



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:45 PM UTC

PDB ID : 5HCD / pdb_00005hcd
Title : Ternary complex of human Complement C5 with Ornithodoros moubata OmCI and Rhipicephalus microplus RaCI2
Authors : Jore, M.M.; Johnson, S.; Lea, S.M.
Deposited on : 2016-01-04
Resolution : 2.98 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

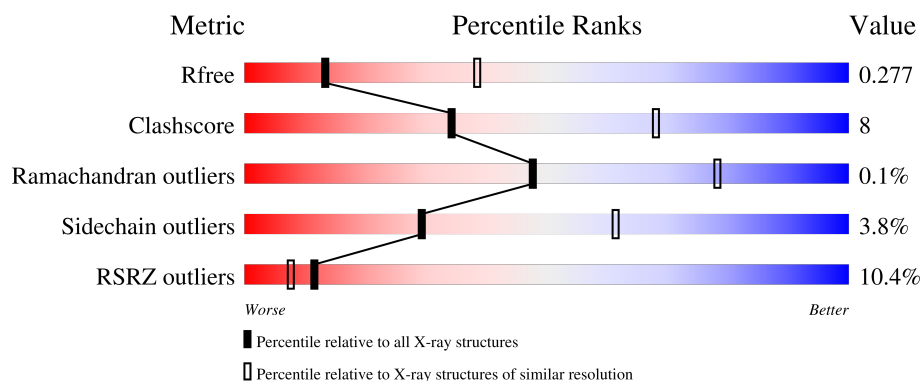
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	10% 77% 21% ..
2	A	998	12% 78% 19% ..
3	C	165	2% 74% 16% 10%
4	D	80	9% 45% 12% 39%
5	E	2	100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14445 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	981	Total	C	N	O	S	0	0	0
			7771	4970	1297	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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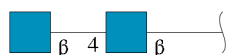
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP Q5YD59
C	78	GLN	ASN	engineered mutation	UNP Q5YD59
C	102	GLN	ASN	engineered mutation	UNP Q5YD59

- Molecule 4 is a protein called Rhipicephalus microplus RaCI2.

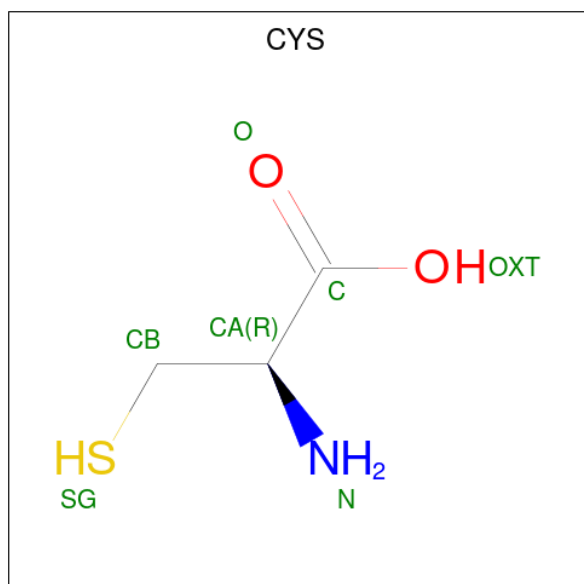
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	49	Total	C	N	O	S	0	0	0
			364	217	70	71	6			

- 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).

