



Full wwPDB/EMDataBank EM Map/Model Validation Report ⓘ

Dec 10, 2019 – 02:46 PM EST

PDB ID : 6D03
EMDB ID: : EMD-7783
Title : Cryo-EM structure of a Plasmodium vivax invasion complex essential for entry into human reticulocytes; one molecule of parasite ligand.
Authors : Gruszczyk, J.; Huang, R.K.; Hong, C.; Yu, Z.; Tham, W.H.
Deposited on : 2018-04-10
Resolution : 3.68 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

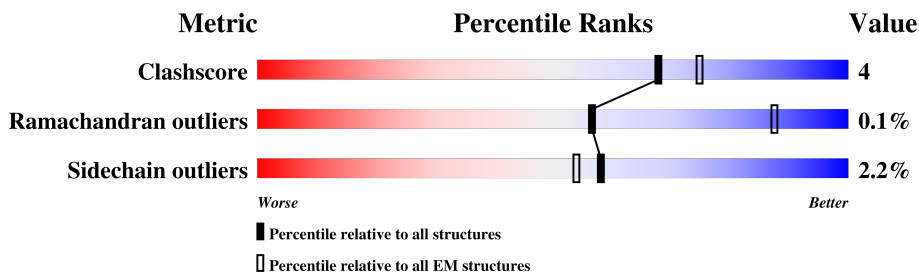
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.68 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	659	83% 14% .
1	B	659	87% 10% .
2	C	698	83% 14% .
2	D	698	86% 11% .
3	E	820	47% 9% 43%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24844 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transferrin receptor protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	641	Total	C	N	O	S	0	0
			5081	3260	855	952	14		
1	B	641	Total	C	N	O	S	0	0
			5081	3260	855	952	14		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	-	expression tag	UNP P02786
A	103	ASP	-	expression tag	UNP P02786
A	104	PRO	-	expression tag	UNP P02786
A	105	HIS	-	expression tag	UNP P02786
A	106	HIS	-	expression tag	UNP P02786
A	107	HIS	-	expression tag	UNP P02786
A	108	HIS	-	expression tag	UNP P02786
A	109	HIS	-	expression tag	UNP P02786
A	110	HIS	-	expression tag	UNP P02786
A	111	SER	-	expression tag	UNP P02786
A	112	SER	-	expression tag	UNP P02786
A	113	GLY	-	expression tag	UNP P02786
A	114	ILE	-	expression tag	UNP P02786
A	115	GLU	-	expression tag	UNP P02786
A	116	GLY	-	expression tag	UNP P02786
A	117	ARG	-	expression tag	UNP P02786
A	118	GLY	-	expression tag	UNP P02786
A	119	GLU	-	expression tag	UNP P02786
A	120	PHE	-	expression tag	UNP P02786
A	142	SER	GLY	variant	UNP P02786
B	102	ALA	-	expression tag	UNP P02786
B	103	ASP	-	expression tag	UNP P02786
B	104	PRO	-	expression tag	UNP P02786
B	105	HIS	-	expression tag	UNP P02786
B	106	HIS	-	expression tag	UNP P02786
B	107	HIS	-	expression tag	UNP P02786

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	HIS	-	expression tag	UNP P02786
B	109	HIS	-	expression tag	UNP P02786
B	110	HIS	-	expression tag	UNP P02786
B	111	SER	-	expression tag	UNP P02786
B	112	SER	-	expression tag	UNP P02786
B	113	GLY	-	expression tag	UNP P02786
B	114	ILE	-	expression tag	UNP P02786
B	115	GLU	-	expression tag	UNP P02786
B	116	GLY	-	expression tag	UNP P02786
B	117	ARG	-	expression tag	UNP P02786
B	118	GLY	-	expression tag	UNP P02786
B	119	GLU	-	expression tag	UNP P02786
B	120	PHE	-	expression tag	UNP P02786
B	142	SER	GLY	variant	UNP P02786

- Molecule 2 is a protein called Serotransferrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	679	Total	C	N	O	S	0	0
			5266	3305	912	1002	47		
2	D	679	Total	C	N	O	S	0	0
			5266	3305	912	1002	47		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	429	VAL	ILE	variant	UNP P02787
D	429	VAL	ILE	variant	UNP P02787

- Molecule 3 is a protein called Reticulocyte binding protein 2, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	466	Total	C	N	O	S	0	0
			3904	2495	650	749	10		

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	150	GLY	-	expression tag	UNP A5K736
E	151	ALA	-	expression tag	UNP A5K736
E	152	MET	-	expression tag	UNP A5K736
E	153	GLY	-	expression tag	UNP A5K736

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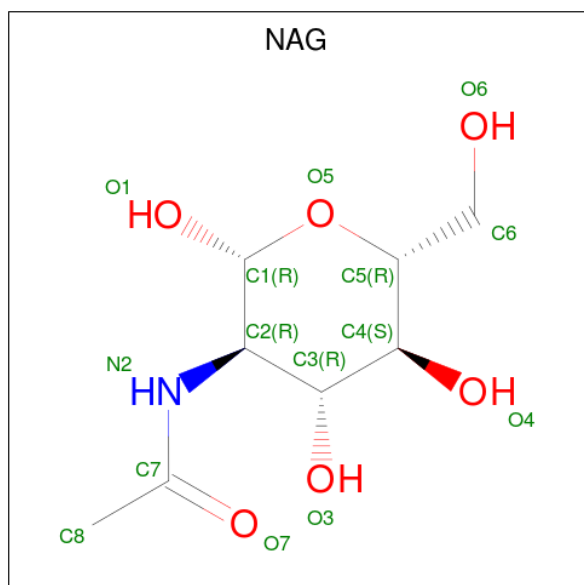
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Chain	Residue	Modelled	Actual	Comment	Reference
E	154	SER	-	expression tag	UNP A5K736
E	155	MET	-	expression tag	UNP A5K736
E	168	SER	ILE	variant	UNP A5K736

