.41
1:A:70:SER:N	1:A:81:GLN:O	2.41	0.41
2:B:53:GLN:HE22	2:B:186:LEU:HD21	1.85	0.41
2:B:266:ASN:HA	2:B:267:PRO:HD3	1.73	0.41
3:C:24:ARG:C	3:C:25:ILE:HD13	2.45	0.41
2:E:40:TRP:N	2:E:59:GLN:OE1	2.50	0.41
2:E:144:TYR:N	2:E:178:THR:O	2.52	0.41
3:C:24:ARG:HD2	3:C:80:TRP:CZ2	2.56	0.41
2:E:114:LYS:HE2	2:E:199:ILE:HD11	2.03	0.41
2:E:148:LYS:HA	2:E:149:PRO:HD3	1.91	0.41
3:C:51:TYR:CZ	3:C:93:THR:HG21	2.56	0.41
3:C:243:LEU:HD23	3:C:243:LEU:HA	1.87	0.41
1:A:26:LEU:HD22	1:A:40:VAL:HG21	2.01	0.41
1:A:121:TYR:CZ	1:A:138:LYS:HD2	2.55	0.41
2:B:14:ILE:HG12	2:B:93:SER:HB2	2.03	0.41
3:C:175:MET:HE3	3:C:175:MET:HB3	1.90	0.41
3:C:180:LEU:N	3:C:180:LEU:CD1	2.83	0.41
2:E:64:LEU:HG	2:E:66:PHE:CE1	2.56	0.41
3:F:5:ASP:HB2	3:F:102:CYS:O	2.21	0.41
1:A:95:MET:HE3	1:A:99:PHE:CB	2.48	0.41
2:B:211:ILE:HG13	2:B:304:ASP:HB3	2.02	0.41
2:E:144:TYR:N	2:E:144:TYR:CD1	2.89	0.41
3:F:71:ARG:HG2	3:F:72:ILE:CG1	2.42	0.41
3:F:205:LEU:HA	3:F:205:LEU:HD12	1.87	0.41
1:A:103:LYS:HD2	1:A:110:LEU:HD23	2.02	0.41
2:B:103:LEU:HD23	2:B:103:LEU:HA	1.85	0.41
2:E:60:HIS:O	2:E:61:LYS:CB	2.62	0.40
2:B:162:ASP:OD1	2:B:162:ASP:N	2.45	0.40
2:E:80:VAL:HB	2:E:89:ARG:HB2	2.02	0.40
2:E:160:VAL:HG11	3:F:171:ILE:HD12	2.03	0.40
1:A:69:LEU:HA	1:A:69:LEU:HD23	1.88	0.40
2:E:97:VAL:HB	2:E:106:ASN:ND2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:ASP:HB2	2:E:300:THR:CG2	2.47	0.40
1:D:95:MET:HE3	1:D:95:MET:HB3	1.57	0.40
2:B:97:VAL:HG23	2:B:97:VAL:O	2.21	0.40
2:B:162:ASP:OD1	2:B:162:ASP:C	2.64	0.40
2:B:207:THR:OG1	2:B:236:GLN:OE1	2.38	0.40
3:C:27:CYS:HA	3:C:28:PRO:HD2	1.70	0.40
3:F:29:LEU:HA	3:F:33:PHE:HB2	2.04	0.40
3:F:46:LEU:HB3	3:F:96:LEU:HD22	2.04	0.40
3:F:96:LEU:HA	3:F:96:LEU:HD23	1.75	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	149/158 (94%)	139 (93%)	9 (6%)	1 (1%)	18	49
1	D	150/158 (95%)	146 (97%)	4 (3%)	0	100	100
2	B	288/321 (90%)	268 (93%)	19 (7%)	1 (0%)	36	67
2	E	304/321 (95%)	284 (93%)	19 (6%)	1 (0%)	36	67
3	C	280/349 (80%)	251 (90%)	28 (10%)	1 (0%)	30	61
3	F	275/349 (79%)	247 (90%)	26 (10%)	2 (1%)	18	49
All	All	1446/1656 (87%)	1335 (92%)	105 (7%)	6 (0%)	30	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	40	THR
1	A	97	LYS
3	C	181	ILE