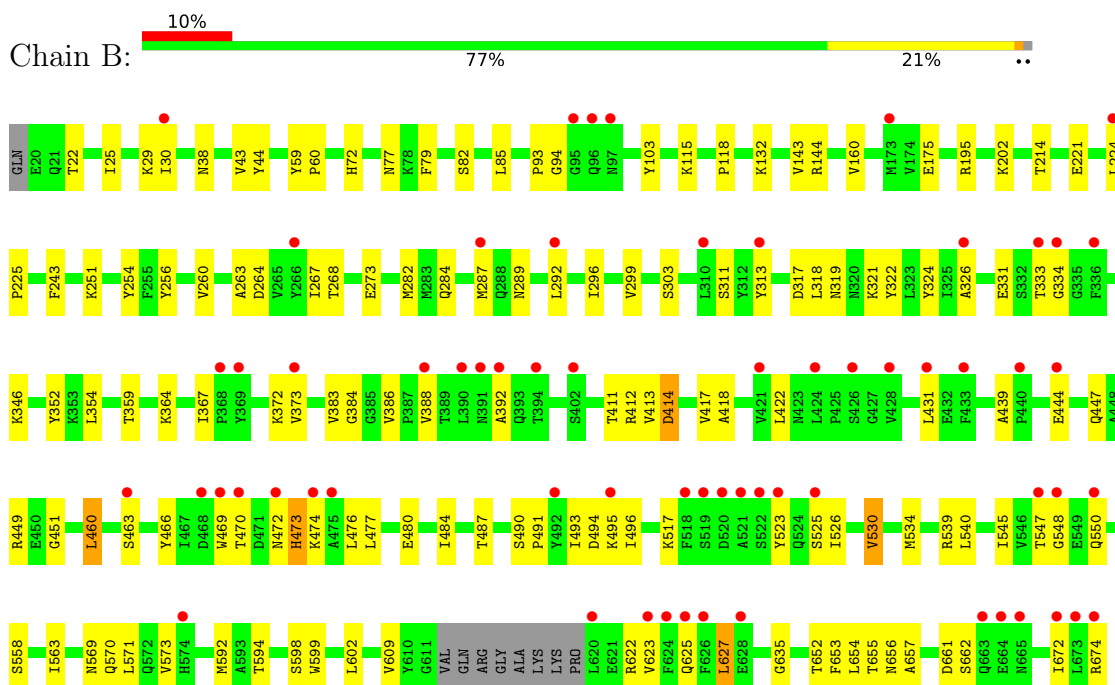


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			6	3	1	1	1		

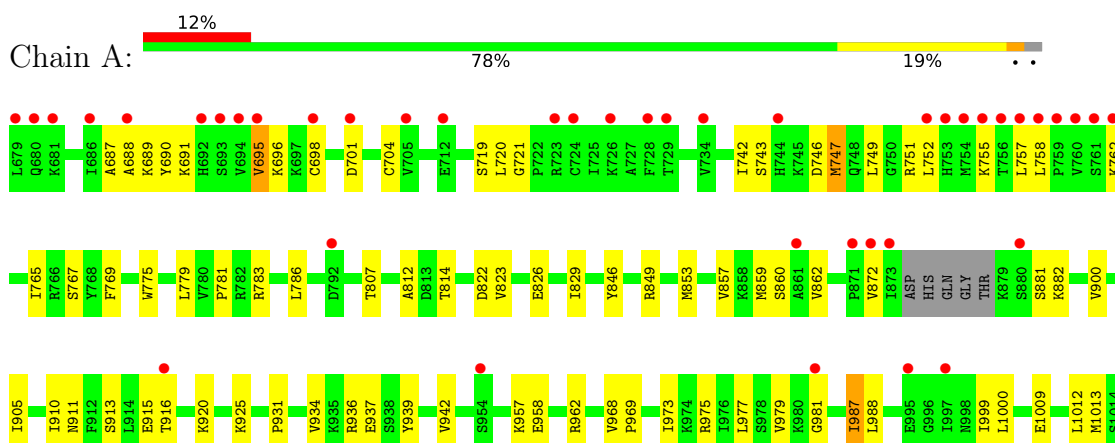
3 Residue-property plots [i](#)

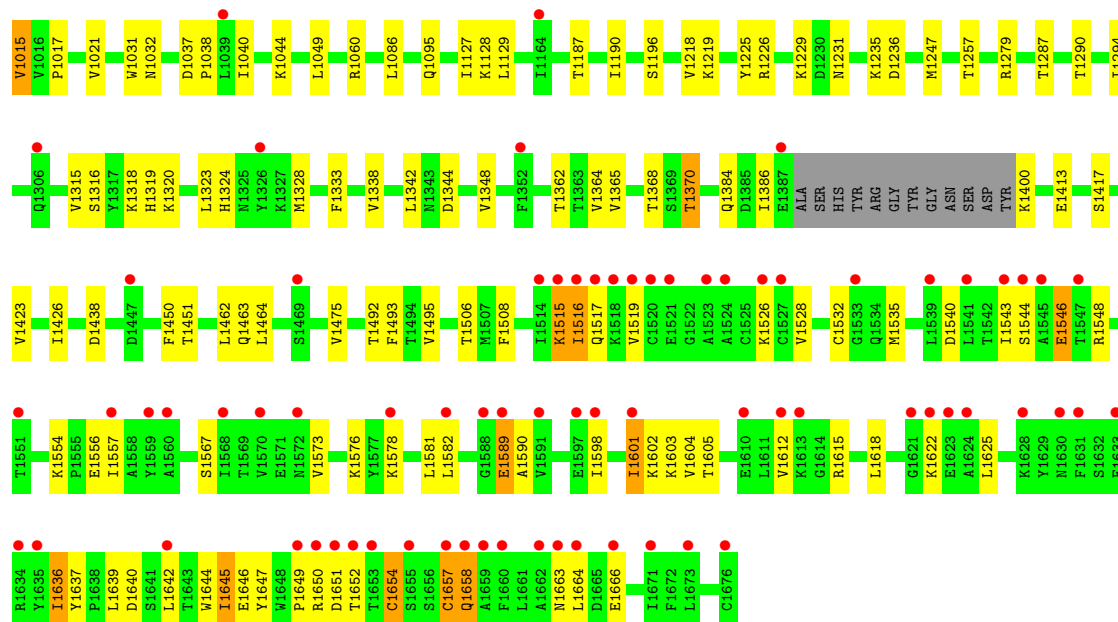
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

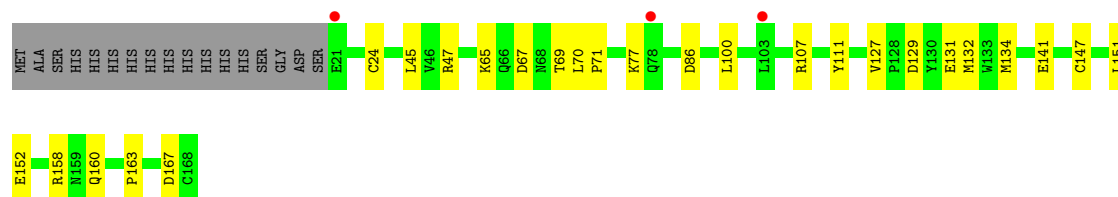
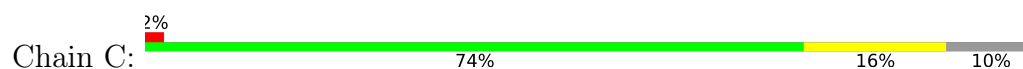


