



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:57 AM UTC

PDB ID : 5HCE / pdb_00005hce
Title : Ternary complex of human Complement C5 with Ornithodoros moubata OmCI and Rhipicephalus appendiculatus RaCI1
Authors : Jore, M.M.; Johnson, S.; Lea, S.M.
Deposited on : 2016-01-04
Resolution : 3.12 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

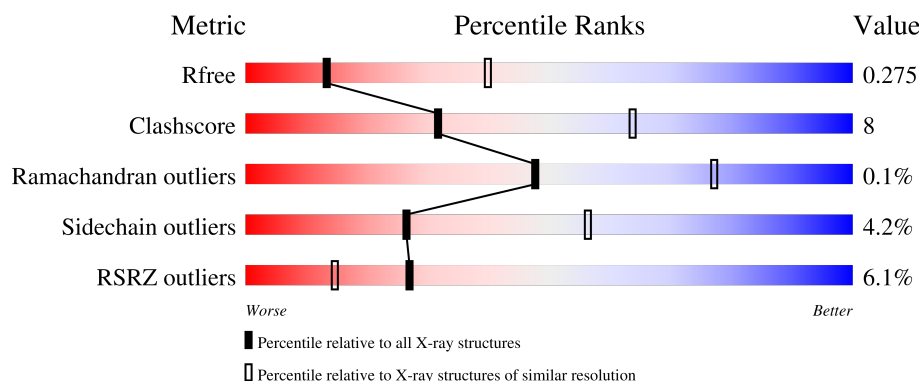
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	B	656	5% 76% 22% ..
2	A	998	7% 77% 20% ..
3	C	165	% 75% 15% 10%
4	D	81	2% 33% 21% 42%
5	E	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14418 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 Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	647	Total	C	N	O	S	0	0	0
			5116	3281	819	1003	13			

- Molecule 2 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	982	Total	C	N	O	S	0	0	0
			7775	4973	1298	1463	41			

- Molecule 3 is a protein called Complement inhibitor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1160	715	195	239	11			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	initiating methionine	UNP Q5YD59
C	5	ALA	-	expression tag	UNP Q5YD59
C	6	SER	-	expression tag	UNP Q5YD59
C	7	HIS	-	expression tag	UNP Q5YD59
C	8	HIS	-	expression tag	UNP Q5YD59
C	9	HIS	-	expression tag	UNP Q5YD59
C	10	HIS	-	expression tag	UNP Q5YD59
C	11	HIS	-	expression tag	UNP Q5YD59
C	12	HIS	-	expression tag	UNP Q5YD59
C	13	HIS	-	expression tag	UNP Q5YD59
C	14	HIS	-	expression tag	UNP Q5YD59
C	15	HIS	-	expression tag	UNP Q5YD59
C	16	HIS	-	expression tag	UNP Q5YD59
C	17	SER	-	expression tag	UNP Q5YD59

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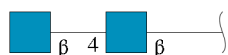
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP Q5YD59
C	78	GLN	ASN	engineered mutation	UNP Q5YD59
C	102	GLN	ASN	engineered mutation	UNP Q5YD59

- Molecule 4 is a protein called Rhipicephalus appendiculatus RaCI1.

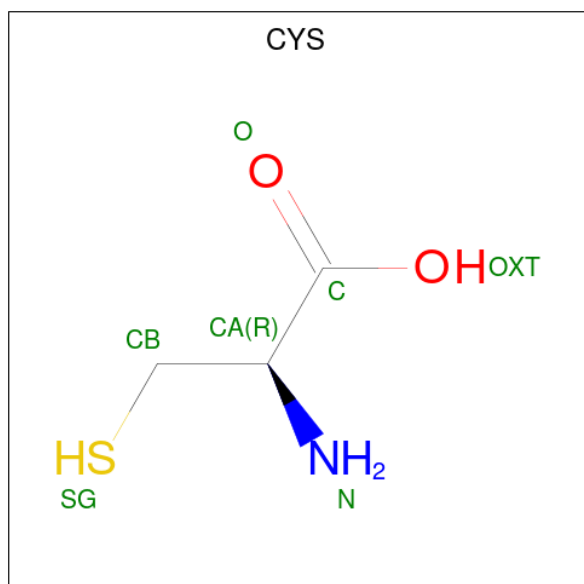
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	47	Total	C	N	O	S	0	0	0
			333	203	62	62	6			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 6 is CYSTEINE (CCD ID: CYS) (formula: C₃H₇NO₂S).