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Mol	Chain	Res	Type
2	B	116	PRO
2	E	28	PRO
3	F	181	ILE

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	128/143 (90%)	118 (92%)	10 (8%)	11	38
1	D	133/143 (93%)	114 (86%)	19 (14%)	3	14
2	B	204/292 (70%)	171 (84%)	33 (16%)	2	11
2	E	265/292 (91%)	224 (84%)	41 (16%)	2	12
3	C	243/320 (76%)	199 (82%)	44 (18%)	2	8
3	F	235/320 (73%)	195 (83%)	40 (17%)	2	10
All	All	1208/1510 (80%)	1021 (84%)	187 (16%)	2	12

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	17	SER
1	A	52	SER
1	A	53	ASN
1	A	93	LYS
1	A	97	LYS
1	A	128	GLU
1	A	129	ASN
1	A	130	MET
1	A	134	LEU
2	B	27	CYS
2	B	29	LEU
2	B	72	GLU
2	B	73	ASP
2	B	108	GLN

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Mol	Chain	Res	Type
2	B	114	LYS
2	B	138	LEU
2	B	163	ARG
2	B	167	MET
2	B	178	THR
2	B	182	SER
2	B	184	THR
2	B	192	ILE
2	B	193	THR
2	B	195	VAL
2	B	199	ILE
2	B	202	GLU
2	B	208	ARG
2	B	219	MET
2	B	226	GLN
2	B	227	ILE
2	B	230	ILE
2	B	238	SER
2	B	248	SER
2	B	249	VAL
2	B	272	ARG
2	B	277	THR
2	B	278	VAL
2	B	282	SER
2	B	284	ILE
2	B	294	THR
2	B	300	THR
2	B	303	ILE
3	C	4	CYS
3	C	13	ARG
3	C	17	VAL
3	C	34	LEU
3	C	35	LYS
3	C	47	THR
3	C	61	GLU
3	C	66	ARG
3	C	69	GLU
3	C	73	SER
3	C	76	LYS
3	C	78	VAL
3	C	86	LEU
3	C	87	ASN

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Mol	Chain	Res	Type
3	C	98	ASN
3	C	99	THR
3	C	103	SER
3	C	112	VAL
3	C	114	LYS
3	C	117	CYS
3	C	129	LEU
3	C	135	ILE
3	C	150	SER
3	C	151	VAL
3	C	154	THR
3	C	161	CYS
3	C	178	SER
3	C	184	ILE
3	C	194	VAL
3	C	195	THR
3	C	202	THR
3	C	205	LEU
3	C	216	SER
3	C	218	LYS
3	C	221	VAL
3	C	226	HIS
3	C	264	ILE
3	C	277	THR
3	C	280	GLU
3	C	282	ILE
3	C	293	THR
3	C	295	ILE
3	C	312	CYS
3	C	323	LYS
1	D	5	SER
1	D	11	ARG
1	D	17	SER
1	D	19	VAL
1	D	34	GLN
1	D	43	SER
1	D	48	GLN
1	D	52	SER
1	D	55	LYS
1	D	63	LYS
1	D	79	THR
1	D	82	LEU

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Mol	Chain	Res	Type
1	D	84	SER
1	D	94	LYS
1	D	97	LYS
1	D	111	GLU
1	D	134	LEU
1	D	138	LYS
1	D	145	ASP
2	E	12	LYS
2	E	13	ILE
2	E	18	SER
2	E	31	PRO
2	E	33	GLU
2	E	38	ILE
2	E	39	THR
2	E	43	ASP
2	E	50	SER
2	E	51	THR
2	E	55	SER
2	E	73	ASP
2	E	80	VAL
2	E	82	ARG
2	E	84	SER
2	E	89	ARG
2	E	114	LYS
2	E	138	LEU
2	E	140	LYS
2	E	151	LEU
2	E	160	VAL
2	E	182	SER
2	E	184	THR
2	E	186	LEU
2	E	195	VAL
2	E	199	ILE
2	E	200	THR
2	E	207	THR
2	E	219	MET
2	E	229	LEU
2	E	230	ILE
2	E	248	SER
2	E	249	VAL
2	E	256	VAL
2	E	282	SER