• Molecule 2: Complement C5

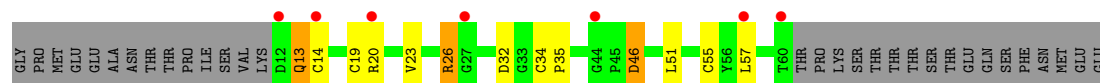




• Molecule 3: Complement inhibitor



• Molecule 4: Rhipicephalus microplus RaCI2



• 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	105.95Å 140.21Å 209.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.54 – 2.98 74.54 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.54-2.98) 99.3 (74.54-2.98)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.257 , 0.282 0.256 , 0.277	Depositor DCC
R_{free} test set	3197 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14445	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.44	0/5234	0.51	0/7119
2	A	0.46	0/7928	0.52	1/10733 (0.0%)
3	C	0.35	0/1183	0.43	0/1599
4	D	0.44	0/368	0.63	0/497
All	All	0.44	0/14713	0.52	1/19948 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1515	LYS	N-CA-C	-7.22	98.03	109.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5116	0	5022	87	0
2	A	7771	0	7817	124	0
3	C	1160	0	1085	13	0
4	D	364	0	352	8	0
5	E	28	0	25	0	0
6	A	6	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14445	0	14304	219	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 (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1515:LYS:HG2	2:A:1516:ILE:HA	1.64	0.79
2:A:942:VAL:HG21	2:A:957:LYS:HG2	1.65	0.77
2:A:1515:LYS:HE3	2:A:1516:ILE:HG23	1.67	0.76
1:B:93:PRO:O	4:D:26:ARG:NH2	2.20	0.75
1:B:487:THR:HG22	1:B:523:TYR:HB3	1.68	0.75
2:A:1625:LEU:HB2	2:A:1636:ILE:HG23	1.68	0.74
1:B:373:VAL:HG21	1:B:388:VAL:HG11	1.70	0.73
1:B:384:GLY:HA3	1:B:413:VAL:HG23	1.70	0.73
2:A:1548:ARG:NH1	2:A:1646:GLU:OE1	2.22	0.71
1:B:359:THR:HG21	1:B:372:LYS:H	1.56	0.71
1:B:469:TRP:HA	1:B:484:ILE:HA	1.74	0.70
4:D:13:GLN:HG3	4:D:14:CYS:H	1.56	0.68
2:A:751:ARG:O	2:A:755:LYS:HB2	1.95	0.67
3:C:77:LYS:NZ	3:C:167:ASP:O	2.27	0.66
1:B:72:HIS:O	1:B:77:ASN:ND2	2.28	0.66
3:C:107:ARG:NH1	3:C:131:GLU:OE1	2.28	0.65
1:B:221:GLU:OE1	2:A:762:LYS:NZ	2.31	0.64
2:A:934:VAL:HG23	2:A:1508:PHE:CZ	2.32	0.64
1:B:655:THR:HG22	1:B:657:ALA:H	1.62	0.63
1:B:268:THR:HG22	1:B:287:MET:HG2	1.79	0.63
1:B:569:ASN:ND2	1:B:598:SER:HB2	2.14	0.63
4:D:20:ARG:NH1	4:D:32:ASP:OD2	2.31	0.62
2:A:1532:CYS:HA	2:A:1640:ASP:HA	1.81	0.62
4:D:14:CYS:SG	4:D:35:PRO:HG2	2.40	0.62
1:B:273:GLU:OE2	1:B:321:LYS:NZ	2.32	0.61
2:A:1535:MET:HG3	2:A:1645:ILE:HD11	1.81	0.61
2:A:1450:PHE:CZ	2:A:1475:VAL:HB	2.35	0.60
2:A:1576:LYS:HE2	2:A:1601:ILE:HD11	1.83	0.60
2:A:1556:GLU:HB3	2:A:1622:LYS:HE2	1.82	0.60
1:B:490:SER:OG	1:B:491:PRO:O	2.07	0.59
1:B:195:ARG:NH2	2:A:1060:ARG:O	2.35	0.59
1:B:386:VAL:H	1:B:411:THR:HB	1.68	0.59
2:A:1544:SER:O	2:A:1546:GLU:N	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ILE:O	1:B:653:PHE:HA	2.03	0.58
1:B:364:LYS:HB3	1:B:367:ILE:HD13	1.84	0.58
1:B:251:LYS:HG2	1:B:296:ILE:HG12	1.84	0.58
1:B:224:LEU:HD12	1:B:225:PRO:HD2	1.85	0.58
2:A:1032:ASN:OD1	2:A:1032:ASN:N	2.37	0.58
2:A:687:ALA:O	2:A:691:LYS:HG3	2.04	0.57
1:B:144:ARG:NH2	1:B:602:LEU:O	2.37	0.57
2:A:743:SER:OG	2:A:746:ASP:OD1	2.20	0.57
1:B:573:VAL:HG12	1:B:592:MET:HG2	1.87	0.57
1:B:592:MET:HE2	2:A:786:LEU:HD22	1.86	0.57
1:B:160:VAL:HG22	1:B:175:GLU:HB3	1.87	0.57
1:B:414:ASP:OD1	1:B:414:ASP:N	2.35	0.57
2:A:747:MET:O	2:A:751:ARG:HG3	2.05	0.56
2:A:1226:ARG:NH1	3:C:141:GLU:OE1	2.38	0.56
1:B:484:ILE:O	1:B:525:SER:HA	2.05	0.56
2:A:1622:LYS:HE3	2:A:1642:LEU:HD23	1.87	0.56
1:B:22:THR:HG21	1:B:545:ILE:HD13	1.87	0.56
2:A:1548:ARG:HH11	2:A:1644:TRP:HH2	1.53	0.55
2:A:915:GLU:OE2	2:A:920:LYS:NZ	2.39	0.55
2:A:915:GLU:HG2	2:A:920:LYS:HG3	1.88	0.54
1:B:115:LYS:HB2	1:B:654:LEU:HD21	1.89	0.54
2:A:1219:LYS:HB2	2:A:1225:TYR:HB2	1.88	0.54
2:A:1370:THR:HG21	2:A:1506:THR:HB	1.90	0.54
2:A:696:LYS:HE2	2:A:758:LEU:O	2.07	0.53
2:A:826:GLU:HG2	2:A:846:TYR:HE1	1.74	0.53