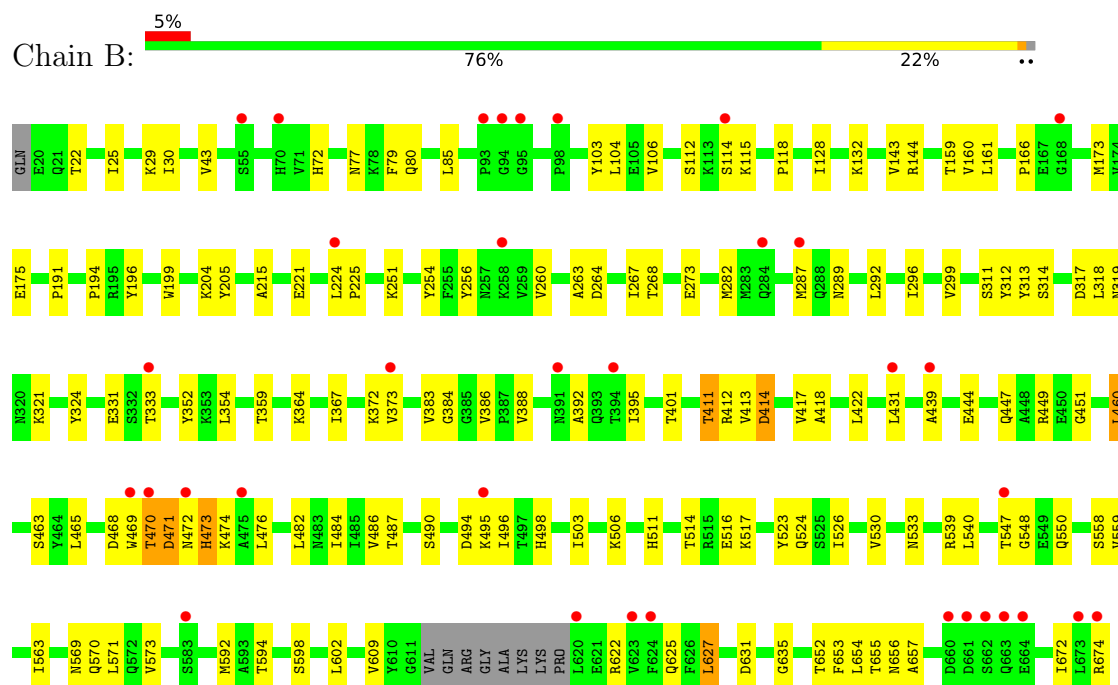


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

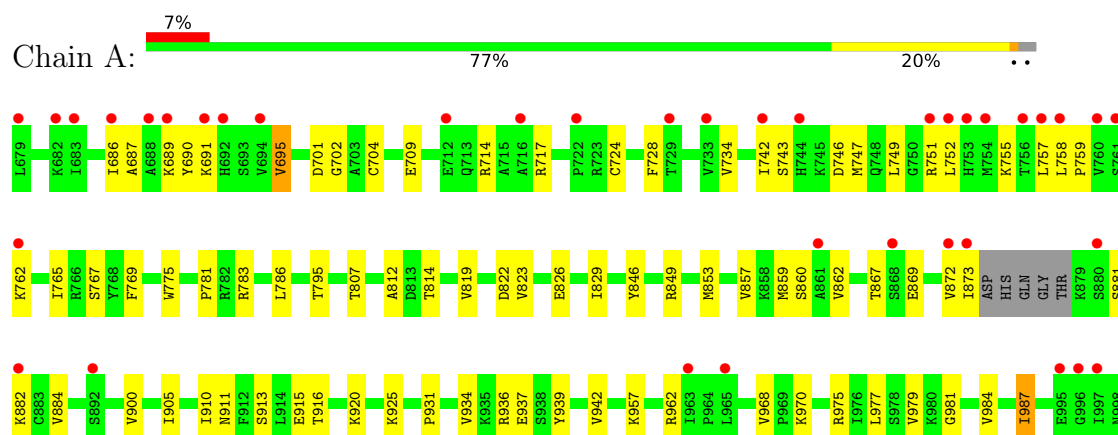
3 Residue-property plots [i](#)

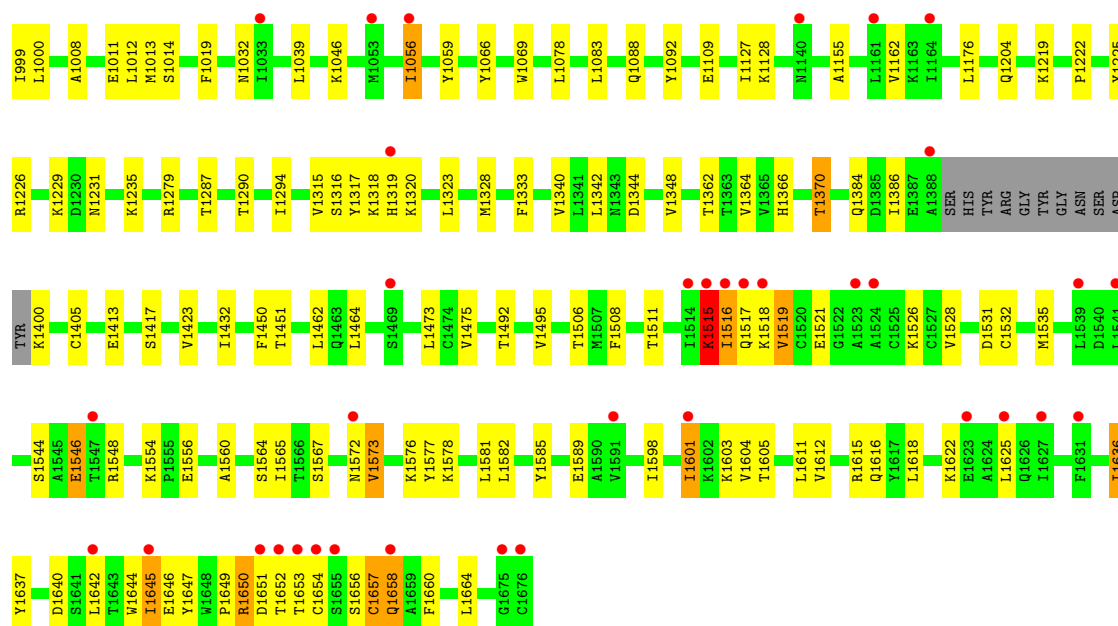
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Complement C5

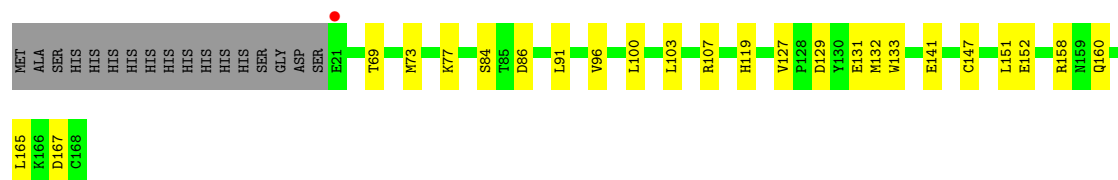
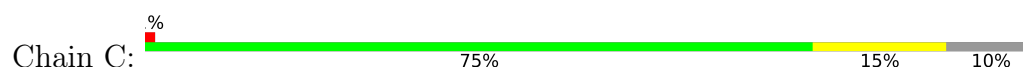


• Molecule 2: Complement C5

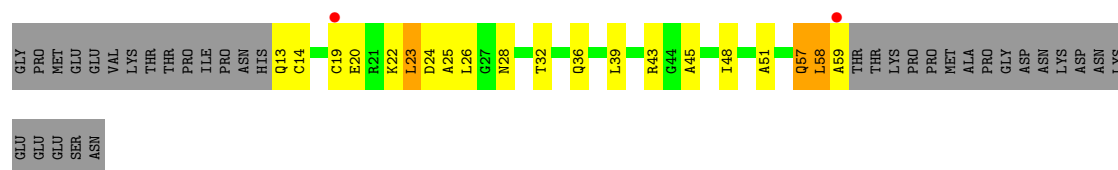
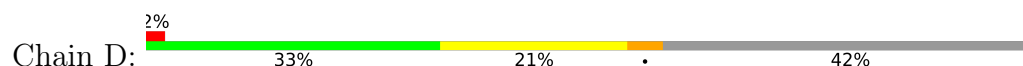