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Mol	Chain	Res	Type
2	E	283	GLU
2	E	286	SER
2	E	295	CYS
2	E	303	ILE
2	E	308	ILE
2	E	314	VAL
3	F	5	ASP
3	F	17	VAL
3	F	24	ARG
3	F	29	LEU
3	F	42	HIS
3	F	46	LEU
3	F	53	THR
3	F	73	SER
3	F	85	LEU
3	F	86	LEU
3	F	99	THR
3	F	100	THR
3	F	103	SER
3	F	113	GLN
3	F	114	LYS
3	F	115	ASP
3	F	120	SER
3	F	129	LEU
3	F	136	GLN
3	F	137	ARG
3	F	138	ILE
3	F	150	SER
3	F	151	VAL
3	F	152	LYS
3	F	155	ILE
3	F	165	GLN
3	F	184	ILE
3	F	194	VAL
3	F	201	ARG
3	F	202	THR
3	F	207	ARG
3	F	209	LEU
3	F	212	LYS
3	F	216	SER
3	F	221	VAL
3	F	233	VAL

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Mol	Chain	Res	Type
3	F	291	THR
3	F	293	THR
3	F	295	ILE
3	F	305	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
2	B	180	HIS
2	B	309	GLN
3	C	16	GLN
3	C	187	ASN
1	D	66	ASN
1	D	149	GLN
2	E	108	GLN
2	E	180	HIS
2	E	236	GLN
2	E	309	GLN
3	F	166	ASN
3	F	169	ASN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
4	NAG	E	401	2	14,14,15	0.60	0	17,19,21	1.08	2 (11%)
4	NAG	F	403	3	14,14,15	0.60	0	17,19,21	1.08	2 (11%)
4	NAG	B	402	2	14,14,15	0.52	0	17,19,21	0.98	2 (11%)
4	NAG	C	401	3	14,14,15	0.59	0	17,19,21	1.09	2 (11%)
4	NAG	F	401	3	14,14,15	0.55	0	17,19,21	1.05	0
4	NAG	C	402	3	14,14,15	0.60	0	17,19,21	0.95	0
4	NAG	E	402	2	14,14,15	0.67	0	17,19,21	1.06	2 (11%)
4	NAG	E	403	2	14,14,15	0.44	0	17,19,21	1.58	2 (11%)
4	NAG	F	402	3	14,14,15	0.50	0	17,19,21	0.60	0
4	NAG	B	403	2	14,14,15	0.60	0	17,19,21	1.07	2 (11%)
4	NAG	B	401	2	14,14,15	0.52	0	17,19,21	1.05	1 (5%)
4	NAG	E	404	2	14,14,15	0.67	0	17,19,21	1.50	1 (5%)
4	NAG	C	403	3	14,14,15	0.86	0	17,19,21	1.11	1 (5%)
4	NAG	C	404	3	14,14,15	0.52	0	17,19,21	0.61	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	401	2	-	1/6/23/26	0/1/1/1
4	NAG	F	403	3	-	0/6/23/26	0/1/1/1
4	NAG	B	402	2	-	2/6/23/26	0/1/1/1
4	NAG	C	401	3	-	0/6/23/26	0/1/1/1
4	NAG	F	401	3	-	2/6/23/26	0/1/1/1
4	NAG	C	402	3	-	5/6/23/26	0/1/1/1
4	NAG	E	402	2	-	1/6/23/26	0/1/1/1
4	NAG	E	403	2	-	0/6/23/26	0/1/1/1
4	NAG	F	402	3	-	4/6/23/26	0/1/1/1
4	NAG	B	403	2	-	1/6/23/26	0/1/1/1
4	NAG	B	401	2	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	404	2	-	1/6/23/26	0/1/1/1
4	NAG	C	403	3	-	0/6/23/26	0/1/1/1
4	NAG	C	404	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	404	NAG	C1-O5-C5	5.05	118.95	112.19
4	E	403	NAG	C2-N2-C7	-4.38	117.02	122.90
4	B	403	NAG	C1-O5-C5	-3.24	107.84	112.19
4	C	401	NAG	C1-O5-C5	-3.24	107.85	112.19
4	E	401	NAG	C1-O5-C5	-3.21	107.89	112.19
4	F	403	NAG	C1-O5-C5	-3.19	107.92	112.19