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Ca 1 1	0
4	A	1	Total Ca 1 1	0

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C N O 70 40 5 25	0
5	A	1	Total C N O 70 40 5 25	0
5	A	1	Total C N O 70 40 5 25	0
5	A	1	Total C N O 70 40 5 25	0
5	A	1	Total C N O 70 40 5 25	0
5	B	1	Total C N O 70 40 5 25	0

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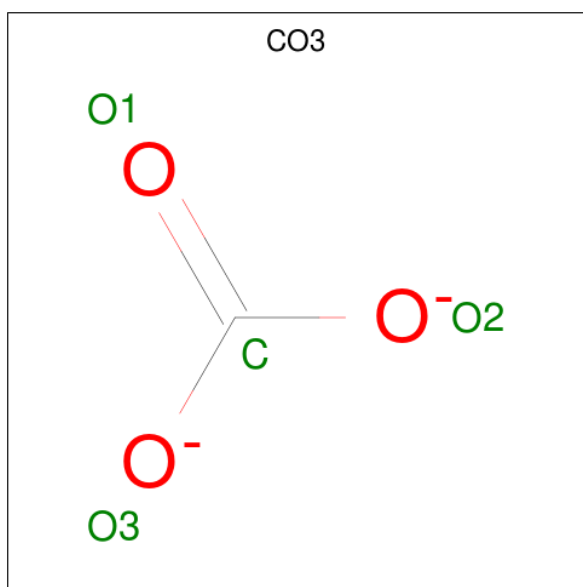
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Mol	Chain	Residues	Atoms				AltConf
5	B	1	Total	C	N	O	0
			70	40	5	25	
5	B	1	Total	C	N	O	0
			70	40	5	25	
5	B	1	Total	C	N	O	0
			70	40	5	25	
5	B	1	Total	C	N	O	0
			70	40	5	25	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	C	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	
5	D	1	Total	C	N	O	0
			42	24	3	15	

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
6	D	2	Total	Fe	0
			2	2	
6	C	2	Total	Fe	0
			2	2	

- Molecule 7 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).

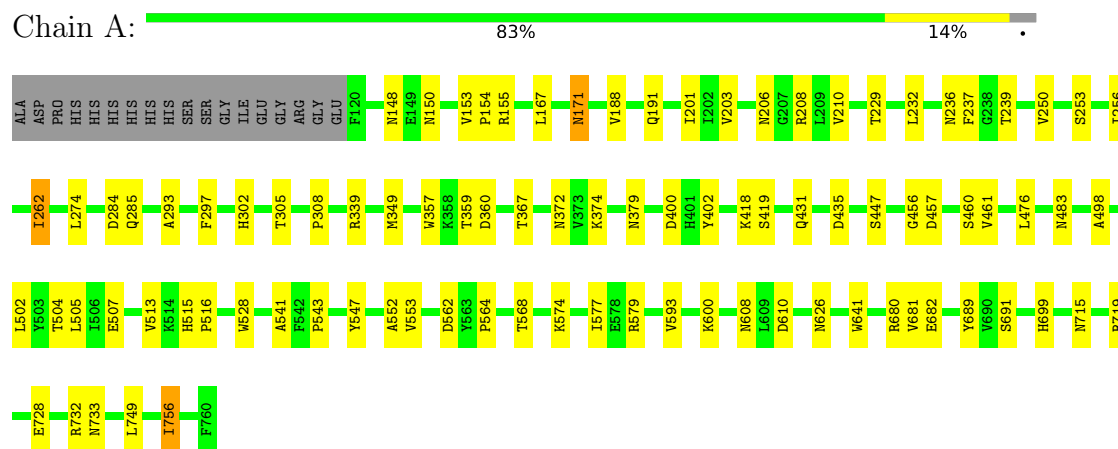


Mol	Chain	Residues	Atoms			AltConf
7	C	1	Total	C	O	0
			8	2	6	
7	C	1	Total	C	O	0
			8	2	6	
7	D	1	Total	C	O	0
			8	2	6	
7	D	1	Total	C	O	0
			8	2	6	

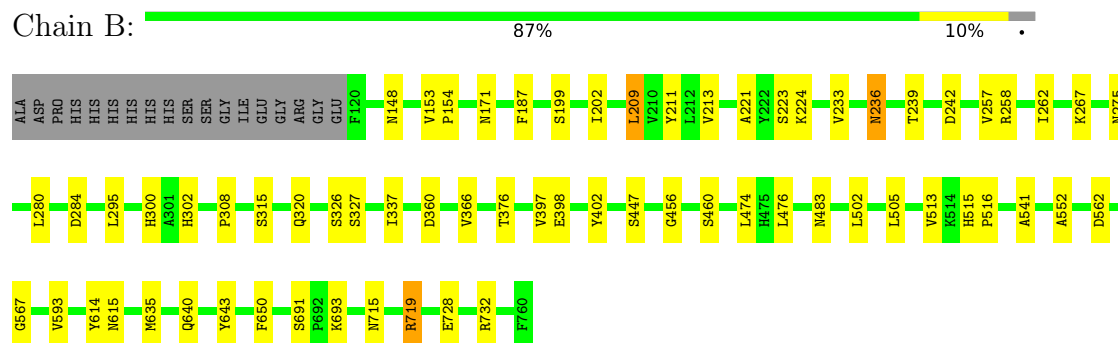
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