• Molecule 3: Complement inhibitor



• Molecule 4: Rhipicephalus appendiculatus RaCI1



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.26Å 140.72Å 210.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.40 – 3.12 74.40 – 3.12	Depositor EDS
% Data completeness (in resolution range)	98.9 (74.40-3.12) 99.1 (74.40-3.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.267 , 0.281 0.267 , 0.275	Depositor DCC
R_{free} test set	2771 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14418	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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	B	0.24	0/5234	0.44	2/7119 (0.0%)
2	A	0.27	0/7932	0.44	1/10740 (0.0%)
3	C	0.20	0/1183	0.35	0/1599
4	D	0.28	0/335	0.48	0/454
All	All	0.26	0/14684	0.43	3/19912 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1515	LYS	N-CA-C	-8.74	95.27	108.99
1	B	470	THR	CA-C-N	-6.28	112.04	122.21
1	B	470	THR	C-N-CA	-6.28	112.04	122.21

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	468	ASP	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	B	5116	0	5022	90	0
2	A	7775	0	7822	129	0
3	C	1160	0	1085	12	0
4	D	333	0	335	13	0
5	E	28	0	25	0	0
6	A	6	0	3	0	0
All	All	14418	0	14292	233	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 8.

All (233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TRP:HA	1:B:484:ILE:HA	1.60	0.84
3:C:77:LYS:NZ	3:C:167:ASP:O	2.17	0.77
1:B:359:THR:HG21	1:B:372:LYS:H	1.49	0.77
2:A:1625:LEU:HB2	2:A:1636:ILE:HG23	1.64	0.77
1:B:384:GLY:HA3	1:B:413:VAL:HG23	1.68	0.76
2:A:1515:LYS:HE3	2:A:1516:ILE:HG23	1.67	0.75
2:A:751:ARG:O	2:A:755:LYS:HB2	1.91	0.71
1:B:373:VAL:HG21	1:B:388:VAL:HG11	1.72	0.70
2:A:1012:LEU:HD21	2:A:1056:ILE:HD12	1.73	0.70
1:B:268:THR:HG22	1:B:287:MET:HG2	1.72	0.70
2:A:942:VAL:HG21	2:A:957:LYS:HG2	1.72	0.70
2:A:695:VAL:HG21	2:A:724:CYS:HA	1.73	0.69
1:B:386:VAL:H	1:B:411:THR:HB	1.57	0.68
1:B:72:HIS:O	1:B:77:ASN:ND2	2.27	0.68
1:B:655:THR:HG22	1:B:657:ALA:H	1.58	0.68
2:A:1517:GLN:NE2	2:A:1604:VAL:O	2.26	0.67
2:A:1532:CYS:HA	2:A:1640:ASP:HA	1.76	0.67
1:B:487:THR:HG22	1:B:523:TYR:HB3	1.79	0.65
2:A:1109:GLU:OE1	4:D:43:ARG:NH2	2.29	0.64
1:B:451:GLY:O	1:B:674:ARG:NH2	2.30	0.63
2:A:1515:LYS:HG2	2:A:1516:ILE:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1128:LYS:NZ	2:A:1417:SER:OG	2.32	0.62
4:D:24:ASP:HB2	4:D:28:ASN:HB2	1.80	0.62
2:A:743:SER:OG	2:A:746:ASP:OD1	2.17	0.62
2:A:1219:LYS:HB2	2:A:1225:TYR:HB2	1.80	0.62
1:B:25:ILE:O	1:B:653:PHE:HA	1.99	0.61
2:A:934:VAL:HG23	2:A:1508:PHE:CZ	2.35	0.60
2:A:1450:PHE:CZ	2:A:1475:VAL:HB	2.37	0.60
1:B:273:GLU:OE2	1:B:321:LYS:NZ	2.36	0.59
2:A:915:GLU:OE2	2:A:920:LYS:NZ	2.36	0.59
1:B:569:ASN:ND2	1:B:598:SER:HB2	2.19	0.58
2:A:1576:LYS:HE2	2:A:1601:ILE:HD11	1.84	0.58
2:A:1612:VAL:HB	2:A:1615:ARG:HD2	1.86	0.57
2:A:1556:GLU:HB3	2:A:1622:LYS:HE2	1.86	0.57
1:B:331:GLU:OE2	1:B:333:THR:OG1	2.19	0.57
2:A:979:VAL:HG12	2:A:1328:MET:HE1	1.87	0.57
1:B:417:VAL:HG21	1:B:473:HIS:CD2	2.39	0.56
1:B:22:THR:HA	1:B:656:ASN:HD21	1.71	0.56
2:A:1567:SER:HB2	2:A:1578:LYS:HD2	1.87	0.56
1:B:414:ASP:OD1	1:B:414:ASP:N	2.36	0.55
1:B:115:LYS:HB2	1:B:654:LEU:HD21	1.86	0.55
2:A:915:GLU:HG2	2:A:920:LYS:HG3	1.87	0.55
1:B:144:ARG:NH2	1:B:602:LEU:O	2.40	0.55
2:A:709:GLU:OE1	2:A:717:ARG:NH2	2.39	0.55
1:B:132:LYS:HD2	1:B:609:VAL:HG11	1.88	0.55
2:A:751:ARG:O	2:A:755:LYS:CB	2.54	0.55
1:B:364:LYS:HB3	1:B:367:ILE:HD13	1.88	0.54
2:A:1370:THR:HG21	2:A:1506:THR:HB	1.90	0.54
2:A:1622:LYS:HE3	2:A:1642:LEU:HD23	1.88	0.54
1:B:221:GLU:OE1	2:A:762:LYS:NZ	2.40	0.54
2:A:1519:VAL:HG13	2:A:1521:GLU:H	1.73	0.54
2:A:1535:MET:HG3	2:A:1645:ILE:HD11	1.90	0.54
1:B:204:LYS:HG2	1:B:205:TYR:H	1.73	0.54
2:A:857:VAL:HA	2:A:913:SER:O	2.07	0.54
2:A:1432:ILE:HG13	2:A:1511:THR:HG21	1.89	0.54
1:B:251:LYS:HG2	1:B:296:ILE:HG12	1.89	0.53
1:B:352:TYR:HE1	1:B:383:VAL:HG11	1.73	0.53
2:A:999:ILE:HG13	2:A:1000:LEU:HG	1.89	0.53
2:A:1226:ARG:NH1	3:C:141:GLU:OE1	2.41	0.53
1:B:592:MET:HE2	2:A:786:LEU:HD22	1.89	0.53
1:B:439:ALA:H	1:B:447:GLN:HE22	1.55	0.53
2:A:975:ARG:NH2	2:A:1344:ASP:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:LYS:HG2	1:B:205:TYR:N	2.23	0.53