1:B:539:ARG:NH2	1:B:635:GLY:O	2.41	0.53
2:A:937:GLU:HG3	2:A:1364:VAL:HG22	1.91	0.53
1:B:439:ALA:H	1:B:447:GLN:HE22	1.57	0.53
2:A:1598:ILE:HD12	2:A:1637:TYR:HE1	1.74	0.53
2:A:719:SER:O	2:A:721:GLY:N	2.42	0.53
2:A:1235:LYS:NZ	2:A:1413:GLU:OE1	2.41	0.53
1:B:412:ARG:N	1:B:417:VAL:O	2.33	0.52
1:B:547:THR:OG1	1:B:548:GLY:N	2.42	0.52
2:A:958:GLU:OE2	2:A:1318:LYS:NZ	2.28	0.52
2:A:979:VAL:HG12	2:A:1328:MET:HE1	1.92	0.52
2:A:1652:THR:HG22	2:A:1658:GLN:HB2	1.92	0.52
2:A:719:SER:C	2:A:721:GLY:H	2.17	0.52
1:B:38:ASN:HD21	1:B:82:SER:HG	1.54	0.52
2:A:1517:GLN:NE2	2:A:1604:VAL:O	2.41	0.52
2:A:1516:ILE:HG22	2:A:1517:GLN:H	1.76	0.52
2:A:1290:THR:O	2:A:1294:ILE:HG12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:THR:HG22	1:B:44:TYR:HB2	1.92	0.51
2:A:749:LEU:HD23	2:A:752:LEU:HD12	1.92	0.51
2:A:999:ILE:HD13	2:A:1017:PRO:HG3	1.91	0.51
1:B:469:TRP:O	1:B:469:TRP:CD1	2.64	0.51
2:A:1612:VAL:HB	2:A:1615:ARG:HD2	1.92	0.51
2:A:1567:SER:HB2	2:A:1578:LYS:HD2	1.92	0.51
1:B:484:ILE:HG22	1:B:526:ILE:O	2.09	0.51
2:A:751:ARG:O	2:A:755:LYS:CB	2.59	0.50
2:A:859:MET:HE2	2:A:910:ILE:HG21	1.93	0.50
2:A:977:LEU:HD21	2:A:1315:VAL:HG11	1.92	0.50
1:B:622:ARG:HB3	1:B:625:GLN:NE2	2.27	0.50
1:B:383:VAL:O	1:B:411:THR:HG21	2.11	0.50
2:A:942:VAL:CG2	2:A:957:LYS:HG2	2.40	0.50
2:A:969:PRO:HG3	2:A:1601:ILE:HG21	1.93	0.50
1:B:284:GLN:NE2	2:A:757:LEU:HD11	2.27	0.50
2:A:857:VAL:HA	2:A:913:SER:O	2.11	0.50
3:C:65:LYS:HE2	3:C:67:ASP:O	2.12	0.49
1:B:451:GLY:O	1:B:674:ARG:NH2	2.46	0.49
2:A:1618:LEU:O	2:A:1645:ILE:HA	2.13	0.49
2:A:905:ILE:HD13	2:A:931:PRO:HG3	1.94	0.49
1:B:444:GLU:O	1:B:449:ARG:NH2	2.46	0.49
2:A:822:ASP:HB2	2:A:849:ARG:HG3	1.93	0.49
2:A:1316:SER:HA	2:A:1323:LEU:H	1.77	0.49
1:B:94:GLY:HA2	4:D:26:ARG:HH21	1.78	0.49
2:A:1384:GLN:O	2:A:1400:LYS:HA	2.12	0.49
2:A:1647:TYR:CE2	2:A:1649:PRO:HG3	2.47	0.49
2:A:1229:LYS:HD2	2:A:1231:ASN:O	2.13	0.49
2:A:1315:VAL:HG23	2:A:1323:LEU:HB3	1.95	0.49
1:B:392:ALA:HB1	1:B:431:LEU:HD11	1.95	0.48
1:B:322:TYR:CE2	1:B:346:LYS:HB2	2.48	0.48
2:A:689:LYS:HD3	2:A:690:TYR:CE1	2.47	0.48
2:A:1196:SER:HB3	2:A:1257:THR:HG23	1.95	0.48
1:B:22:THR:HA	1:B:656:ASN:HD21	1.78	0.47
2:A:1320:LYS:HG2	2:A:1342:LEU:HD13	1.95	0.47
2:A:1602:LYS:HB3	2:A:1639:LEU:HD12	1.97	0.47
3:C:86:ASP:O	3:C:100:LEU:HD13	2.14	0.47
1:B:29:LYS:HD2	1:B:652:THR:HG23	1.96	0.47
1:B:623:VAL:HG12	1:B:627:LEU:HD22	1.96	0.47
2:A:1645:ILE:O	2:A:1645:ILE:HG13	2.14	0.47
1:B:417:VAL:HG21	1:B:473:HIS:NE2	2.29	0.47
1:B:463:SER:HA	1:B:490:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:TYR:HA	2:A:846:TYR:HE2	1.79	0.47
2:A:1451:THR:HG22	2:A:1463:GLN:O	2.14	0.47
1:B:318:LEU:HA	1:B:321:LYS:HG3	1.96	0.47
2:A:1589:GLU:OE1	2:A:1590:ALA:N	2.48	0.47
1:B:490:SER:O	1:B:493:ILE:HG13	2.15	0.46
1:B:38:ASN:ND2	1:B:82:SER:OG	2.38	0.46
2:A:695:VAL:HG23	2:A:698:CYS:SG	2.55	0.46
2:A:781:PRO:C	2:A:783:ARG:H	2.23	0.46
2:A:1086:LEU:HD22	2:A:1095:GLN:OE1	2.16	0.46
2:A:1315:VAL:HG12	2:A:1348:VAL:HG22	1.97	0.46
1:B:571:LEU:HG	2:A:812:ALA:HB2	1.97	0.46
3:C:129:ASP:OD1	3:C:158:ARG:NH2	2.45	0.46
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.98	0.46
2:A:1450:PHE:HA	2:A:1464:LEU:HD13	1.98	0.46
1:B:352:TYR:HE1	1:B:383:VAL:HG11	1.80	0.46
2:A:829:ILE:HG13	2:A:925:LYS:HG2	1.98	0.46
2:A:999:ILE:HG13	2:A:1000:LEU:HG	1.97	0.46
2:A:1218:VAL:HG12	2:A:1226:ARG:HG3	1.96	0.46
2:A:1554:LYS:HG3	2:A:1556:GLU:H	1.81	0.46
1:B:477:LEU:HB2	1:B:480:GLU:HG3	1.98	0.45
2:A:975:ARG:HA	2:A:1362:THR:O	2.16	0.45
3:C:152:GLU:HG2	3:C:160:GLN:HE22	1.81	0.45
1:B:599:TRP:CZ3	2:A:779:LEU:HB2	2.51	0.45
2:A:1451:THR:HG22	2:A:1463:GLN:C	2.42	0.45
1:B:570:GLN:O	1:B:594:THR:HA	2.17	0.45
2:A:934:VAL:HG22	2:A:1492:THR:HG21	1.99	0.45
2:A:981:GLY:HA3	2:A:1333:PHE:CD2	2.51	0.45
2:A:1386:ILE:HD12	2:A:1386:ILE:HA	1.83	0.45