4	E	402	NAG	C2-N2-C7	-3.14	118.69	122.90
4	B	401	NAG	C1-O5-C5	2.87	116.03	112.19
4	B	402	NAG	C2-N2-C7	-2.75	119.22	122.90
4	E	402	NAG	C1-O5-C5	2.39	115.39	112.19
4	B	402	NAG	C1-O5-C5	2.39	115.38	112.19
4	F	403	NAG	O5-C1-C2	-2.11	108.03	111.29
4	C	401	NAG	O5-C1-C2	-2.11	108.03	111.29
4	E	401	NAG	O5-C1-C2	-2.09	108.05	111.29
4	E	403	NAG	C1-O5-C5	2.07	114.96	112.19
4	B	403	NAG	O5-C1-C2	-2.06	108.11	111.29
4	C	403	NAG	O5-C5-C4	-2.05	105.85	110.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	402	NAG	C8-C7-N2-C2
4	B	402	NAG	O7-C7-N2-C2
4	C	402	NAG	C3-C2-N2-C7
4	C	402	NAG	C8-C7-N2-C2
4	C	402	NAG	O7-C7-N2-C2
4	E	401	NAG	C3-C2-N2-C7
4	F	402	NAG	C8-C7-N2-C2
4	F	402	NAG	O7-C7-N2-C2
4	F	402	NAG	O5-C5-C6-O6
4	F	402	NAG	C4-C5-C6-O6
4	B	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	B	401	NAG	C8-C7-N2-C2
4	B	401	NAG	C4-C5-C6-O6
4	C	402	NAG	C4-C5-C6-O6
4	B	401	NAG	O7-C7-N2-C2
4	F	401	NAG	O5-C5-C6-O6
4	E	404	NAG	O5-C5-C6-O6
4	F	401	NAG	C4-C5-C6-O6
4	C	402	NAG	O5-C5-C6-O6
4	E	402	NAG	C4-C5-C6-O6
4	B	403	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	NAG	1	0
4	C	401	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	151/158 (95%)	-0.21	0	100 100	41, 62, 87, 96	0
1	D	152/158 (96%)	-0.61	0	100 100	24, 38, 65, 73	0
2	B	296/321 (92%)	0.04	3 (1%)	79 61	42, 71, 93, 116	0
2	E	307/321 (95%)	-0.45	1 (0%)	90 80	20, 43, 71, 90	1 (0%)
3	C	287/349 (82%)	-0.36	2 (0%)	84 68	18, 46, 73, 83	1 (0%)
3	F	289/349 (82%)	-0.20	2 (0%)	84 68	24, 55, 83, 95	0
All	All	1482/1656 (89%)	-0.28	8 (0%)	87 73	18, 53, 84, 116	2 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	36	PHE	2.9
3	C	33	PHE	2.6
3	F	202	THR	2.5
2	B	85	SER	2.4
2	B	84	SER	2.2
2	B	83	ASN	2.2
2	E	34	HIS	2.2
3	C	296	LEU	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 oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	NAG	F	403	14/15	0.61	0.18	94,101,110,113	0
4	NAG	B	403	14/15	0.64	0.15	67,79,83,85	0
4	NAG	C	404	14/15	0.66	0.16	81,92,104,106	0
4	NAG	C	401	14/15	0.80	0.15	64,69,75,79	0
4	NAG	F	401	14/15	0.81	0.11	55,76,89,93	0
4	NAG	F	402	14/15	0.82	0.12	57,84,92,93	0
4	NAG	C	402	14/15	0.85	0.13	29,50,61,66	0
4	NAG	E	401	14/15	0.86	0.12	28,51,59,67	0
4	NAG	B	402	14/15	0.88	0.10	62,75,82,83	0
4	NAG	E	404	14/15	0.89	0.12	42,67,83,87	0
4	NAG	C	403	14/15	0.90	0.09	42,59,67,68	0
4	NAG	B	401	14/15	0.91	0.08	56,72,78,78	0
4	NAG	E	402	14/15	0.94	0.09	29,43,48,60	0
4	NAG	E	403	14/15	0.96	0.06	28,36,44,47	0

6.5 Other polymers

There are no such residues in this entry.