2:A:1515:LYS:CE	2:A:1516:ILE:HG23	2.36	0.53
2:A:1069:TRP:CD1	2:A:1451:THR:HG1	2.27	0.52
2:A:1544:SER:O	2:A:1546:GLU:N	2.38	0.52
3:C:107:ARG:NH1	3:C:131:GLU:OE1	2.42	0.52
1:B:25:ILE:HG13	1:B:106:VAL:HG21	1.91	0.52
2:A:1657:CYS:O	2:A:1660:PHE:HB3	2.10	0.52
2:A:1162:VAL:HG21	4:D:57:GLN:HG2	1.92	0.52
2:A:1320:LYS:HG2	2:A:1342:LEU:HD13	1.91	0.51
1:B:444:GLU:O	1:B:449:ARG:NH2	2.43	0.51
4:D:48:ILE:HG22	4:D:51:ALA:HB2	1.93	0.51
2:A:975:ARG:HG3	2:A:1340:VAL:HB	1.93	0.51
3:C:152:GLU:HG2	3:C:160:GLN:HE22	1.75	0.51
4:D:24:ASP:OD1	4:D:25:ALA:N	2.43	0.51
1:B:417:VAL:HG21	1:B:473:HIS:NE2	2.26	0.50
2:A:1316:SER:HA	2:A:1323:LEU:H	1.76	0.50
2:A:1652:THR:HG22	2:A:1658:GLN:HB2	1.92	0.50
1:B:29:LYS:HD2	1:B:652:THR:HG23	1.93	0.50
2:A:1011:GLU:O	2:A:1014:SER:OG	2.21	0.50
1:B:573:VAL:HG12	1:B:592:MET:HG2	1.93	0.50
2:A:687:ALA:O	2:A:691:LYS:HG3	2.12	0.50
2:A:1618:LEU:O	2:A:1645:ILE:HA	2.12	0.50
1:B:104:LEU:O	1:B:114:SER:HA	2.12	0.50
2:A:1032:ASN:OD1	2:A:1032:ASN:N	2.45	0.50
2:A:970:LYS:NZ	2:A:1531:ASP:OD2	2.38	0.50
1:B:484:ILE:HG22	1:B:526:ILE:O	2.12	0.49
2:A:1548:ARG:HH11	2:A:1644:TRP:HH2	1.60	0.49
1:B:503:ILE:HB	1:B:511:HIS:HB2	1.94	0.49
2:A:689:LYS:HD3	2:A:690:TYR:CE1	2.47	0.49
2:A:1013:MET:HE3	2:A:1287:THR:HB	1.93	0.49
2:A:691:LYS:HE2	2:A:757:LEU:HD13	1.94	0.49
1:B:43:VAL:HG23	1:B:79:PHE:HB3	1.95	0.48
2:A:1235:LYS:NZ	2:A:1413:GLU:OE1	2.45	0.48
1:B:318:LEU:HA	1:B:321:LYS:HG3	1.95	0.48
1:B:106:VAL:O	1:B:112:SER:HA	2.13	0.48
2:A:749:LEU:HD23	2:A:752:LEU:HD12	1.95	0.48
2:A:860:SER:HB2	2:A:911:ASN:HB2	1.95	0.48
2:A:1290:THR:O	2:A:1294:ILE:HG12	2.12	0.48
2:A:1516:ILE:HG22	2:A:1517:GLN:H	1.79	0.48
1:B:412:ARG:N	1:B:417:VAL:O	2.45	0.48
1:B:539:ARG:NH2	1:B:635:GLY:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:ILE:HG12	1:B:540:LEU:HD13	1.95	0.48
1:B:547:THR:OG1	1:B:548:GLY:N	2.47	0.47
1:B:516:GLU:O	1:B:524:GLN:NE2	2.33	0.47
2:A:1066:TYR:HB3	2:A:1078:LEU:HD23	1.96	0.47
3:C:132:MET:HE3	3:C:147:CYS:HB2	1.94	0.47
1:B:224:LEU:HD12	1:B:225:PRO:HD2	1.95	0.47
1:B:256:TYR:HA	2:A:846:TYR:HE2	1.79	0.47
1:B:471:ASP:OD1	1:B:473:HIS:CE1	2.68	0.47
2:A:781:PRO:C	2:A:783:ARG:H	2.22	0.47
2:A:859:MET:HE2	2:A:910:ILE:HG21	1.96	0.47
2:A:1616:GLN:OE1	2:A:1650:ARG:NH2	2.47	0.47
1:B:383:VAL:O	1:B:411:THR:HG21	2.15	0.47
2:A:714:ARG:HA	2:A:717:ARG:HH21	1.79	0.47
2:A:1315:VAL:HG12	2:A:1348:VAL:HG22	1.96	0.47
2:A:975:ARG:HA	2:A:1362:THR:O	2.15	0.46
4:D:19:CYS:SG	4:D:20:GLU:N	2.88	0.46
2:A:1554:LYS:HG3	2:A:1556:GLU:H	1.80	0.46
4:D:24:ASP:N	4:D:28:ASN:O	2.48	0.46
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.98	0.46
1:B:392:ALA:HB1	1:B:431:LEU:HD11	1.98	0.46
1:B:463:SER:HA	1:B:490:SER:HB2	1.98	0.46
1:B:160:VAL:HG22	1:B:175:GLU:HB3	1.97	0.46
1:B:282:MET:HE1	1:B:324:TYR:HE2	1.81	0.46
2:A:1405:CYS:HA	2:A:1473:LEU:O	2.16	0.46
2:A:1598:ILE:HD12	2:A:1637:TYR:HE1	1.80	0.46
1:B:267:ILE:HD13	1:B:299:VAL:HG21	1.97	0.46
2:A:860:SER:CB	2:A:911:ASN:HB2	2.46	0.46
2:A:934:VAL:HG22	2:A:1492:THR:HG21	1.98	0.46
2:A:937:GLU:HG3	2:A:1364:VAL:HG22	1.97	0.46
2:A:1647:TYR:CE2	2:A:1649:PRO:HG3	2.50	0.45
2:A:984:VAL:HG23	2:A:987:ILE:HD12	1.97	0.45
2:A:869:GLU:N	2:A:869:GLU:OE1	2.50	0.45
2:A:1222:PRO:HG2	3:C:165:LEU:HD11	1.98	0.45
2:A:867:THR:HG22	2:A:900:VAL:HG12	1.99	0.45
1:B:571:LEU:HG	2:A:812:ALA:HB2	1.98	0.45
2:A:829:ILE:HG13	2:A:925:LYS:HG2	1.99	0.45
2:A:981:GLY:HA3	2:A:1333:PHE:CD2	2.51	0.45
3:C:129:ASP:OD1	3:C:158:ARG:NH2	2.47	0.45
2:A:1647:TYR:CZ	2:A:1649:PRO:HG3	2.52	0.44
2:A:1516:ILE:HG22	2:A:1517:GLN:N	2.32	0.44
2:A:1423:VAL:O	2:A:1495:VAL:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:THR:HG21	1:B:372:LYS:N	2.24	0.44
1:B:412:ARG:HH11	1:B:412:ARG:HB2	1.82	0.44
2:A:942:VAL:CG2	2:A:957:LYS:HG2	2.45	0.44
1:B:317:ASP:C	1:B:319:ASN:H	2.26	0.44
1:B:469:TRP:CD1	1:B:482:LEU:HD11	2.53	0.44
2:A:1645:ILE:O	2:A:1645:ILE:HG13	2.17	0.44
4:D:45:ALA:HB3	4:D:48:ILE:HG12	1.98	0.44
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.99	0.43
2:A:1229:LYS:HD2	2:A:1231:ASN:O	2.18	0.43
3:C:91:LEU:HG	3:C:96:VAL:HG22	2.00	0.43