2:A:968:VAL:HG22	2:A:1368:THR:HG22	1.97	0.45
1:B:331:GLU:OE2	1:B:333:THR:OG1	2.22	0.45
2:A:1012:LEU:O	2:A:1015:VAL:HG12	2.17	0.45
2:A:1128:LYS:NZ	2:A:1417:SER:OG	2.49	0.45
3:C:24:CYS:O	3:C:111:TYR:OH	2.31	0.45
2:A:1324:HIS:HE1	2:A:1338:VAL:HG11	1.82	0.44
2:A:939:TYR:CZ	2:A:1279:ARG:HD3	2.52	0.44
1:B:540:LEU:O	1:B:558:SER:HA	2.18	0.44
1:B:282:MET:HE1	1:B:324:TYR:HE2	1.83	0.44
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.83	0.44
1:B:460:LEU:HA	1:B:460:LEU:HD12	1.70	0.44
2:A:1426:ILE:HG12	2:A:1493:PHE:CD1	2.53	0.44
2:A:1517:GLN:NE2	2:A:1605:THR:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:691:LYS:HE2	2:A:757:LEU:HD13	1.99	0.44
2:A:1013:MET:HE3	2:A:1287:THR:HB	1.99	0.44
1:B:333:THR:OG1	1:B:334:GLY:N	2.51	0.44
1:B:609:VAL:HG12	2:A:769:PHE:CG	2.53	0.44
1:B:254:TYR:CE2	1:B:260:VAL:HA	2.52	0.44
2:A:822:ASP:OD1	2:A:822:ASP:N	2.46	0.44
2:A:823:VAL:HG21	2:A:853:MET:SD	2.58	0.43
2:A:1129:LEU:HD23	2:A:1129:LEU:HA	1.84	0.43
1:B:43:VAL:HG23	1:B:79:PHE:HB3	2.00	0.43
1:B:311:SER:O	1:B:313:TYR:N	2.51	0.43
2:A:1037:ASP:OD2	2:A:1040:ILE:HG13	2.17	0.43
1:B:132:LYS:HD2	1:B:609:VAL:HG11	1.99	0.43
1:B:317:ASP:C	1:B:319:ASN:H	2.27	0.43
1:B:496:ILE:O	1:B:517:LYS:HD3	2.18	0.43
2:A:1015:VAL:HG22	2:A:1049:LEU:HD12	2.00	0.43
3:C:134:MET:HE3	3:C:134:MET:HB2	1.87	0.43
1:B:268:THR:OG1	1:B:326:ALA:HB3	2.17	0.43
2:A:1319:HIS:N	2:A:1344:ASP:OD2	2.49	0.43
3:C:47:ARG:NH1	3:C:160:GLN:OE1	2.48	0.43
1:B:144:ARG:HG2	2:A:775:TRP:CZ2	2.53	0.43
3:C:132:MET:HE3	3:C:147:CYS:HB2	1.99	0.43
2:A:765:ILE:HG13	2:A:767:SER:H	1.84	0.43
2:A:988:LEU:HD23	2:A:1021:VAL:HG22	2.00	0.43
1:B:627:LEU:HD12	1:B:627:LEU:HA	1.82	0.43
1:B:661:ASP:OD1	1:B:662:SER:N	2.45	0.43
4:D:19:CYS:HB3	4:D:55:CYS:SG	2.58	0.43
2:A:973:ILE:HG23	2:A:1365:VAL:HG12	2.01	0.42
2:A:1187:THR:HA	2:A:1190:ILE:HG22	2.01	0.42
2:A:1576:LYS:HG2	2:A:1601:ILE:HG12	2.01	0.42
2:A:987:ILE:HD13	2:A:1294:ILE:HG23	2.02	0.42
1:B:94:GLY:HA2	4:D:26:ARG:NH2	2.34	0.42
2:A:1654:CYS:HB2	2:A:1657:CYS:HB3	1.95	0.42
1:B:59:TYR:HA	1:B:60:PRO:HA	1.79	0.42
2:A:881:SER:OG	2:A:882:LYS:N	2.52	0.42
4:D:46:ASP:OD1	4:D:46:ASP:N	2.50	0.42
2:A:1031:TRP:HB3	2:A:1038:PRO:HB3	2.01	0.42
1:B:263:ALA:HB3	1:B:292:LEU:HB3	2.01	0.42
1:B:282:MET:HE1	1:B:324:TYR:CE2	2.54	0.42
2:A:688:ALA:HA	2:A:691:LYS:HD2	2.02	0.42
2:A:860:SER:HB3	2:A:911:ASN:H	1.85	0.42
2:A:701:ASP:HA	2:A:704:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1554:LYS:HB3	2:A:1557:ILE:HG12	2.01	0.41
1:B:267:ILE:HD13	1:B:299:VAL:HG21	2.01	0.41
2:A:859:MET:HE1	2:A:900:VAL:HG11	2.02	0.41
2:A:1009:GLU:OE2	2:A:1287:THR:OG1	2.30	0.41
2:A:1540:ASP:HB3	2:A:1543:ILE:HD13	2.01	0.41
2:A:1516:ILE:HG22	2:A:1517:GLN:N	2.35	0.41
1:B:202:LYS:HE3	1:B:214:THR:OG1	2.21	0.41
2:A:872:VAL:HG22	2:A:881:SER:O	2.21	0.41
2:A:1423:VAL:O	2:A:1495:VAL:HA	2.20	0.41
1:B:243:PHE:O	1:B:303:SER:HB2	2.21	0.41
3:C:45:LEU:HG	3:C:163:PRO:HG2	2.01	0.41
2:A:1044:LYS:HE2	2:A:1044:LYS:HB3	1.86	0.40
2:A:1229:LYS:NZ	2:A:1236:ASP:O	2.54	0.40
1:B:466:TYR:HD2	1:B:487:THR:OG1	2.04	0.40
1:B:476:LEU:HB2	1:B:563:ILE:HG12	2.03	0.40
2:A:987:ILE:H	2:A:987:ILE:HG13	1.53	0.40
2:A:1663:ASN:O	2:A:1666:GLU:HB2	2.22	0.40
1:B:30:ILE:HD12	1:B:118:PRO:HB2	2.02	0.40
1:B:311:SER:HA	1:B:313:TYR:CE2	2.56	0.40
2:A:1438:ASP:OD1	2:A:1438:ASP:N	2.55	0.40
1:B:530:VAL:HA	1:B:534:MET:SD	2.61	0.40
3:C:70:LEU:HA	3:C:71:PRO:HD3	1.97	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%)	615 (96%)	28 (4%)	0	100	100
2	A	975/998 (98%)	924 (95%)	50 (5%)	1 (0%)	48	78
3	C	146/165 (88%)	138 (94%)	8 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	47/80 (59%)	43 (92%)	3 (6%)	1 (2%)	5	25
All	All	1811/1899 (95%)	1720 (95%)	89 (5%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	720	LEU
4	D	13	GLN