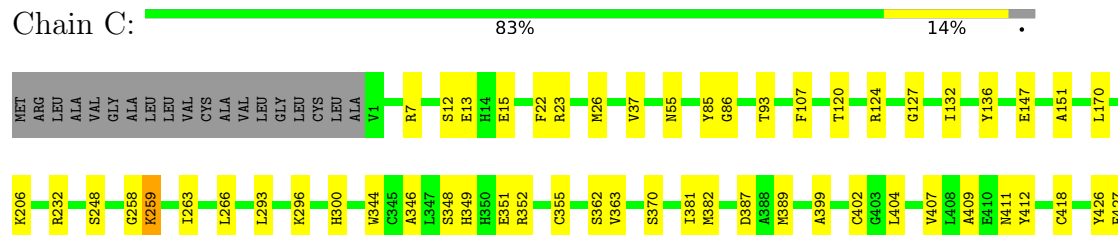
- Molecule 1: Transferrin receptor protein 1

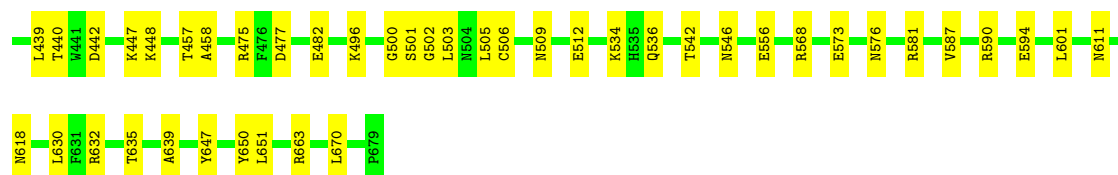


- Molecule 1: Transferrin receptor protein 1



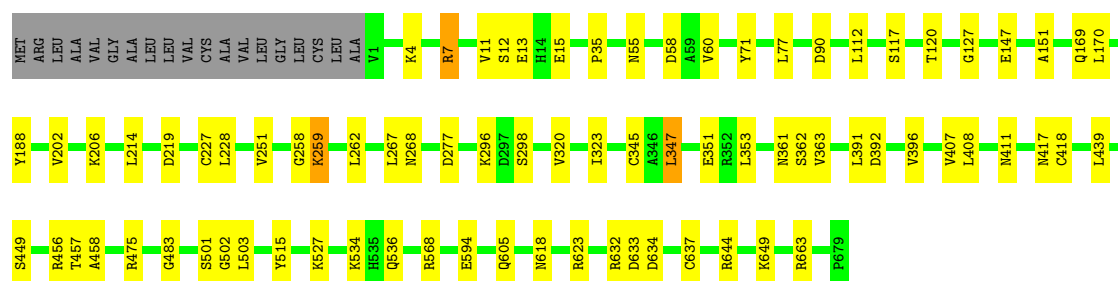
- Molecule 2: Serotransferrin





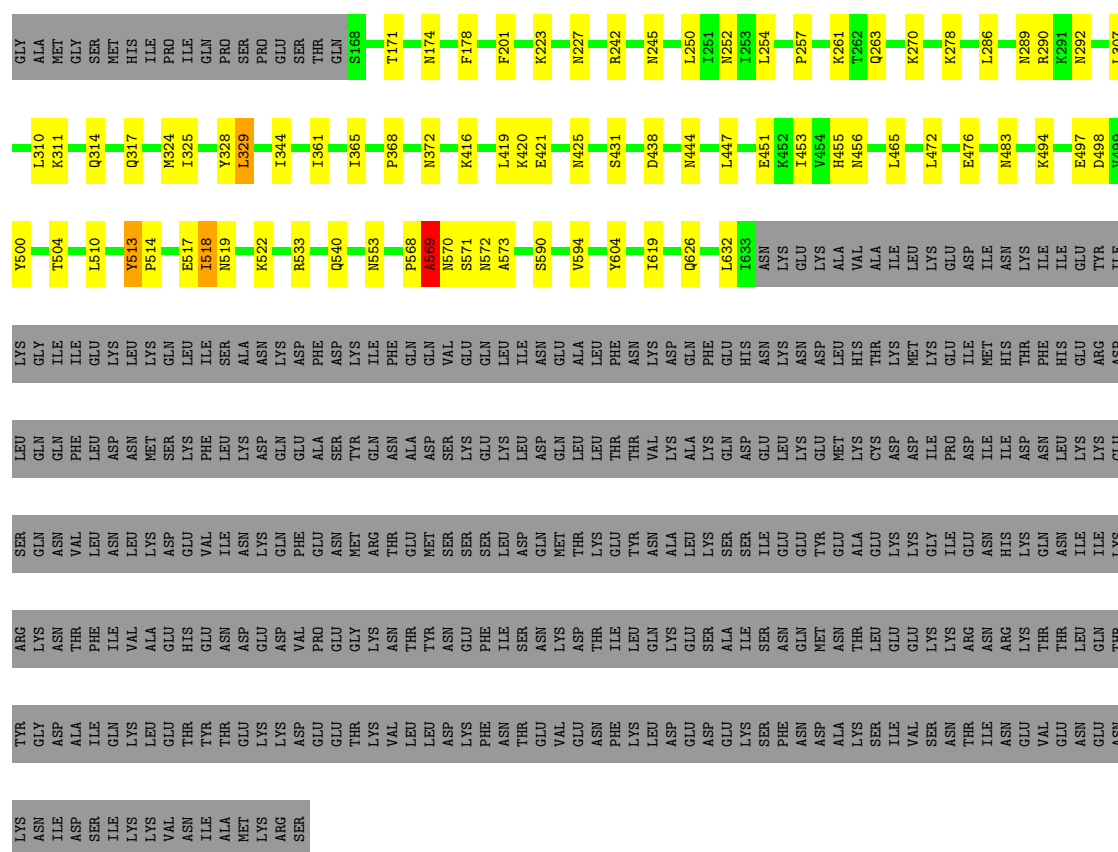
• Molecule 2: Serotransferrin

Chain D: 86% 11% .



