



# Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2016 – 05:24 PM EDT

PDB ID : 5HCE  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027457  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

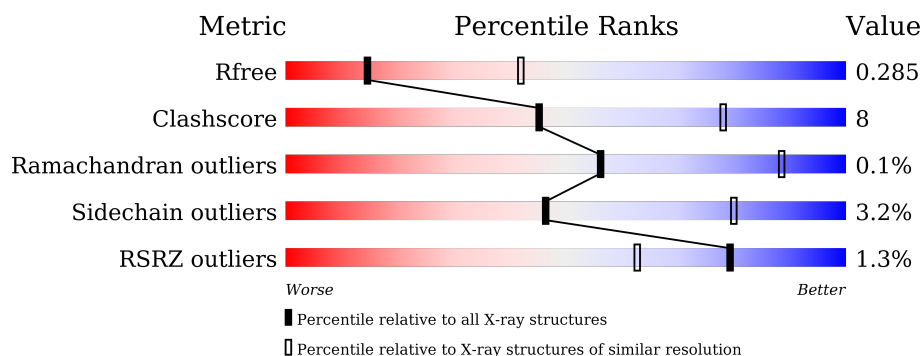
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1112 (3.16-3.08)
Clashscore	102246	1218 (3.16-3.08)
Ramachandran outliers	100387	1175 (3.16-3.08)
Sidechain outliers	100360	1175 (3.16-3.08)
RSRZ outliers	91569	1114 (3.16-3.08)

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

Mol	Chain	Length	Quality of chain
1	B	656	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>..</div> </div> </div>
2	A	998	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
3	C	165	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>12%</div> <div>10%</div> </div> </div>
4	D	81	<div> <div></div> <div> <div>33%</div> <div>20%</div> <div>5%</div> <div>42%</div> </div> </div>

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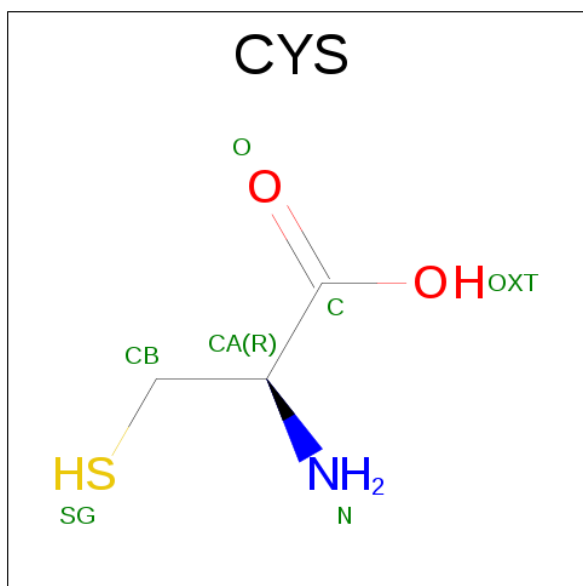
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP Q5YD59
C	78	GLN	ASN	engineered mutation	UNP Q5YD59
C	102	GLN	ASN	engineered mutation	UNP Q5YD59

- Molecule 4 is a protein called Rhipicephalus appendiculatus RaCI1.

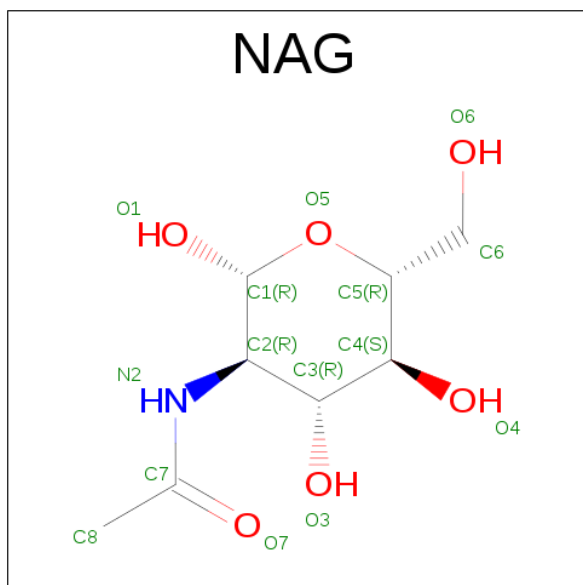
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	47	Total	C	N	O	S	0	0	0
			333	203	62	62	6			

- Molecule 5 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).



