



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2016 – 09:18 AM EDT

PDB ID : 5HCD  
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](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

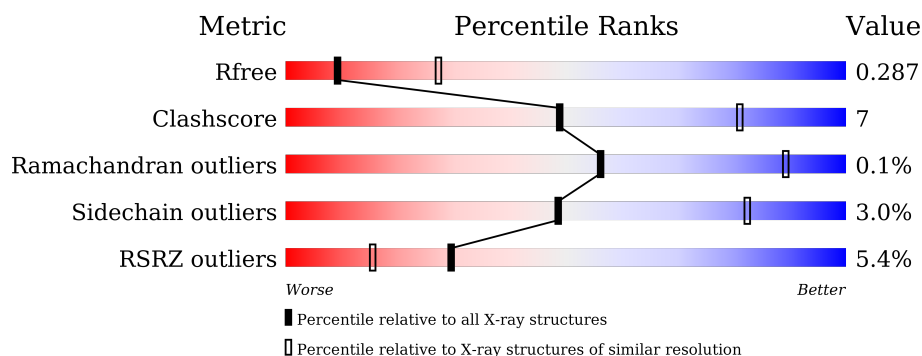
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (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 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>5%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>.</div> </div> </div>
2	A	998	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>..</div> </div> </div>
3	C	165	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>13%</div> <div>10%</div> </div> </div>
4	D	80	<div> <div></div> <div> <div>45%</div> <div>13%</div> <div>.</div> <div>39%</div> </div> </div>

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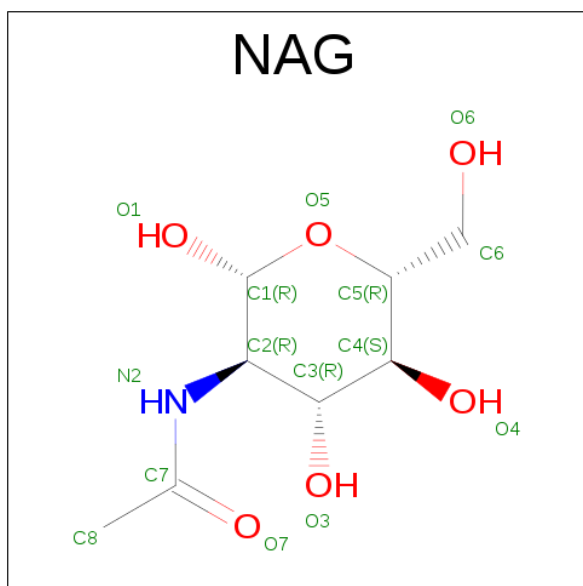
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Chain	Residue	Modelled	Actual	Comment	Reference
C	18	GLY	-	expression tag	UNP Q5YD59
C	78	GLN	ASN	engineered mutation	UNP Q5YD59
C	102	GLN	ASN	engineered mutation	UNP Q5YD59

- Molecule 4 is a protein called Rhipicephalus microplus RaCI2.

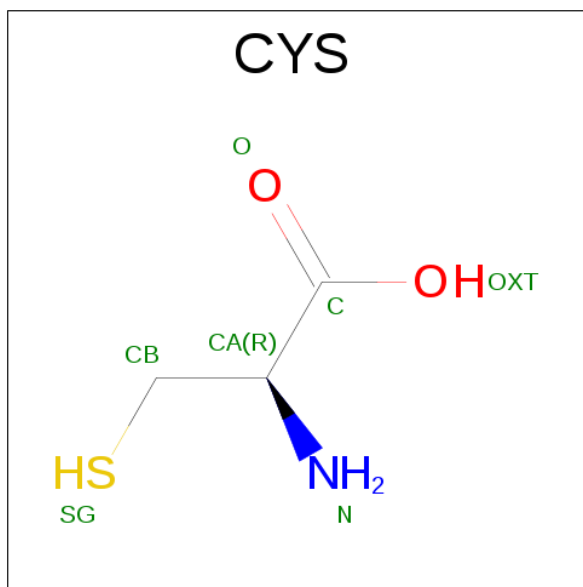
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	49	Total	C	N	O	S	0	0	0
			364	217	70	71	6			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 6 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).