2:A:1577:TYR:CE1	2:A:1611:LEU:HB2	2.53	0.43
1:B:496:ILE:O	1:B:517:LYS:HD3	2.18	0.43
2:A:765:ILE:HG13	2:A:767:SER:H	1.83	0.43
1:B:540:LEU:O	1:B:558:SER:HA	2.19	0.43
1:B:622:ARG:HB3	1:B:625:GLN:NE2	2.34	0.43
2:A:1176:LEU:HD22	2:A:1204:GLN:HB3	2.00	0.43
4:D:23:LEU:HD13	4:D:23:LEU:HA	1.84	0.43
2:A:1083:LEU:O	2:A:1155:ALA:HB2	2.19	0.43
1:B:128:ILE:HB	1:B:215:ALA:HB2	2.01	0.43
2:A:701:ASP:HA	2:A:704:CYS:SG	2.59	0.43
1:B:609:VAL:HG12	2:A:769:PHE:CG	2.53	0.43
2:A:968:VAL:HG23	2:A:1366:HIS:O	2.18	0.43
1:B:196:TYR:CZ	1:B:221:GLU:HB2	2.54	0.43
2:A:822:ASP:HB2	2:A:849:ARG:HG3	2.00	0.43
1:B:254:TYR:CE2	1:B:260:VAL:HA	2.54	0.43
1:B:539:ARG:NH1	1:B:631:ASP:OD2	2.52	0.43
2:A:826:GLU:HG2	2:A:846:TYR:HE1	1.84	0.43
2:A:939:TYR:CZ	2:A:1279:ARG:HD3	2.54	0.43
4:D:25:ALA:HB3	4:D:26:LEU:HD12	1.99	0.43
1:B:30:ILE:HD12	1:B:118:PRO:HB2	2.01	0.42
1:B:627:LEU:HD12	1:B:627:LEU:HA	1.85	0.42
2:A:905:ILE:HD13	2:A:931:PRO:HG3	2.01	0.42
1:B:144:ARG:HG2	2:A:775:TRP:CZ2	2.53	0.42
1:B:159:THR:O	1:B:175:GLU:HA	2.19	0.42
1:B:484:ILE:HD12	1:B:540:LEU:HD23	2.01	0.42
1:B:498:HIS:CE1	1:B:516:GLU:HG2	2.54	0.42
1:B:460:LEU:HD12	1:B:460:LEU:HA	1.76	0.42
2:A:1162:VAL:HG22	4:D:59:ALA:HB2	2.02	0.42
2:A:1318:LYS:HE3	2:A:1319:HIS:CE1	2.54	0.42
2:A:1229:LYS:HG2	2:A:1231:ASN:H	1.84	0.42
2:A:1576:LYS:HG2	2:A:1601:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:TYR:O	1:B:314:SER:N	2.45	0.42
1:B:311:SER:O	1:B:313:TYR:N	2.53	0.42
2:A:881:SER:OG	2:A:882:LYS:N	2.52	0.42
1:B:166:PRO:HD3	1:B:199:TRP:CD1	2.55	0.42
2:A:822:ASP:OD1	2:A:822:ASP:N	2.47	0.42
2:A:1019:PHE:CZ	2:A:1088:GLN:HB3	2.54	0.42
2:A:1386:ILE:HD12	2:A:1386:ILE:HA	1.86	0.42
2:A:795:THR:H	2:A:819:VAL:HG23	1.83	0.42
2:A:1517:GLN:NE2	2:A:1605:THR:HA	2.35	0.42
3:C:119:HIS:CE1	3:C:133:TRP:HB2	2.54	0.42
2:A:1654:CYS:HB2	2:A:1657:CYS:HB3	1.87	0.42
1:B:570:GLN:O	1:B:594:THR:HA	2.20	0.42
2:A:1046:LYS:NZ	2:A:1092:TYR:O	2.53	0.42
3:C:86:ASP:O	3:C:100:LEU:HD13	2.20	0.42
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.85	0.41
2:A:1564:SER:HB2	2:A:1616:GLN:HG2	2.01	0.41
3:C:73:MET:HE3	3:C:84:SER:OG	2.19	0.41
4:D:20:GLU:HG3	4:D:22:LYS:HG2	2.02	0.41
2:A:872:VAL:HG23	2:A:873:ILE:HG22	2.02	0.41
2:A:1565:ILE:CD1	2:A:1611:LEU:HB3	2.50	0.41
3:C:103:LEU:HD23	3:C:103:LEU:HA	1.81	0.41
1:B:592:MET:SD	1:B:602:LEU:HD11	2.60	0.41
2:A:1315:VAL:HG23	2:A:1323:LEU:HB3	2.02	0.41
1:B:191:PRO:HD2	1:B:194:PRO:HB3	2.02	0.41
1:B:465:LEU:HD11	1:B:486:VAL:HG13	2.02	0.41
2:A:823:VAL:HA	2:A:846:TYR:O	2.21	0.41
2:A:1008:ALA:HB2	2:A:1059:TYR:CG	2.55	0.41
2:A:823:VAL:HG21	2:A:853:MET:SD	2.60	0.41
2:A:987:ILE:H	2:A:987:ILE:HG13	1.52	0.41
1:B:506:LYS:NZ	1:B:533:ASN:O	2.49	0.41
2:A:758:LEU:HB2	2:A:759:PRO:HD3	2.03	0.41
2:A:1572:ASN:HB3	2:A:1573:VAL:H	1.70	0.41
2:A:702:GLY:HA2	2:A:728:PHE:CE2	2.56	0.41
2:A:860:SER:HB3	2:A:911:ASN:H	1.85	0.41
2:A:1548:ARG:NH1	2:A:1646:GLU:OE1	2.54	0.41
2:A:1384:GLN:O	2:A:1400:LYS:HA	2.20	0.41
1:B:395:ILE:HG12	1:B:401:THR:HG22	2.02	0.40
1:B:469:TRP:HZ3	1:B:559:VAL:HB	1.86	0.40
2:A:686:ILE:HD11	2:A:734:VAL:HG11	2.03	0.40
2:A:1317:TYR:CD1	2:A:1344:ASP:HB3	2.56	0.40
4:D:39:LEU:HB2	4:D:58:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLN:NE2	1:B:514:THR:OG1	2.55	0.40
1:B:373:VAL:CG2	1:B:418:ALA:HB3	2.52	0.40
2:A:977:LEU:HD21	2:A:1315:VAL:HG11	2.03	0.40
2:A:1560:ALA:O	2:A:1585:TYR:HB2	2.21	0.40
1:B:161:LEU:O	1:B:173:MET:HA	2.21	0.40
1:B:476:LEU:HB2	1:B:563:ILE:HG12	2.04	0.40
2:A:1464:LEU:HD12	2:A:1464:LEU:HA	1.81	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	B	643/656 (98%)	616 (96%)	27 (4%)	0	100	100
2	A	976/998 (98%)	924 (95%)	52 (5%)	0	100	100
3	C	146/165 (88%)	138 (94%)	8 (6%)	0	100	100
4	D	45/81 (56%)	39 (87%)	5 (11%)	1 (2%)	5	22
All	All	1810/1900 (95%)	1717 (95%)	92 (5%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	14	CYS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	574/581 (99%)	554 (96%)	20 (4%)	32	60
2	A	872/885 (98%)	834 (96%)	38 (4%)	25	54
3	C	128/143 (90%)	125 (98%)	3 (2%)	44	68
4	D	37/68 (54%)	31 (84%)	6 (16%)	2	10
All	All	1611/1677 (96%)	1544 (96%)	67 (4%)	26	56