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

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

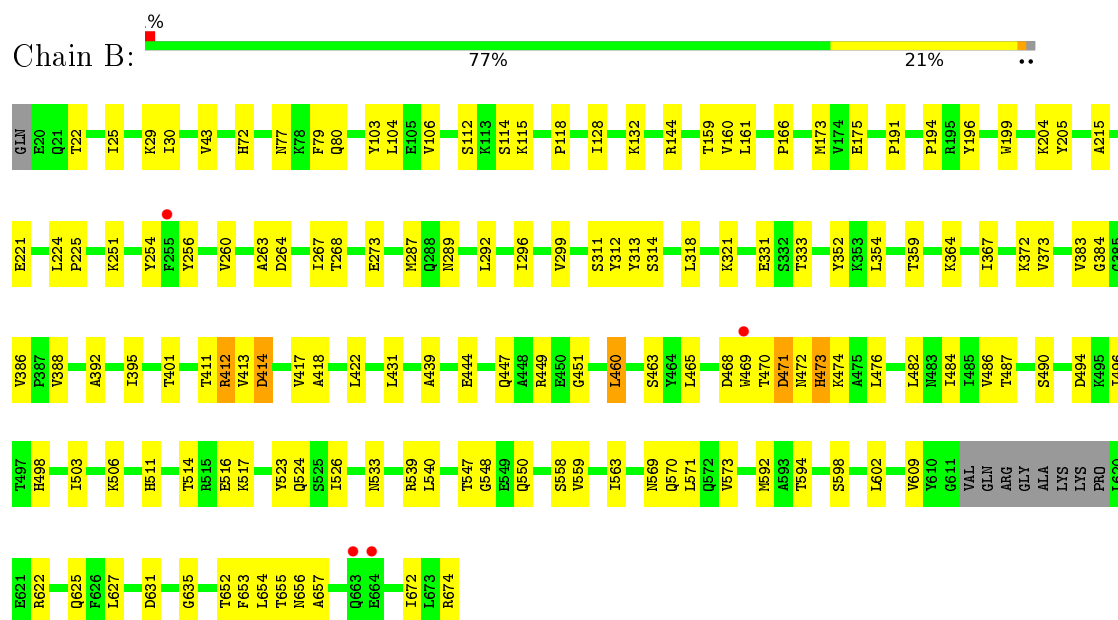


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

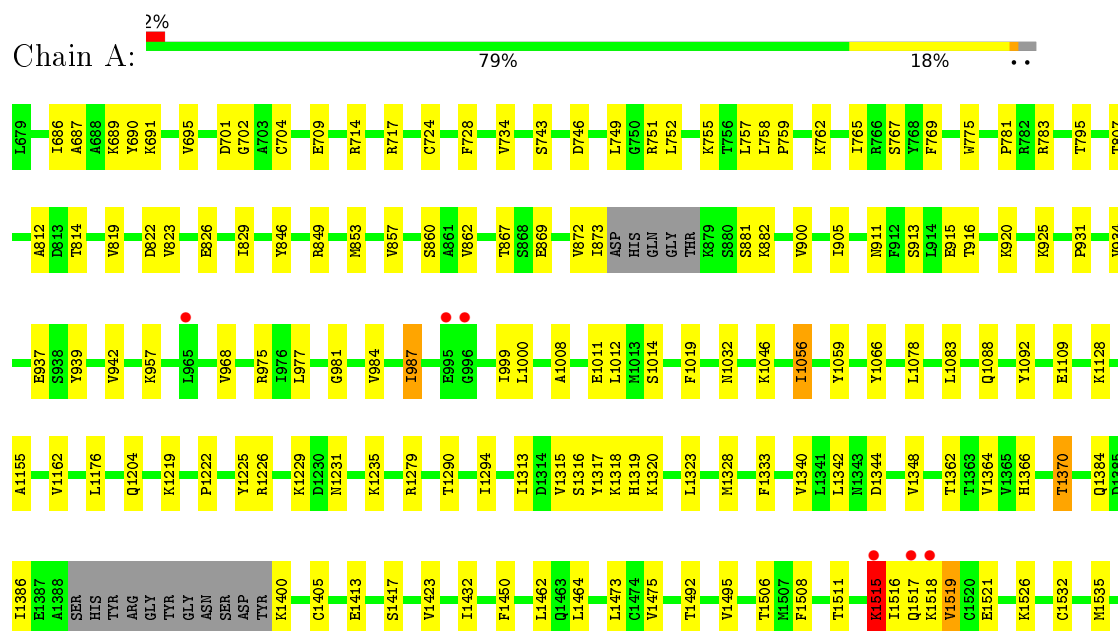
### 3 Residue-property plots

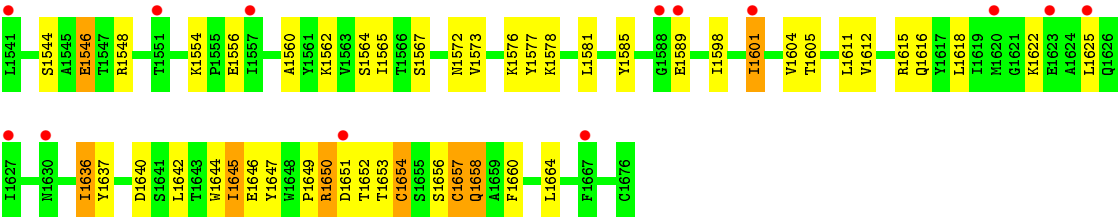
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

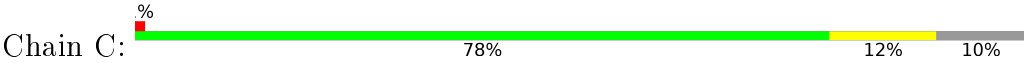


#### • Molecule 2: Complement C5

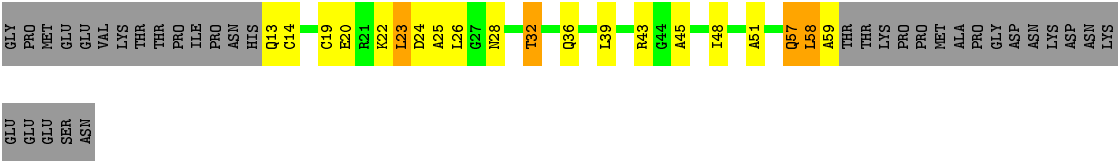
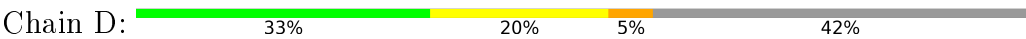




● Molecule 3: Complement inhibitor



● Molecule 4: Rhipicephalus appendiculatus RaCl1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.26Å 140.72Å 210.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.40 – 3.12 94.13 – 3.12	Depositor EDS
% Data completeness (in resolution range)	98.9 (74.40-3.12) 99.1 (94.13-3.12)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.267 , 0.281 0.274 , 0.285	Depositor DCC
$R_{free}$ test set	5264 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.2	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 23.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	14418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.34	0/5234	0.51	0/7119
2	A	0.36	0/7932	0.50	1/10740 (0.0%)
3	C	0.30	0/1183	0.47	0/1599
4	D	0.39	0/335	0.55	0/454
All	All	0.35	0/14684	0.51	1/19912 (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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	1515	LYS	N-CA-C	-5.83	95.27	111.00