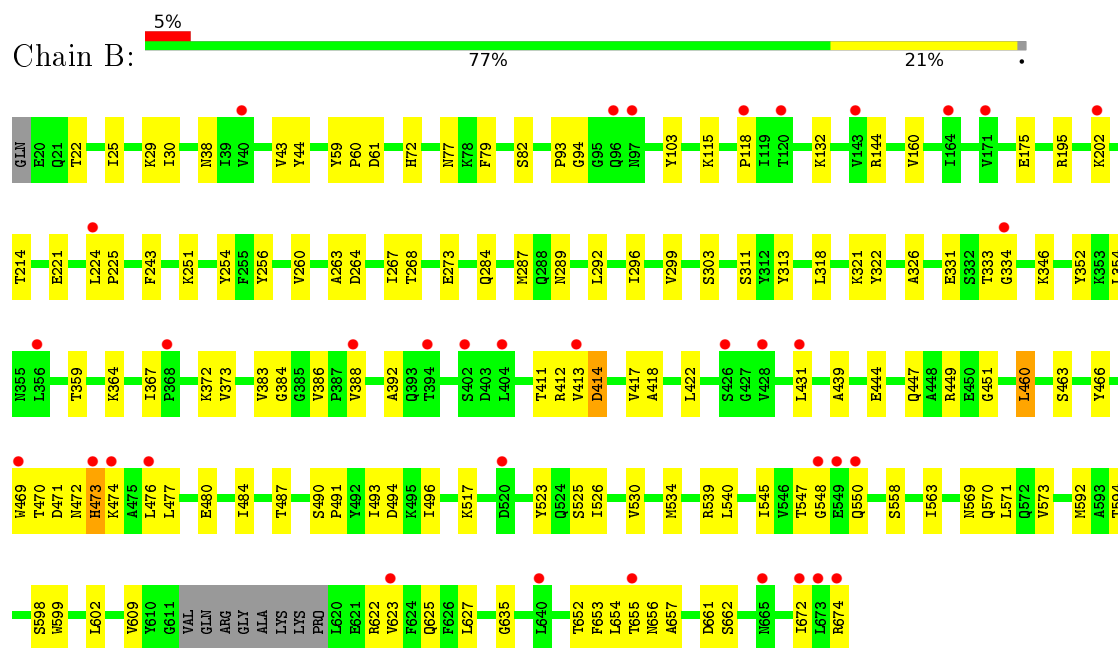


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
6	A	1	6	3	1	1	1	0	0

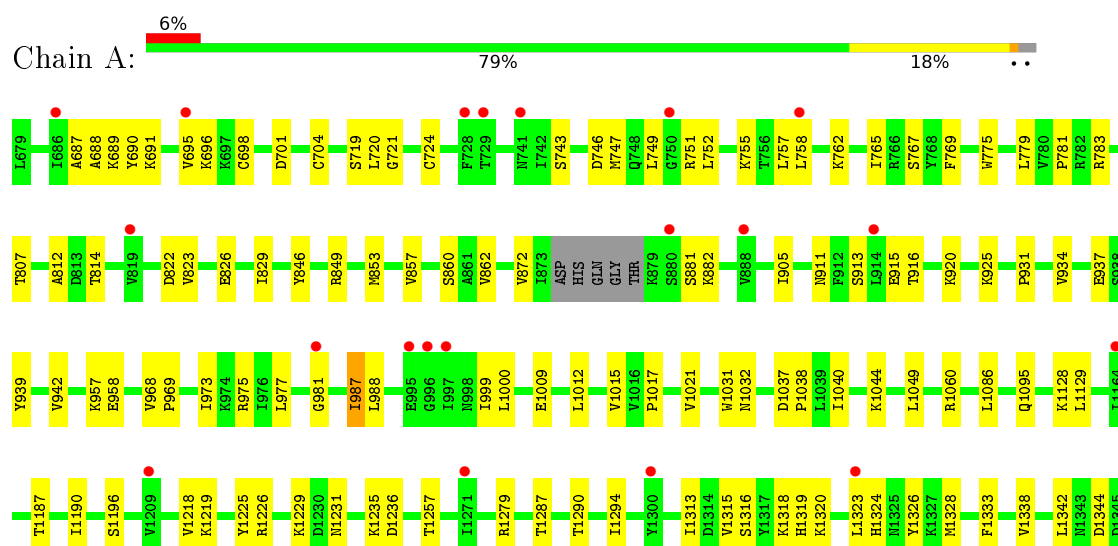
### 3 Residue-property plots

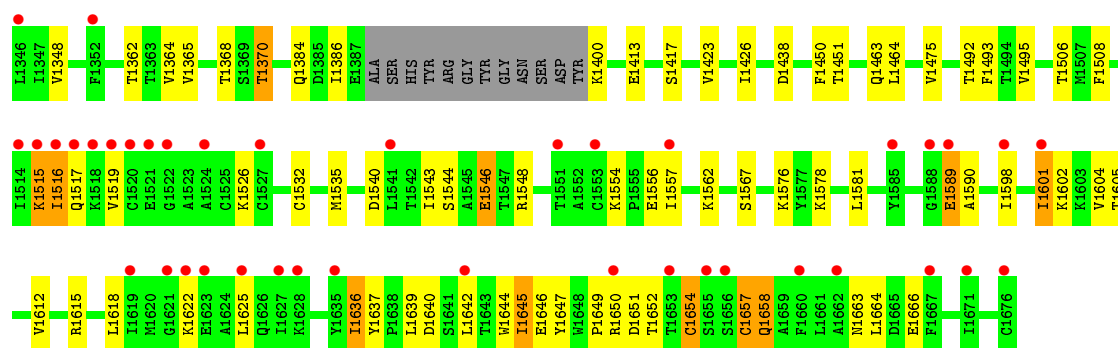
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

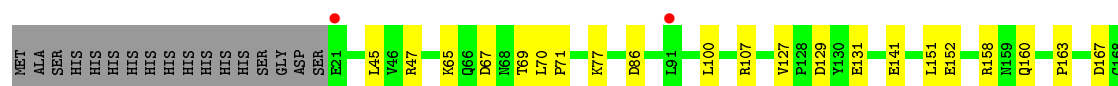
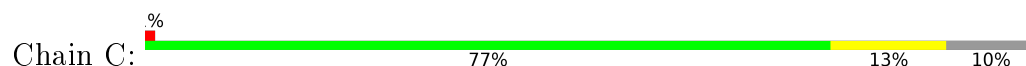


#### • Molecule 2: Complement C5





• Molecule 3: Complement inhibitor



• Molecule 4: Rhinoceros microplus RaCI2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.95Å 140.21Å 209.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.54 – 2.98 116.57 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.54-2.98) 99.3 (116.57-2.98)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.62 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.257 , 0.282 0.263 , 0.287	Depositor DCC
$R_{free}$ test set	6091 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.6	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 22.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	14445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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	0.54	0/5234	0.56	0/7119
2	A	0.55	1/7928 (0.0%)	0.56	0/10733
3	C	0.44	0/1183	0.51	0/1599
4	D	0.54	0/368	0.63	0/497
All	All	0.54	1/14713 (0.0%)	0.56	0/19948

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	724	CYS	CB-SG	-5.24	1.73	1.81

There are no bond angle outliers.