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	85	LEU
1	B	103	TYR
1	B	143	VAL
1	B	264	ASP
1	B	289	ASN
1	B	354	LEU
1	B	411	THR
1	B	414	ASP
1	B	460	LEU
1	B	470	THR
1	B	471	ASP
1	B	472	ASN
1	B	473	HIS
1	B	474	LYS
1	B	494	ASP
1	B	495	LYS
1	B	530	VAL
1	B	550	GLN
1	B	627	LEU
1	B	672	ILE
2	A	695	VAL
2	A	742	ILE
2	A	747	MET
2	A	807	THR
2	A	814	THR
2	A	862	VAL
2	A	884	VAL
2	A	916	THR
2	A	936	ARG
2	A	962	ARG

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Mol	Chain	Res	Type
2	A	987	ILE
2	A	1039	LEU
2	A	1056	ILE
2	A	1127	ILE
2	A	1370	THR
2	A	1462	LEU
2	A	1515	LYS
2	A	1516	ILE
2	A	1518	LYS
2	A	1519	VAL
2	A	1526	LYS
2	A	1528	VAL
2	A	1546	GLU
2	A	1573	VAL
2	A	1581	LEU
2	A	1582	LEU
2	A	1589	GLU
2	A	1601	ILE
2	A	1603	LYS
2	A	1636	ILE
2	A	1645	ILE
2	A	1650	ARG
2	A	1651	ASP
2	A	1653	THR
2	A	1656	SER
2	A	1657	CYS
2	A	1658	GLN
2	A	1664	LEU
3	C	69	THR
3	C	127	VAL
3	C	151	LEU
4	D	13	GLN
4	D	23	LEU
4	D	32	THR
4	D	36	GLN
4	D	57	GLN
4	D	58	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	HIS

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Mol	Chain	Res	Type
1	B	434	ASN
1	B	472	ASN
1	B	473	HIS
1	B	481	HIS
1	B	527	ASN
1	B	591	ASN
1	B	665	ASN
2	A	680	GLN
2	A	785	GLN
2	A	886	GLN
2	A	1204	GLN
2	A	1319	HIS
2	A	1448	GLN
2	A	1674	ASN
3	C	66	GLN

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 ⓘ

2 monosaccharides 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	$\# Z > 2$
5	NAG	E	1	2,5	14,14,15	0.49	0	17,19,21	0.54	0
5	NAG	E	2	5	14,14,15	0.27	0	17,19,21	0.44	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
5	NAG	E	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