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	87	0
2	A	7775	0	7822	124	0
3	C	1160	0	1085	10	0
4	D	333	0	335	14	0
5	A	6	0	3	0	0
6	A	28	0	25	0	0
All	All	14418	0	14292	225	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 (225) 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: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
4:D:20:GLU:H	4:D:32:THR:HG1	1.50	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
1:B:414:ASP:OD1	1:B:414:ASP:N	2.36	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
2:A:915:GLU:HG2	2:A:920:LYS:HG3	1.87	0.55
1:B:115:LYS:HB2	1:B:654:LEU:HD21	1.86	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
2:A:743:SER:OG	2:A:746:ASP:OD1	2.17	0.55
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:364:LYS:HB3	1:B:367:ILE:HD13	1.88	0.54
2:A:1519:VAL:HG13	2:A:1521:GLU:H	1.73	0.54
1:B:221:GLU:OE1	2:A:762:LYS:NZ	2.40	0.54
2:A:1535:MET:HG3	2:A:1645:ILE:HD11	1.90	0.54
2:A:1432:ILE:HG13	2:A:1511:THR:HG21	1.89	0.54
2:A:857:VAL:HA	2:A:913:SER:O	2.07	0.54
1:B:204:LYS:HG2	1:B:205:TYR:H	1.73	0.54
2:A:1226:ARG:NH1	3:C:141:GLU:OE1	2.41	0.53
2:A:999:ILE:HG13	2:A:1000:LEU:HG	1.89	0.53
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:975:ARG:NH2	2:A:1344:ASP:O	2.40	0.53
1:B:439:ALA:H	1:B:447:GLN:HE22	1.55	0.53
1:B:204:LYS:HG2	1:B:205:TYR:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1515:LYS:CE	2:A:1516:ILE:HG23	2.36	0.53
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
2:A:1657:CYS:O	2:A:1660:PHE:HB3	2.10	0.52
1:B:25:ILE:HG13	1:B:106:VAL:HG21	1.91	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
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:417:VAL:HG21	1:B:473:HIS:NE2	2.26	0.50
2:A:1011:GLU:O	2:A:1014:SER:OG	2.21	0.50
1:B:29:LYS:HD2	1:B:652:THR:HG23	1.93	0.50
2:A:1618:LEU:O	2:A:1645:ILE:HA	2.12	0.50
2:A:687:ALA:O	2:A:691:LYS:HG3	2.12	0.50
1:B:573:VAL:HG12	1:B:592:MET:HG2	1.93	0.50
2:A:1032:ASN:N	2:A:1032:ASN:OD1	2.45	0.50
1:B:104:LEU:O	1:B:114:SER:HA	2.12	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:691:LYS:HE2	2:A:757:LEU:HD13	1.94	0.49
2:A:1235:LYS:NZ	2:A:1413:GLU:OE1	2.45	0.48
1:B:43:VAL:HG23	1:B:79:PHE:HB3	1.95	0.48
1:B:318:LEU:HA	1:B:321:LYS:HG3	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
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
1:B:106:VAL:O	1:B:112:SER:HA	2.13	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
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
2:A:1066:TYR:HB3	2:A:1078:LEU:HD23	1.96	0.47
1:B:516:GLU:O	1:B:524:GLN:NE2	2.33	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
1:B:224:LEU:HD12	1:B:225:PRO:HD2	1.95	0.47
1:B:471:ASP:OD1	1:B:473:HIS:CE1	2.68	0.47
2:A:1616:GLN:OE1	2:A:1650:ARG:NH2	2.47	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
1:B:383:VAL:O	1:B:411:THR:HG21	2.15	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
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:160:VAL:HG22	1:B:175:GLU:HB3	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
1:B:267:ILE:HD13	1:B:299:VAL:HG21	1.97	0.46
2:A:937:GLU:HG3	2:A:1364:VAL:HG22	1.97	0.46
2:A:1313:ILE:HD12	2:A:1328:MET:HE3	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
2:A:981:GLY:HA3	2:A:1333:PHE:CD2	2.51	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