• Molecule 3: Reticulocyte binding protein 2, putative

Chain E: 47% 9% 43%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	637649	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, FE, 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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.49	0/5203	0.64	2/7053 (0.0%)
1	B	0.50	0/5203	0.62	3/7053 (0.0%)
2	C	0.43	0/5386	0.61	3/7280 (0.0%)
2	D	0.42	0/5386	0.62	6/7280 (0.1%)
3	E	0.40	0/3973	0.60	3/5337 (0.1%)
All	All	0.45	0/25151	0.62	17/34003 (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	A	0	1
1	B	0	1
3	E	0	2
All	All	0	4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	476	LEU	CA-CB-CG	6.79	130.92	115.30
1	B	209	LEU	CA-CB-CG	6.55	130.37	115.30
2	D	112	LEU	CA-CB-CG	6.22	129.61	115.30
2	D	347	LEU	CA-CB-CG	6.12	129.38	115.30
2	C	503	LEU	CA-CB-CG	6.04	129.19	115.30
3	E	317	GLN	C-N-CA	6.00	136.69	121.70
2	D	503	LEU	CA-CB-CG	5.94	128.97	115.30
1	A	756	ILE	C-N-CA	5.74	136.04	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	419	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	262	ILE	CG1-CB-CG2	-5.68	98.90	111.40
1	B	295	LEU	CB-CG-CD2	-5.65	101.39	111.00
2	C	505	LEU	CA-CB-CG	5.52	128.01	115.30
3	E	569	ALA	C-N-CA	5.50	135.44	121.70
2	D	277	ASP	CB-CG-OD1	5.29	123.07	118.30
2	D	353	LEU	CA-CB-CG	5.21	127.29	115.30
2	C	670	LEU	CA-CB-CG	5.16	127.16	115.30
2	D	267	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	756	ILE	Peptide
1	B	567	GLY	Peptide
3	E	513	TYR	Peptide
3	E	569	ALA	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	5081	0	5009	47	0
1	B	5081	0	5010	32	0
2	C	5266	0	5086	56	0
2	D	5266	0	5085	38	0
3	E	3904	0	3918	39	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	70	0	63	0	0
5	B	70	0	63	0	0
5	C	42	0	37	0	0
5	D	42	0	38	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
7	C	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	8	0	0	1	0
All	All	24844	0	24309	208	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 4.