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	B	574/581 (99%)	556 (97%)	18 (3%)	35	66
2	A	872/885 (98%)	838 (96%)	34 (4%)	28	60
3	C	128/143 (90%)	125 (98%)	3 (2%)	44	72
4	D	42/71 (59%)	36 (86%)	6 (14%)	3	14
All	All	1616/1680 (96%)	1555 (96%)	61 (4%)	29	61

All (61) 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	414	ASP
1	B	460	LEU
1	B	470	THR
1	B	472	ASN
1	B	473	HIS
1	B	474	LYS

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Mol	Chain	Res	Type
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	916	THR
2	A	936	ARG
2	A	962	ARG
2	A	987	ILE
2	A	1015	VAL
2	A	1127	ILE
2	A	1247	MET
2	A	1370	THR
2	A	1462	LEU
2	A	1516	ILE
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	1654	CYS
2	A	1657	CYS
2	A	1658	GLN
2	A	1664	LEU
3	C	69	THR
3	C	127	VAL

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Mol	Chain	Res	Type
3	C	151	LEU
4	D	23	VAL
4	D	26	ARG
4	D	34	CYS
4	D	46	ASP
4	D	51	LEU
4	D	57	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	355	ASN
1	B	374	GLN
1	B	472	ASN
1	B	481	HIS
1	B	527	ASN
1	B	591	ASN
1	B	665	ASN
2	A	737	GLN
2	A	785	GLN
2	A	909	ASN
2	A	1204	GLN
2	A	1448	GLN
2	A	1674	ASN
4	D	16	ASN
4	D	50	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](#)

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	0.29	0	17,19,21	0.55	0
5	NAG	E	2	5	14,14,15	0.30	0	17,19,21	0.49	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.

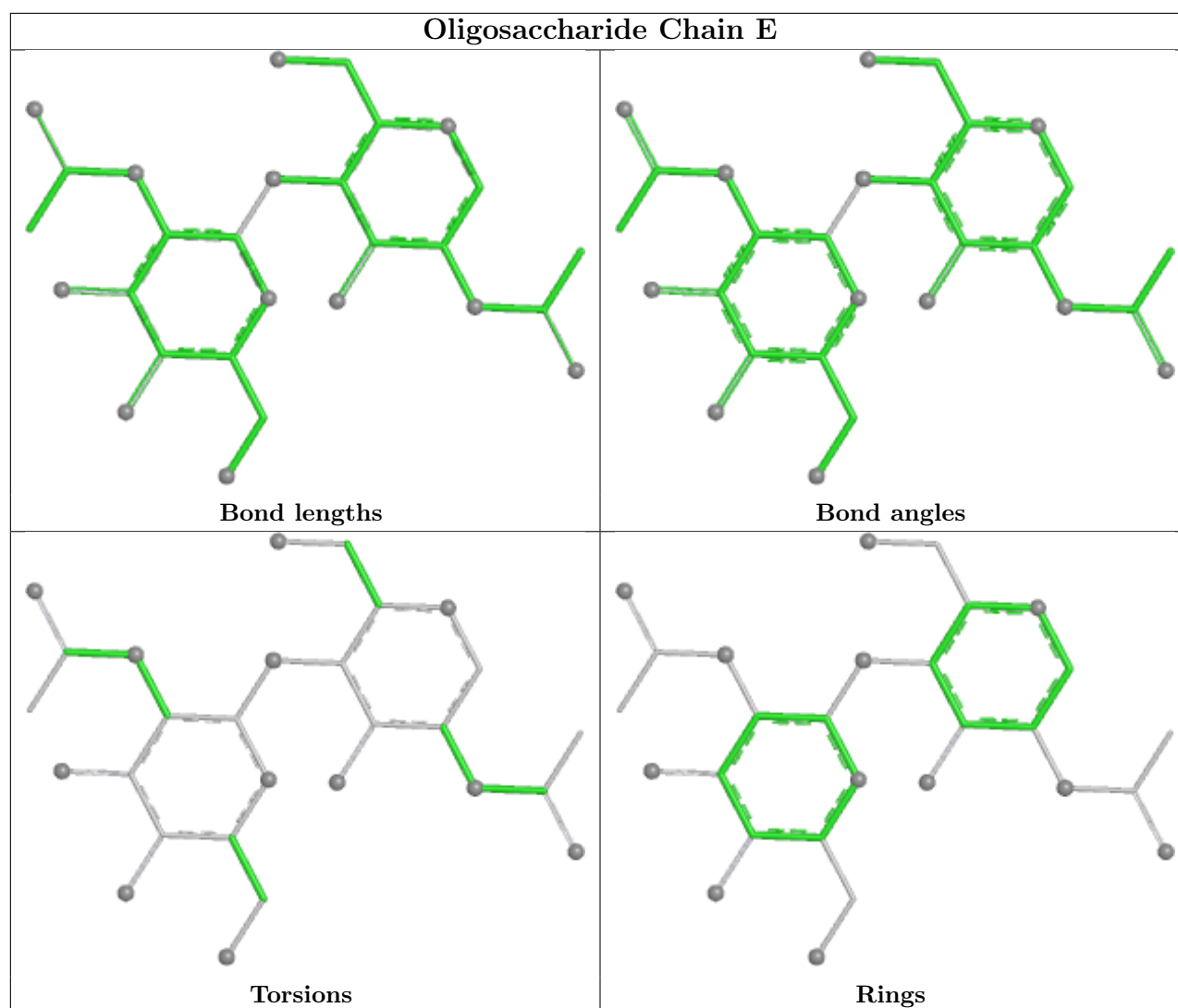
There are no chirality outliers.