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
1:B:359:THR:HG21	1:B:372:LYS:N	2.24	0.44
2:A:942:VAL:CG2	2:A:957:LYS:HG2	2.45	0.44
1:B:412:ARG:HH11	1:B:412:ARG:HB2	1.82	0.44
2:A:1645:ILE:HG13	2:A:1645:ILE:O	2.17	0.44
1:B:469:TRP:CD1	1:B:482:LEU:HD11	2.53	0.44
4:D:45:ALA:HB3	4:D:48:ILE:HG12	1.98	0.44
2:A:1229:LYS:HD2	2:A:1231:ASN:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.99	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
2:A:765:ILE:HG13	2:A:767:SER:H	1.83	0.43
1:B:496:ILE:O	1:B:517:LYS:HD3	2.18	0.43
2:A:1176:LEU:HD22	2:A:1204:GLN:HB3	2.00	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
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
2:A:701:ASP:HA	2:A:704:CYS:SG	2.59	0.43
1:B:128:ILE:HB	1:B:215:ALA:HB2	2.01	0.43
2:A:968:VAL:HG23	2:A:1366:HIS:O	2.18	0.43
1:B:609:VAL:HG12	2:A:769:PHE:CG	2.53	0.43
2:A:822:ASP:HB2	2:A:849:ARG:HG3	2.00	0.43
1:B:196:TYR:CZ	1:B:221:GLU:HB2	2.54	0.43
2:A:939:TYR:CZ	2:A:1279:ARG:HD3	2.54	0.43
2:A:826:GLU:HG2	2:A:846:TYR:HE1	1.84	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
4:D:25:ALA:HB3	4:D:26:LEU:HD12	1.99	0.43
2:A:781:PRO:C	2:A:783:ARG:H	2.22	0.42
2:A:905:ILE:HD13	2:A:931:PRO:HG3	2.01	0.42
1:B:30:ILE:HD12	1:B:118:PRO:HB2	2.01	0.42
1:B:627:LEU:HA	1:B:627:LEU:HD12	1.85	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
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
1:B:460:LEU:HD12	1:B:460:LEU:HA	1.76	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
1:B:312:TYR:O	1:B:314:SER:N	2.45	0.42
2:A:881:SER:OG	2:A:882:LYS:N	2.52	0.42
1:B:311:SER:O	1:B:313:TYR:N	2.53	0.42
2:A:1019:PHE:CZ	2:A:1088:GLN:HB3	2.54	0.42
2:A:1386:ILE:HA	2:A:1386:ILE:HD12	1.86	0.42
2:A:822:ASP:OD1	2:A:822:ASP:N	2.47	0.42
1:B:166:PRO:HD3	1:B:199:TRP:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1517:GLN:NE2	2:A:1605:THR:HA	2.35	0.42
2:A:795:THR:H	2:A:819:VAL:HG23	1.83	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
2:A:1046:LYS:NZ	2:A:1092:TYR:O	2.53	0.42
1:B:570:GLN:O	1:B:594:THR:HA	2.20	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
4:D:20:GLU:HG3	4:D:22:LYS:HG2	2.02	0.41
2:A:1565:ILE:CD1	2:A:1611:LEU:HB3	2.50	0.41
2:A:872:VAL:HG23	2:A:873:ILE:HG22	2.02	0.41
3:C:103:LEU:HA	3:C:103:LEU:HD23	1.81	0.41
2:A:1315:VAL:HG23	2:A:1323:LEU:HB3	2.02	0.41
1:B:592:MET:SD	1:B:602:LEU:HD11	2.60	0.41
2:A:1008:ALA:HB2	2:A:1059:TYR:CG	2.55	0.41
2:A:823:VAL:HA	2:A:846:TYR:O	2.21	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:HG21	2:A:853:MET:SD	2.60	0.41
2:A:987:ILE:HG13	2:A:987:ILE:H	1.52	0.41
2:A:1572:ASN:HB3	2:A:1573:VAL:H	1.70	0.41
2:A:758:LEU:HB2	2:A:759:PRO:HD3	2.03	0.41
1:B:506:LYS:NZ	1:B:533:ASN:O	2.49	0.41
2:A:1548:ARG:NH1	2:A:1646:GLU:OE1	2.54	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:1384:GLN:O	2:A:1400:LYS:HA	2.20	0.41
2:A:1317:TYR:CD1	2:A:1344:ASP:HB3	2.56	0.40
2:A:686:ILE:HD11	2:A:734:VAL:HG11	2.03	0.40
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
4:D:39:LEU:HB2	4:D:58:LEU:HD21	2.03	0.40
1:B:80:GLN:NE2	1:B:514:THR:OG1	2.55	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:373:VAL:CG2	1:B:418:ALA:HB3	2.52	0.40
2:A:1464:LEU:HD12	2:A:1464:LEU:HA	1.81	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