All (208) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PRO:O	1:A:547:TYR:HB3	1.77	0.84
2:C:132:ILE:O	2:C:136:TYR:HB2	1.82	0.79
1:A:203:VAL:O	1:A:372:ASN:HB3	1.82	0.79
2:D:449:SER:O	2:D:483:GLY:HA2	1.90	0.71
3:E:421:GLU:O	3:E:425:ASN:HB2	1.91	0.70
3:E:517:GLU:HG2	3:E:518:ILE:HG13	1.72	0.70
1:A:504:THR:O	1:A:507:GLU:HB2	1.93	0.69
1:A:681:VAL:HG23	1:A:749:LEU:HD21	1.75	0.68
1:A:682:GLU:OE2	1:A:699:HIS:NE2	2.30	0.64
2:C:448:LYS:HG2	2:C:482:GLU:HB2	1.81	0.63
2:C:500:GLY:HA3	2:C:512:GLU:HG2	1.80	0.62
2:D:439:LEU:O	2:D:568:ARG:NH1	2.33	0.61
3:E:500:TYR:OH	3:E:533:ARG:NH2	2.35	0.60
3:E:500:TYR:O	3:E:504:THR:HB	2.02	0.59
1:A:476:LEU:HD11	1:A:680:ARG:HB3	1.83	0.59
3:E:324:MET:O	3:E:328:TYR:HB3	2.03	0.59
2:C:346:ALA:O	2:C:370:SER:HA	2.03	0.58
2:D:411:ASN:ND2	2:D:418:CYS:O	2.36	0.58
3:E:171:THR:OG1	3:E:252:ASN:ND2	2.37	0.58
1:A:153:VAL:HG13	1:A:154:PRO:HD3	1.85	0.57
2:D:623:ARG:NH2	2:D:633:ASP:O	2.37	0.57
2:C:439:LEU:HD11	2:C:447:LYS:HG2	1.85	0.57
1:A:402:TYR:HB3	1:A:447:SER:HB2	1.87	0.56
1:B:456:GLY:HA2	1:B:460:SER:HA	1.86	0.56
1:A:641:TRP:HD1	1:B:320:GLN:HE21	1.53	0.56
1:B:258:ARG:NH1	1:B:284:ASP:OD2	2.39	0.56
1:B:502:LEU:O	1:B:505:LEU:HB3	2.06	0.56
2:C:348:SER:OG	2:C:509:ASN:ND2	2.39	0.56
2:C:542:THR:HG21	2:C:556:GLU:HB2	1.88	0.55
2:C:611:ASN:OD1	2:C:611:ASN:N	2.40	0.55
2:D:12:SER:OG	2:D:13:GLU:N	2.39	0.55
1:A:155:ARG:NH2	1:A:419:SER:OG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:PHE:HB3	1:A:568:THR:HG22	1.87	0.54
1:A:239:THR:HG22	1:A:262:ILE:HD11	1.90	0.54
3:E:178:PHE:HE1	3:E:278:LYS:HE2	1.72	0.54
1:A:600:LYS:O	1:A:608:ASN:ND2	2.39	0.54
2:C:411:ASN:ND2	2:C:418:CYS:O	2.40	0.54
2:D:534:LYS:NZ	2:D:634:ASP:OD2	2.40	0.54
1:A:456:GLY:HA2	1:A:460:SER:HA	1.90	0.54
2:C:37:VAL:HG22	2:C:266:LEU:HD21	1.88	0.54
2:C:15:GLU:HG2	2:C:293:LEU:HG	1.89	0.54
2:D:120:THR:HG22	2:D:127:GLY:HA3	1.90	0.53
1:B:239:THR:HG22	1:B:262:ILE:HD11	1.90	0.53
3:E:361:ILE:HD11	3:E:465:LEU:HD11	1.90	0.53
2:C:344:TRP:HE1	2:C:630:LEU:HD22	1.74	0.53
2:C:352:ARG:HD3	2:C:370:SER:HB3	1.89	0.53
2:D:457:THR:OG1	2:D:458:ALA:N	2.42	0.53
3:E:451:GLU:OE2	3:E:455:HIS:NE2	2.42	0.52
1:A:293:ALA:HB2	1:A:339:ARG:HH21	1.74	0.52
2:C:412:TYR:OH	2:C:632:ARG:NH2	2.42	0.52
2:D:407:VAL:HG12	2:D:408:LEU:HD12	1.91	0.52
2:C:124:ARG:NE	7:C:704:CO3:O2	2.42	0.52
2:D:188:TYR:HE2	2:D:296:LYS:HE2	1.75	0.52
2:D:392:ASP:O	2:D:396:VAL:N	2.40	0.52
3:E:368:PRO:O	3:E:372:ASN:ND2	2.43	0.51
1:A:515:HIS:CD2	1:A:516:PRO:HD2	2.46	0.51
2:D:147:GLU:HB3	2:D:170:LEU:HD11	1.92	0.51
3:E:472:LEU:O	3:E:476:GLU:HB2	2.10	0.51
2:C:439:LEU:O	2:C:568:ARG:NH1	2.44	0.51
2:C:93:THR:O	2:C:248:SER:OG	2.27	0.51
3:E:494:LYS:O	3:E:498:ASP:HB2	2.10	0.51
1:B:221:ALA:HB3	1:B:300:HIS:HA	1.92	0.51
2:D:206:LYS:NZ	2:D:298:SER:OG	2.44	0.51
1:B:562:ASP:N	1:B:562:ASP:OD1	2.44	0.51
2:C:409:ALA:O	2:C:639:ALA:HB3	2.10	0.51
1:B:236:ASN:N	1:B:242:ASP:OD2	2.39	0.50
2:D:4:LYS:HB3	2:D:35:PRO:HA	1.93	0.50
1:B:153:VAL:HG13	1:B:154:PRO:HD3	1.91	0.50
2:C:120:THR:HG22	2:C:127:GLY:HA3	1.93	0.50
2:C:534:LYS:HG3	2:C:536:GLN:H	1.75	0.50
3:E:568:PRO:HB2	3:E:571:SER:HB3	1.93	0.50
2:D:534:LYS:HG3	2:D:536:GLN:H	1.75	0.50
3:E:286:LEU:HG	3:E:290:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LEU:O	1:A:505:LEU:HB3	2.12	0.49
2:C:107:PHE:H	2:C:232:ARG:HH21	1.59	0.49
1:A:236:ASN:HB3	1:A:357:TRP:CE2	2.47	0.49
1:B:515:HIS:CD2	1:B:516:PRO:HD2	2.46	0.49
2:C:389:MET:O	2:C:587:VAL:HA	2.12	0.49
1:A:564:PRO:HG2	1:A:579:ARG:HH12	1.77	0.49
1:B:640:GLN:HA	1:B:643:TYR:HD2	1.77	0.49
3:E:325:ILE:O	3:E:329:LEU:HB2	2.13	0.49
3:E:254:LEU:HD12	3:E:270:LYS:HG3	1.94	0.49
2:D:11:VAL:HB	2:D:15:GLU:HG3	1.94	0.49
1:A:513:VAL:HG21	1:A:593:VAL:HG22	1.94	0.48
1:B:402:TYR:HB3	1:B:447:SER:HB2	1.95	0.48
2:C:477:ASP:OD1	2:C:477:ASP:N	2.44	0.48
2:C:506:CYS:N	2:C:512:GLU:OE2	2.43	0.48
2:D:457:THR:OG1	7:D:702:CO3:O3	2.31	0.48
2:C:147:GLU:O	2:C:151:ALA:HB2	2.13	0.48
2:C:426:TYR:OH	7:C:702:CO3:O1	2.27	0.48
1:B:199:SER:H	1:B:376:THR:HG23	1.79	0.48
2:C:399:ALA:HB1	2:C:404:LEU:HD12	1.95	0.48
2:C:346:ALA:HB1	2:C:351:GLU:HB3	1.94	0.48
1:B:280:LEU:HD23	1:B:337:ILE:HD13	1.96	0.47
2:C:407:VAL:HG22	2:C:594:GLU:HG3	1.94	0.47
2:D:258:GLY:HA3	2:D:259:LYS:HA	1.65	0.47
1:A:236:ASN:OD1	1:A:237:PHE:N	2.45	0.47
2:D:151:ALA:HB1	2:D:169:GLN:HB2	1.96	0.47
1:B:728:GLU:OE2	1:B:732:ARG:NE	2.43	0.47
3:E:497:GLU:OE2	3:E:540:GLN:NE2	2.44	0.47
3:E:513:TYR:OH	3:E:632:LEU:O	2.32	0.46
2:C:457:THR:OG1	2:C:458:ALA:N	2.47	0.46
2:D:347:LEU:H	2:D:351:GLU:HB2	1.79	0.46
2:D:227:CYS:SG	2:D:228:LEU:N	2.88	0.46
3:E:310:LEU:HB3	3:E:416:LYS:HD2	1.96	0.46