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	2003	2	4,5,6	0.81	0	1,5,7	0.50	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	2003	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	2003	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%)	0.95	64 (9%) 13 8	43, 68, 106, 155	0
2	A	981/998 (98%)	0.87	115 (11%) 9 6	39, 59, 148, 208	0
3	C	148/165 (89%)	0.68	3 (2%) 65 45	56, 78, 116, 178	0
4	D	49/80 (61%)	1.01	7 (14%) 6 4	49, 69, 92, 173	0
All	All	1825/1899 (96%)	0.89	189 (10%) 11 8	39, 64, 134, 208	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1517	GLN	6.4
1	B	624	PHE	5.6
2	A	1518	LYS	5.3
2	A	1655	SER	5.0
2	A	1516	ILE	4.9
1	B	623	VAL	4.6
2	A	1570	VAL	4.5
2	A	1662	ALA	4.4
2	A	1591	VAL	4.3
2	A	762	LYS	4.3
2	A	1653	THR	4.3
3	C	21	GLU	4.2
2	A	760	VAL	4.2
2	A	729	THR	4.1
2	A	995	GLU	4.1
2	A	679	LEU	4.0
2	A	1514	ILE	4.0
2	A	1520	CYS	4.0
4	D	12	ASP	4.0
2	A	1541	LEU	4.0
1	B	394	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	A	997	ILE	3.9
1	B	96	GLN	3.8
2	A	1519	VAL	3.8
2	A	761	SER	3.8
2	A	880	SER	3.8
2	A	757	LEU	3.7
1	B	421	VAL	3.7
2	A	873	ILE	3.7
1	B	470	THR	3.6
2	A	755	LYS	3.6
4	D	60	THR	3.5
2	A	758	LEU	3.5
1	B	334	GLY	3.4
2	A	1524	ALA	3.4
1	B	310	LEU	3.3
2	A	1521	GLU	3.3
2	A	1539	LEU	3.3
2	A	1642	LEU	3.3
1	B	97	ASN	3.3
2	A	694	VAL	3.2
2	A	734	VAL	3.2
2	A	726	LYS	3.2
2	A	872	VAL	3.2
1	B	525	SER	3.1
2	A	1352	PHE	3.1
2	A	981	GLY	3.1
1	B	547	THR	3.1
2	A	1589	GLU	3.1
1	B	521	ALA	3.1
1	B	224	LEU	3.1
1	B	472	ASN	3.1
1	B	495	LYS	3.1
2	A	1657	CYS	3.0
2	A	728	PHE	3.0
1	B	469	TRP	3.0
2	A	954	SER	3.0
2	A	1658	GLN	3.0
2	A	1663	ASN	3.0
2	A	753	HIS	3.0
1	B	431	LEU	2.9
1	B	665	ASN	2.9
2	A	712	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	522	SER	2.9
2	A	695	VAL	2.9
2	A	1523	ALA	2.9
2	A	744	HIS	2.9
2	A	1649	PRO	2.9
1	B	391	ASN	2.9
2	A	1572	ASN	2.9
2	A	1659	ALA	2.9
1	B	519	SER	2.9
2	A	871	PRO	2.8
1	B	474	LYS	2.8
2	A	1387	GLU	2.8
2	A	1635	TYR	2.8
2	A	723	ARG	2.8
1	B	475	ALA	2.8
2	A	686	ILE	2.8
1	B	463	SER	2.7
1	B	326	ALA	2.7
1	B	392	ALA	2.7
2	A	1545	ALA	2.7
2	A	1164	ILE	2.7
2	A	692	HIS	2.7
2	A	1515	LYS	2.7
2	A	705	VAL	2.7
2	A	1527	CYS	2.7
2	A	1621	GLY	2.7
2	A	1612	VAL	2.7
1	B	287	MET	2.7
2	A	1652	THR	2.7
2	A	1651	ASP	2.7
1	B	620	LEU	2.7
2	A	1673	LEU	2.7
2	A	1622	LYS	2.6
1	B	428	VAL	2.6
2	A	1543	ILE	2.6
2	A	1628	LYS	2.6
1	B	333	THR	2.6
2	A	1547	THR	2.6
2	A	1623	GLU	2.6
1	B	433	PHE	2.6
2	A	1650	ARG	2.6
2	A	1676	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	444	GLU	2.6
2	A	1533	GLY	2.6
2	A	1559	TYR	2.6
2	A	756	THR	2.6
2	A	916	THR	2.6
1	B	674	ARG	2.5
1	B	368	PRO	2.5
2	A	1598	ILE	2.5
2	A	1560	ALA	2.5
2	A	701	ASP	2.5
1	B	672	ILE	2.5
2	A	1660	PHE	2.5
1	B	673	LEU	2.4
2	A	759	PRO	2.4
2	A	1601	ILE	2.4
2	A	792	ASP	2.4
4	D	27	GLY	2.4
1	B	625	GLN	2.4
1	B	313	TYR	2.4
2	A	1588	GLY	2.4
1	B	468	ASP	2.4
3	C	103	LEU	2.4
1	B	388	VAL	2.3
2	A	681	LYS	2.3
2	A	1630	ASN	2.3
1	B	548	GLY	2.3
4	D	14	CYS	2.3
1	B	426	SER	2.3
1	B	266	TYR	2.3
1	B	424	LEU	2.3
2	A	1447	ASP	2.3
1	B	292	LEU	2.3
1	B	390	LEU	2.3
2	A	1664	LEU	2.3
2	A	1671	ILE	2.3
1	B	336	PHE	2.3
2	A	1631	PHE	2.3
1	B	626	PHE	2.3
1	B	550	GLN	2.3
1	B	663	GLN	2.3
1	B	574	HIS	2.3
4	D	57	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	A	1613	LYS	2.2
2	A	752	LEU	2.2
2	A	1039	LEU	2.2
2	A	1526	LYS	2.2
1	B	30	ILE	2.2
2	A	1326	TYR	2.2
2	A	754	MET	2.2
2	A	1306	GLN	2.2
2	A	1551	THR	2.2
1	B	369	TYR	2.2
1	B	402	SER	2.2
2	A	693	SER	2.2
4	D	44	GLY	2.2
2	A	1582	LEU	2.2
1	B	628	GLU	2.2
2	A	688	ALA	2.2
2	A	1624	ALA	2.2
1	B	173	MET	2.2
1	B	95	GLY	2.2
2	A	861	ALA	2.2
2	A	724	CYS	2.1
2	A	1469	SER	2.1
1	B	492	TYR	2.1
4	D	20	ARG	2.1
1	B	664	GLU	2.1
2	A	1557	ILE	2.1
2	A	1597	GLU	2.1
2	A	680	GLN	2.1
1	B	520	ASP	2.1
2	A	698	CYS	2.1
2	A	1544	SER	2.1
1	B	440	PRO	2.1
1	B	518	PHE	2.1
2	A	1633	PHE	2.1
2	A	1568	ILE	2.1
3	C	78	GLN	2.0
2	A	1634	ARG	2.0
2	A	1610	GLU	2.0
1	B	523	TYR	2.0
2	A	1578	LYS	2.0
1	B	373	VAL	2.0
2	A	1666	GLU	2.0