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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%)	8	37
All	All	1810/1900 (95%)	1717 (95%)	92 (5%)	1 (0%)	56	88

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	14	CYS

### 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%)	559 (97%)	15 (3%)	54	83
2	A	872/885 (98%)	845 (97%)	27 (3%)	47	80
3	C	128/143 (90%)	125 (98%)	3 (2%)	58	85
4	D	37/68 (54%)	31 (84%)	6 (16%)	3	12
All	All	1611/1677 (96%)	1560 (97%)	51 (3%)	46	80

All (51) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	103	TYR
1	B	264	ASP
1	B	289	ASN
1	B	354	LEU
1	B	412	ARG
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	550	GLN
1	B	672	ILE
2	A	807	THR
2	A	814	THR
2	A	862	VAL
2	A	916	THR
2	A	987	ILE
2	A	1056	ILE
2	A	1370	THR
2	A	1462	LEU
2	A	1515	LYS
2	A	1518	LYS
2	A	1519	VAL
2	A	1526	LYS
2	A	1546	GLU
2	A	1562	LYS
2	A	1581	LEU
2	A	1589	GLU
2	A	1601	ILE
2	A	1636	ILE
2	A	1645	ILE
2	A	1650	ARG
2	A	1651	ASP
2	A	1653	THR
2	A	1654	CYS
2	A	1656	SER
2	A	1657	CYS
2	A	1658	GLN
2	A	1664	LEU
3	C	69	THR

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Mol	Chain	Res	Type
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	CYS	A	2101	2	3,5,6	0.72	0	3,5,7	1.31	1 (33%)
6	NAG	A	2102	2,6	14,14,15	0.47	0	15,19,21	0.50	0
6	NAG	A	2103	6	14,14,15	0.26	0	15,19,21	0.36	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	CYS	A	2101	2	-	0/1/4/6	0/0/0/0
6	NAG	A	2102	2,6	-	0/6/23/26	0/1/1/1
6	NAG	A	2103	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2101	CYS	O-C-CA	-2.04	120.26	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	B	647/656 (98%)	0.18	4 (0%) 90 81	49, 76, 118, 157	0
2	A	982/998 (98%)	0.30	19 (1%) 70 48	44, 66, 160, 215	0
3	C	148/165 (89%)	0.14	1 (0%) 89 79	61, 85, 123, 138	0
4	D	47/81 (58%)	0.01	0 100 100	63, 78, 98, 121	0
All	All	1824/1900 (96%)	0.24	24 (1%) 79 63	44, 72, 144, 215	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1518	LYS	9.1
2	A	1517	GLN	7.5
2	A	996	GLY	4.6
3	C	21	GLU	3.9
2	A	995	GLU	3.5
1	B	664	GLU	3.4
2	A	1541	LEU	3.3
1	B	663	GLN	3.3
2	A	1589	GLU	3.2
2	A	1623	GLU	3.1
2	A	1627	ILE	3.1
2	A	1588	GLY	3.0
2	A	1625	LEU	2.7
2	A	965	LEU	2.7
2	A	1630	ASN	2.6
2	A	1515	LYS	2.5
2	A	1651	ASP	2.3
2	A	1557	ILE	2.3
1	B	469	TRP	2.2
2	A	1667	PHE	2.2
2	A	1620	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	255	PHE	2.1
2	A	1601	ILE	2.0
2	A	1551	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CYS	A	2101	6/7	0.75	0.25	0.25	106,111,116,122	0
6	NAG	A	2102	14/15	0.91	0.18	-0.98	60,67,87,98	0
6	NAG	A	2103	14/15	0.86	0.17	-	89,98,108,110	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.