2:C:573:GLU:OE2	2:C:576:ASN:ND2	2.46	0.46
1:B:233:VAL:HG22	1:B:366:VAL:HG12	1.98	0.46
3:E:514:PRO:HG2	3:E:522:LYS:HE3	1.97	0.46
1:A:250:VAL:O	1:A:253:SER:OG	2.33	0.46
1:A:574:LYS:HA	1:A:577:ILE:HG22	1.98	0.46
1:A:691:SER:HB2	1:B:691:SER:HB2	1.97	0.46
1:B:202:ILE:N	1:B:211:TYR:O	2.48	0.46
1:B:223:SER:OG	1:B:224:LYS:N	2.48	0.46
1:B:397:VAL:HG12	1:B:398:GLU:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:412:TYR:HE1	2:C:632:ARG:HG2	1.81	0.46
2:C:85:TYR:HE1	2:C:296:LYS:HD3	1.80	0.46
3:E:569:ALA:H	3:E:570:ASN:HB3	1.81	0.46
2:C:86:GLY:O	2:C:300:HIS:ND1	2.49	0.45
3:E:201:PHE:HB2	3:E:431:SER:HB3	1.97	0.45
1:A:302:HIS:CD2	1:A:308:PRO:HB3	2.52	0.45
1:A:359:THR:OG1	1:A:360:ASP:N	2.49	0.45
1:B:360:ASP:OD1	1:B:360:ASP:N	2.49	0.45
2:C:206:LYS:HD3	2:C:296:LYS:HZ1	1.81	0.45
2:D:71:TYR:HA	2:D:77:LEU:H	1.81	0.45
1:A:201:ILE:HD11	1:A:210:VAL:HG13	1.98	0.45
2:D:117:SER:HA	2:D:202:VAL:O	2.17	0.45
1:A:507:GLU:OE2	1:A:528:TRP:NE1	2.50	0.45
2:C:440:THR:HG22	2:C:442:ASP:H	1.82	0.45
1:B:541:ALA:HB1	1:B:552:ALA:HB1	1.99	0.45
3:E:361:ILE:HG13	3:E:365:ILE:HD13	1.99	0.45
1:A:305:THR:HG21	1:A:543:PRO:HG3	1.99	0.45
2:D:407:VAL:HG22	2:D:594:GLU:HG3	1.99	0.45
1:A:349:MET:HG2	1:A:367:THR:HA	1.99	0.45
2:D:214:LEU:HD13	2:D:219:ASP:HB3	1.98	0.45
2:D:347:LEU:HD23	2:D:351:GLU:HG3	1.99	0.45
2:D:90:ASP:N	2:D:90:ASP:OD1	2.47	0.44
1:B:326:SER:OG	1:B:327:SER:N	2.51	0.44
2:D:534:LYS:NZ	2:D:632:ARG:HD3	2.33	0.44
2:D:60:VAL:O	2:D:251:VAL:HA	2.18	0.44
2:C:381:ILE:HD11	2:C:389:MET:HB2	2.00	0.44
1:A:188:VAL:HG11	1:A:461:VAL:HG21	2.00	0.44
1:A:728:GLU:OE2	1:A:732:ARG:NH2	2.44	0.44
1:B:513:VAL:HG21	1:B:593:VAL:HG22	2.00	0.44
2:D:320:VAL:HA	2:D:323:ILE:HG22	1.99	0.44
1:B:284:ASP:OD1	1:B:284:ASP:N	2.49	0.44
2:C:382:MET:SD	2:C:402:CYS:HB3	2.58	0.44
3:E:310:LEU:HD23	3:E:416:LYS:HG3	2.00	0.44
3:E:324:MET:O	3:E:328:TYR:CB	2.65	0.44
1:B:187:PHE:O	1:B:315:SER:OG	2.36	0.44
1:B:615:ASN:HD21	1:B:650:PHE:HD1	1.64	0.44
3:E:510:LEU:HD21	3:E:626:GLN:HG3	2.00	0.44
3:E:289:ASN:HD22	3:E:292:ASN:HD22	1.65	0.43
1:A:191:GLN:HE21	1:A:379:ASN:HB2	1.82	0.43
3:E:223:LYS:O	3:E:227:ASN:HB2	2.19	0.43
3:E:572:ASN:HA	3:E:573:ALA:HA	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:348:SER:O	2:C:349:HIS:ND1	2.52	0.43
2:C:501:SER:HA	2:C:502:GLY:HA2	1.74	0.43
3:E:344:ILE:HD12	3:E:344:ILE:HA	1.89	0.43
3:E:510:LEU:HD13	3:E:510:LEU:HA	1.87	0.43
1:B:635:MET:HG3	1:B:719:ARG:HH12	1.84	0.42
2:C:351:GLU:O	2:C:355:CYS:HB2	2.18	0.42
2:C:147:GLU:O	2:C:151:ALA:CB	2.67	0.42
3:E:365:ILE:HD11	3:E:465:LEU:HG	2.01	0.42
1:A:284:ASP:OD1	1:A:284:ASP:N	2.52	0.42
3:E:361:ILE:HD12	3:E:361:ILE:HA	1.89	0.42
2:D:449:SER:O	2:D:483:GLY:CA	2.63	0.42
2:D:605:GLN:HE21	2:D:637:CYS:HB2	1.84	0.42
3:E:590:SER:OG	3:E:590:SER:O	2.38	0.42
1:A:689:TYR:HB3	1:B:693:LYS:HD2	2.02	0.42
2:C:258:GLY:HA3	2:C:259:LYS:HA	1.65	0.42
2:D:362:SER:OG	2:D:363:VAL:N	2.53	0.42
1:A:167:LEU:O	1:A:171:ASN:HB2	2.19	0.42
1:A:431:GLN:O	1:A:435:ASP:HB2	2.20	0.42
2:C:647:TYR:O	2:C:651:LEU:HB2	2.20	0.42
2:D:12:SER:H	2:D:15:GLU:HB2	1.85	0.42
1:A:400:ASP:OD1	1:A:400:ASP:N	2.53	0.42
1:A:504:THR:OG1	1:A:610:ASP:OD2	2.31	0.42
1:A:498:ALA:HB2	1:A:553:VAL:HG23	2.02	0.41
1:B:213:VAL:O	3:E:604:TYR:OH	2.34	0.41
2:C:147:GLU:HB3	2:C:170:LEU:HD11	2.02	0.41
2:D:456:ARG:NH2	2:D:515:TYR:OH	2.53	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.93	0.41
2:C:534:LYS:HG3	2:C:536:GLN:N	2.35	0.41
1:A:262:ILE:HG21	1:A:262:ILE:HD13	1.87	0.41
2:D:644:ARG:HA	2:D:649:LYS:HE3	2.02	0.41
2:D:501:SER:HA	2:D:502:GLY:HA2	1.69	0.41
1:A:541:ALA:HB1	1:A:552:ALA:HB1	2.02	0.41
1:A:562:ASP:OD1	1:A:562:ASP:N	2.52	0.41
2:C:412:TYR:CE1	2:C:632:ARG:HG2	2.56	0.41
1:A:229:THR:HG22	1:A:374:LYS:HB2	2.02	0.41
1:A:232:LEU:HD21	1:A:256:ILE:HB	2.02	0.41
1:B:302:HIS:CE1	1:B:308:PRO:HB3	2.56	0.41
2:D:7:ARG:O	2:D:58:ASP:N	2.50	0.41
2:C:362:SER:OG	2:C:363:VAL:N	2.54	0.41
3:E:553:ASN:HD21	3:E:594:VAL:HG13	1.86	0.41
2:C:355:CYS:HB2	2:C:630:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:632:ARG:HB3	2:C:635:THR:HG23	2.02	0.41
3:E:257:PRO:O	3:E:261:LYS:HB2	2.20	0.41
2:C:12:SER:OG	2:C:13:GLU:N	2.54	0.40
2:C:387:ASP:OD1	2:C:590:ARG:NH2	2.53	0.40
2:C:650:TYR:HD2	2:C:651:LEU:HD22	1.86	0.40
2:C:22:PHE:O	2:C:26:MET:HB2	2.20	0.40
3:E:307:LEU:HD13	3:E:420:LYS:HG3	2.04	0.40
1:B:257:VAL:HG21	1:B:267:LYS:HD3	2.02	0.40
2:C:601:LEU:HD23	2:C:601:LEU:HA	1.88	0.40
1:A:418:LYS:NZ	1:A:457:ASP:OD1	2.41	0.40
3:E:438:ASP:N	3:E:438:ASP:OD1	2.54	0.40
2:C:427:PHE:HE1	2:C:581:ARG:HE	1.70	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 PDB entries followed by that with respect to all EM entries.