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

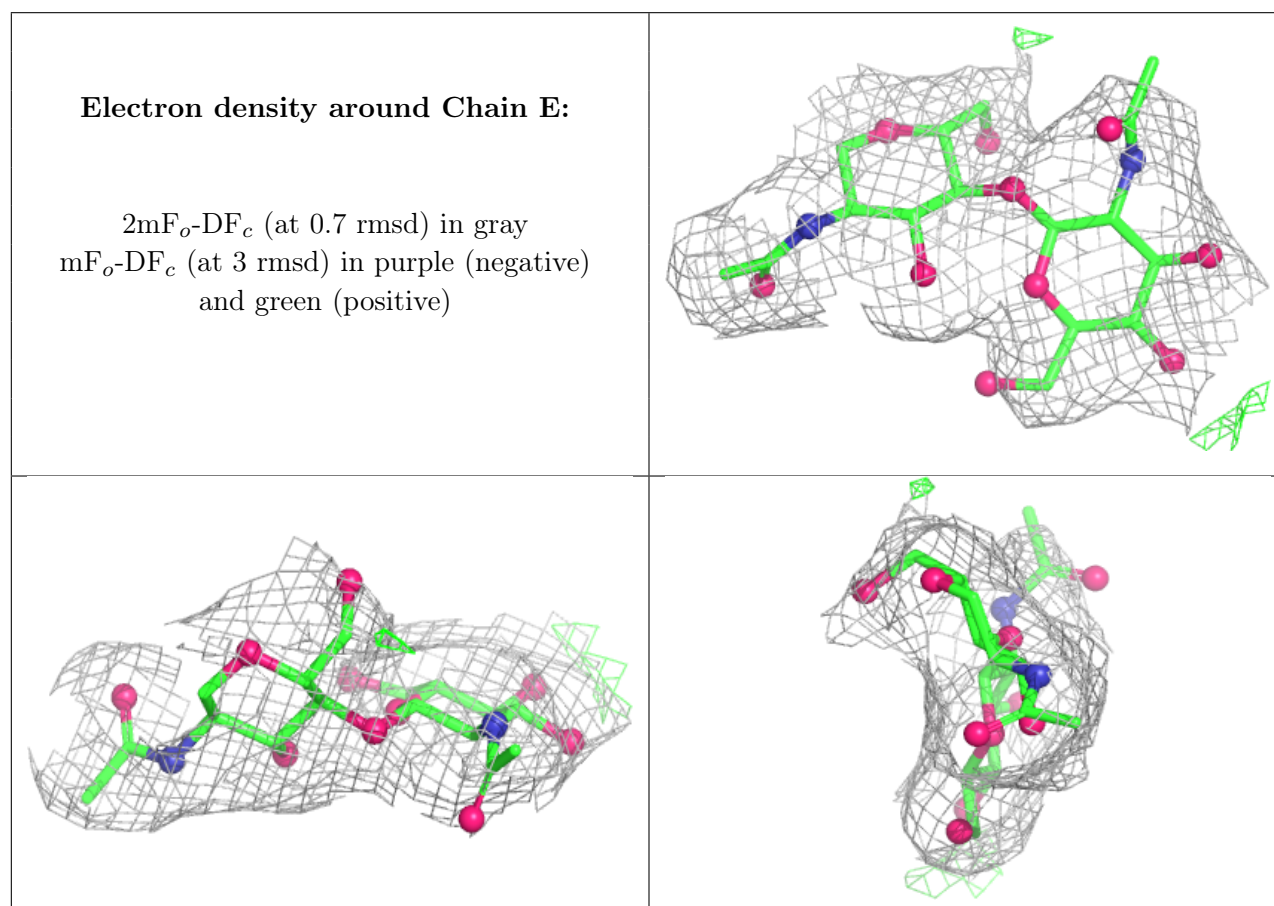
There are no non-standard protein/DNA/RNA residues in this entry.

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	0.72	0.13	76,91,102,112	0
5	NAG	E	1	14/15	0.90	0.09	36,54,78,81	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

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	2003	6/7	0.73	0.22	85,92,98,99	0

6.5 Other polymers

There are no such residues in this entry.