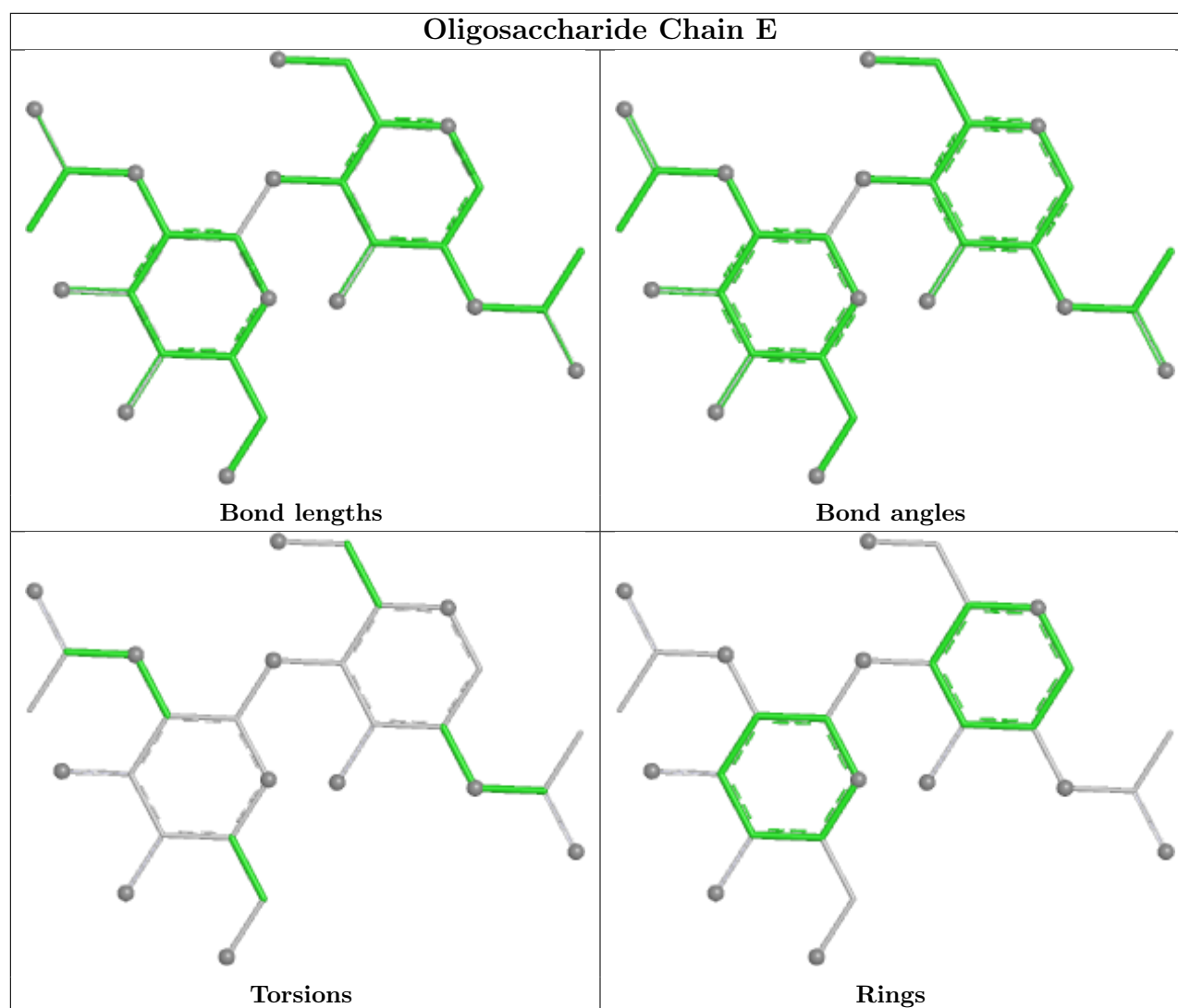
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
6	CYS	A	2101	2	4,5,6	0.80	0	1,5,7	1.02	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
6	CYS	A	2101	2	-	1/1/4/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2101	CYS	N-CA-CB-SG

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.