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	639/659 (97%)	606 (95%)	33 (5%)	0	100	100
1	B	639/659 (97%)	608 (95%)	31 (5%)	0	100	100
2	C	677/698 (97%)	633 (94%)	44 (6%)	0	100	100
2	D	677/698 (97%)	632 (93%)	45 (7%)	0	100	100
3	E	464/820 (57%)	450 (97%)	12 (3%)	2 (0%)	36	74
All	All	3096/3534 (88%)	2929 (95%)	165 (5%)	2 (0%)	56	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	519	ASN
3	E	518	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 PDB entries followed by that with respect to all EM entries.

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	550/564 (98%)	539 (98%)	11 (2%)	58	82
1	B	550/564 (98%)	540 (98%)	10 (2%)	62	84
2	C	572/585 (98%)	562 (98%)	10 (2%)	63	85
2	D	572/585 (98%)	559 (98%)	13 (2%)	53	80
3	E	442/775 (57%)	428 (97%)	14 (3%)	42	74
All	All	2686/3073 (87%)	2628 (98%)	58 (2%)	58	80

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	ASN
1	A	150	ASN
1	A	171	ASN
1	A	206	ASN
1	A	208	ARG
1	A	285	GLN
1	A	483	ASN
1	A	626	ASN
1	A	715	ASN
1	A	719	ARG
1	A	733	ASN
1	B	148	ASN
1	B	171	ASN
1	B	209	LEU
1	B	236	ASN
1	B	275	ASN
1	B	474	LEU
1	B	483	ASN
1	B	614	TYR
1	B	715	ASN
1	B	719	ARG
2	C	7	ARG
2	C	23	ARG

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Mol	Chain	Res	Type
2	C	55	ASN
2	C	259	LYS
2	C	263	ILE
2	C	475	ARG
2	C	496	LYS
2	C	546	ASN
2	C	618	ASN
2	C	663	ARG
2	D	7	ARG
2	D	55	ASN
2	D	259	LYS
2	D	262	LEU
2	D	268	ASN
2	D	345	CYS
2	D	361	ASN
2	D	391	LEU
2	D	417	ASN
2	D	475	ARG
2	D	527	LYS
2	D	618	ASN
2	D	663	ARG
3	E	174	ASN
3	E	242	ARG
3	E	245	ASN
3	E	250	LEU
3	E	263	GLN
3	E	311	LYS
3	E	314	GLN
3	E	329	LEU
3	E	444	ASN
3	E	447	LEU
3	E	453	ILE
3	E	456	ASN
3	E	483	ASN
3	E	619	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	171	ASN
1	A	206	ASN

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Mol	Chain	Res	Type
1	A	348	ASN
1	A	379	ASN
1	A	515	HIS
1	A	626	ASN
1	A	715	ASN
1	A	733	ASN
1	B	171	ASN
1	B	236	ASN
1	B	275	ASN
1	B	302	HIS
1	B	401	HIS
1	B	483	ASN
1	B	715	ASN
2	C	25	HIS
2	C	55	ASN
2	C	213	ASN
2	C	509	ASN
2	C	546	ASN
2	C	604	GLN
2	C	618	ASN
2	D	55	ASN
2	D	268	ASN
2	D	361	ASN
2	D	417	ASN
2	D	469	ASN
2	D	618	ASN
3	E	174	ASN
3	E	245	ASN
3	E	252	ASN
3	E	289	ASN
3	E	314	GLN
3	E	372	ASN
3	E	428	ASN
3	E	444	ASN
3	E	483	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 6 are monoatomic - leaving 20 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	$\# Z > 2$
5	NAG	A	802	1	14,14,15	0.49	0	17,19,21	0.57	0
5	NAG	A	803	1,5	14,14,15	0.27	0	17,19,21	1.51	2 (11%)
5	NAG	A	804	5	14,14,15	0.23	0	17,19,21	0.53	0
5	NAG	A	805	1,5	14,14,15	0.53	0	17,19,21	1.06	1 (5%)
5	NAG	A	806	5	14,14,15	0.69	1 (7%)	17,19,21	0.66	0
5	NAG	B	802	1	14,14,15	0.50	0	17,19,21	0.64	1 (5%)
5	NAG	B	803	1,5	14,14,15	0.61	0	17,19,21	0.57	0
5	NAG	B	804	5	14,14,15	0.41	0	17,19,21	0.40	0
5	NAG	B	805	1,5	14,14,15	0.57	0	17,19,21	1.07	1 (5%)
5	NAG	B	806	5	14,14,15	0.39	0	17,19,21	0.43	0
7	CO3	C	702	6	0,3,3	0.00	-	0,3,3	0.00	-
7	CO3	C	704	6	0,3,3	0.00	-	0,3,3	0.00	-
5	NAG	C	705	2,5	14,14,15	0.42	0	17,19,21	0.88	1 (5%)
5	NAG	C	706	5	14,14,15	0.59	0	17,19,21	0.92	1 (5%)
5	NAG	C	707	2	14,14,15	0.36	0	17,19,21	0.65	1 (5%)
7	CO3	D	702	6	0,3,3	0.00	-	0,3,3	0.00	-
7	CO3	D	704	6	0,3,3	0.00	-	0,3,3	0.00	-
5	NAG	D	705	2,5	14,14,15	0.41	0	17,19,21	0.67	0
5	NAG	D	706	5	14,14,15	1.35	1 (7%)	17,19,21	1.47	1 (5%)
5	NAG	D	707	2	14,14,15	1.22	1 (7%)	17,19,21	1.30	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	802	1	-	2/6/23/26	0/1/1/1
5	NAG	A	803	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	804	5	-	0/6/23/26	0/1/1/1
5	NAG	A	805	1,5	-	1/6/23/26	0/1/1/1
5	NAG	A	806	5	-	4/6/23/26	0/1/1/1
5	NAG	B	802	1	-	2/6/23/26	0/1/1/1
5	NAG	B	803	1,5	-	2/6/23/26	0/1/1/1
5	NAG	B	804	5	-	2/6/23/26	0/1/1/1
5	NAG	B	805	1,5	-	2/6/23/26	0/1/1/1
5	NAG	B	806	5	-	2/6/23/26	0/1/1/1
5	NAG	C	705	2,5	-	2/6/23/26	0/1/1/1
5	NAG	C	706	5	-	3/6/23/26	0/1/1/1
5	NAG	C	707	2	-	2/6/23/26	0/1/1/1
5	NAG	D	705	2,5	-	4/6/23/26	0/1/1/1
5	NAG	D	706	5	-	2/6/23/26	0/1/1/1
5	NAG	D	707	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	706	NAG	O5-C1	4.84	1.51	1.43
5	D	707	NAG	O5-C1	4.15	1.50	1.43
5	A	806	NAG	C1-C2	2.35	1.55	1.52

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	706	NAG	C1-O5-C5	5.72	119.97	112.20
5	D	707	NAG	C1-O5-C5	5.10	119.13	112.20
5	A	803	NAG	C1-O5-C5	4.81	118.74	112.20
5	B	805	NAG	C2-N2-C7	3.18	127.48	122.92
5	C	706	NAG	C2-N2-C7	3.15	127.43	122.92
5	A	805	NAG	C2-N2-C7	3.11	127.38	122.92
5	C	705	NAG	C1-O5-C5	3.02	116.31	112.20
5	A	803	NAG	C2-N2-C7	2.99	127.21	122.92
5	C	707	NAG	C1-O5-C5	2.28	115.30	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	NAG	C1-O5-C5	2.12	115.08	112.20

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	802	NAG	O5-C5-C6-O6
5	A	802	NAG	C4-C5-C6-O6
5	B	806	NAG	O5-C5-C6-O6
5	C	706	NAG	O5-C5-C6-O6
5	B	806	NAG	C4-C5-C6-O6
5	A	806	NAG	C8-C7-N2-C2
5	A	806	NAG	O7-C7-N2-C2
5	D	705	NAG	C8-C7-N2-C2
5	D	705	NAG	O7-C7-N2-C2
5	C	706	NAG	C4-C5-C6-O6
5	D	706	NAG	C4-C5-C6-O6
5	D	705	NAG	O5-C5-C6-O6
5	B	802	NAG	O5-C5-C6-O6
5	B	804	NAG	O5-C5-C6-O6
5	D	705	NAG	C4-C5-C6-O6
5	C	705	NAG	O5-C5-C6-O6
5	B	805	NAG	O5-C5-C6-O6
5	D	706	NAG	O5-C5-C6-O6
5	B	804	NAG	C4-C5-C6-O6
5	C	705	NAG	C4-C5-C6-O6
5	A	806	NAG	C4-C5-C6-O6
5	A	806	NAG	O5-C5-C6-O6
5	B	803	NAG	C4-C5-C6-O6
5	C	707	NAG	O5-C5-C6-O6
5	C	707	NAG	C4-C5-C6-O6
5	B	802	NAG	C4-C5-C6-O6
5	B	803	NAG	O5-C5-C6-O6
5	A	803	NAG	C3-C2-N2-C7
5	C	706	NAG	C3-C2-N2-C7
5	B	805	NAG	C3-C2-N2-C7
5	A	805	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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.