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	B	647/656 (98%)	0.73	35 (5%)	31	17	49, 76, 118, 157	0
2	A	982/998 (98%)	0.64	74 (7%)	20	11	44, 66, 160, 215	0
3	C	148/165 (89%)	0.38	1 (0%)	84	68	61, 85, 123, 138	0
4	D	47/81 (58%)	0.68	2 (4%)	40	22	63, 78, 98, 121	0
All	All	1824/1900 (96%)	0.65	112 (6%)	27	15	44, 72, 144, 215	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1388	ALA	5.9
2	A	694	VAL	5.3
2	A	760	VAL	5.0
2	A	679	LEU	4.8
2	A	1517	GLN	4.6
2	A	1053	MET	4.3
2	A	1653	THR	4.2
1	B	624	PHE	4.1
2	A	1518	LYS	4.0
2	A	995	GLU	3.8
2	A	873	ILE	3.7
1	B	94	GLY	3.7
2	A	752	LEU	3.7
1	B	95	GLY	3.6
2	A	757	LEU	3.6
3	C	21	GLU	3.6
2	A	682	LYS	3.5
2	A	683	ILE	3.4
1	B	662	SER	3.4
1	B	93	PRO	3.3
2	A	761	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	1516	ILE	3.2
2	A	1524	ALA	3.2
1	B	664	GLU	3.1
2	A	762	LYS	3.1
2	A	997	ILE	3.1
4	D	59	ALA	3.1
1	B	469	TRP	3.1
2	A	1591	VAL	3.0
2	A	965	LEU	3.0
2	A	1627	ILE	3.0
2	A	712	GLU	2.9
1	B	623	VAL	2.9
2	A	1601	ILE	2.9
1	B	168	GLY	2.8
2	A	1676	CYS	2.8
2	A	1541	LEU	2.8
2	A	744	HIS	2.7
2	A	689	LYS	2.7
2	A	753	HIS	2.7
1	B	661	ASP	2.7
2	A	1655	SER	2.6
1	B	660	ASP	2.6
1	B	333	THR	2.6
2	A	1514	ILE	2.5
1	B	258	LYS	2.5
2	A	688	ALA	2.5
2	A	861	ALA	2.5
1	B	472	ASN	2.5
2	A	742	ILE	2.5
2	A	963	ILE	2.5
2	A	756	THR	2.5
1	B	663	GLN	2.5
1	B	475	ALA	2.5
2	A	1642	LEU	2.5
2	A	733	VAL	2.5
1	B	224	LEU	2.4
2	A	1625	LEU	2.4
2	A	996	GLY	2.4
1	B	439	ALA	2.4
2	A	1623	GLU	2.4
2	A	686	ILE	2.4
2	A	1319	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	A	1675	GLY	2.4
2	A	1539	LEU	2.4
2	A	1658	GLN	2.4
2	A	1140	ASN	2.3
2	A	892	SER	2.3
2	A	722	PRO	2.3
1	B	55	SER	2.3
2	A	1469	SER	2.3
2	A	1654	CYS	2.3
2	A	729	THR	2.2
1	B	674	ARG	2.2
2	A	872	VAL	2.2
1	B	394	THR	2.2
1	B	495	LYS	2.2
2	A	692	HIS	2.2
2	A	882	LYS	2.2
1	B	583	SER	2.2
2	A	1164	ILE	2.2
4	D	19	CYS	2.2
1	B	673	LEU	2.2
2	A	1645	ILE	2.2
1	B	391	ASN	2.2
2	A	754	MET	2.2
1	B	431	LEU	2.2
1	B	470	THR	2.1
2	A	716	ALA	2.1
2	A	1572	ASN	2.1
2	A	1631	PHE	2.1
1	B	70	HIS	2.1
2	A	1652	THR	2.1
2	A	751	ARG	2.1
2	A	880	SER	2.1
2	A	1651	ASP	2.1
1	B	547	THR	2.1
1	B	620	LEU	2.1
2	A	1161	LEU	2.1
1	B	287	MET	2.1
1	B	98	PRO	2.1
2	A	868	SER	2.1
2	A	758	LEU	2.1
2	A	691	LYS	2.1
1	B	284	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	373	VAL	2.0
1	B	114	SER	2.0
2	A	1033	ILE	2.0
2	A	1523	ALA	2.0
2	A	1547	THR	2.0
2	A	1515	LYS	2.0
2	A	1056	ILE	2.0

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

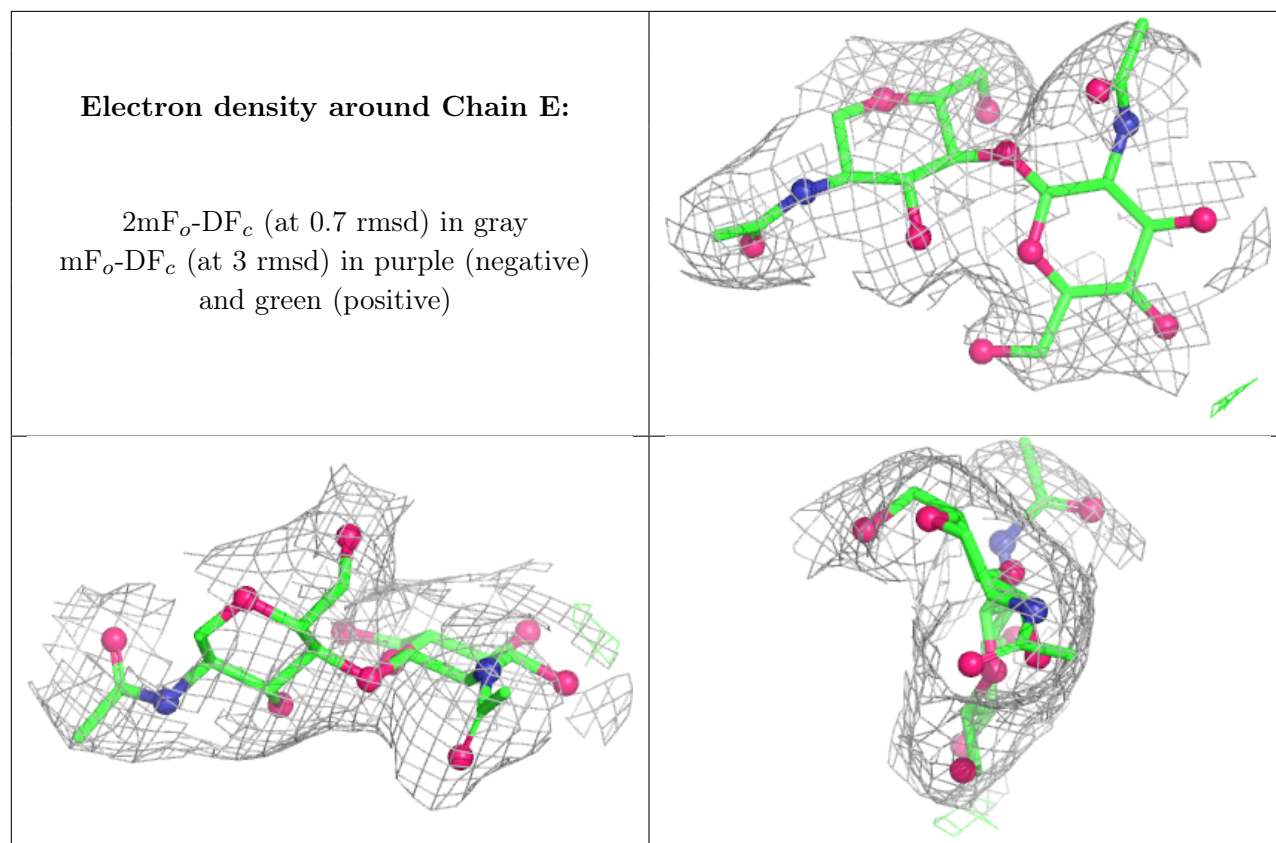
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
5	NAG	E	2	14/15	0.75	0.11	89,98,108,110	0
5	NAG	E	1	14/15	0.87	0.10	60,67,87,98	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



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. 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($\text{\AA}^2$)	Q<0.9
6	CYS	A	2101	6/7	0.69	0.24	106,111,116,122	0

6.5 Other polymers [i](#)

There are no such residues in this entry.