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	82	0
2	A	7771	0	7817	120	0
3	C	1160	0	1085	10	0
4	D	364	0	352	8	0
5	A	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	208	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:487:THR:HG22	1:B:523:TYR:HB3	1.68	0.75
1:B:93:PRO:O	4:D:26:ARG:NH2	2.20	0.75
2:A:1625:LEU:HB2	2:A:1636:ILE:HG23	1.68	0.74
1:B:384:GLY:HA3	1:B:413:VAL:HG23	1.70	0.73
1:B:373:VAL:HG21	1:B:388:VAL:HG11	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:490:SER:OG	1:B:491:PRO:O	2.07	0.70
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: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:N	2:A:1032:ASN:OD1	2.37	0.58
2:A:687:ALA:O	2:A:691:LYS:HG3	2.04	0.57
2:A:743:SER:OG	2:A:746:ASP:OD1	2.20	0.57
1:B:144:ARG:NH2	1:B:602:LEU:O	2.37	0.57
1:B:573:VAL:HG12	1:B:592:MET:HG2	1.87	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
2:A:1598:ILE:HD12	2:A:1637:TYR:HE1	1.74	0.53
1:B:439:ALA:H	1:B:447:GLN:HE22	1.57	0.53
2:A:1235:LYS:NZ	2:A:1413:GLU:OE1	2.41	0.53
2:A:719:SER:O	2:A:721:GLY:N	2.42	0.53
2:A:1652:THR:HG22	2:A:1658:GLN:HB2	1.92	0.52
2:A:958:GLU:OE2	2:A:1318:LYS:NZ	2.28	0.52
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: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
2:A:749:LEU:HD23	2:A:752:LEU:HD12	1.92	0.51
1:B:22:THR:HG22	1:B:44:TYR:HB2	1.92	0.51
2:A:999:ILE:HD13	2:A:1017:PRO:HG3	1.91	0.51
2:A:1612:VAL:HB	2:A:1615:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:TRP:O	1:B:469:TRP:CD1	2.64	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: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
2:A:942:VAL:CG2	2:A:957:LYS:HG2	2.40	0.50
1:B:383:VAL:O	1:B:411:THR:HG21	2.11	0.50
2:A:969:PRO:HG3	2:A:1601:ILE:HG21	1.93	0.50
2:A:857:VAL:HA	2:A:913:SER:O	2.11	0.50
1:B:284:GLN:NE2	2:A:757:LEU:HD11	2.27	0.50
3:C:65:LYS:HE2	3:C:67:ASP:O	2.12	0.49
2:A:1618:LEU:O	2:A:1645:ILE:HA	2.13	0.49
1:B:451:GLY:O	1:B:674:ARG:NH2	2.46	0.49
2:A:905:ILE:HD13	2:A:931:PRO:HG3	1.94	0.49
2:A:1316:SER:HA	2:A:1323:LEU:H	1.77	0.49
2:A:822:ASP:HB2	2:A:849:ARG:HG3	1.93	0.49
1:B:444:GLU:O	1:B:449:ARG:NH2	2.46	0.49
2:A:1384:GLN:O	2:A:1400:LYS:HA	2.12	0.49
1:B:94:GLY:HA2	4:D:26:ARG:HH21	1.78	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
2:A:1313:ILE:HD12	2:A:1328:MET:HE3	1.96	0.47
2:A:1320:LYS:HG2	2:A:1342:LEU:HD13	1.95	0.47
1:B:22:THR:HA	1:B:656:ASN:HD21	1.78	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
2:A:1645:ILE:HG13	2:A:1645:ILE:O	2.14	0.47
2:A:719:SER:C	2:A:721:GLY:H	2.17	0.47
1:B:623:VAL:HG12	1:B:627:LEU:HD22	1.96	0.47
1:B:463:SER:HA	1:B:490:SER:HB2	1.97	0.47
1:B:417:VAL:HG21	1:B:473:HIS:NE2	2.29	0.47
2:A:1451:THR:HG22	2:A:1463:GLN:O	2.14	0.47
1:B:256:TYR:HA	2:A:846:TYR:HE2	1.79	0.47
2:A:1589:GLU:OE1	2:A:1590:ALA:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:LEU:HA	1:B:321:LYS:HG3	1.96	0.47
1:B:490:SER:O	1:B:493:ILE:HG13	2.15	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
2:A:695:VAL:HG23	2:A:698:CYS:SG	2.55	0.46
1:B:38:ASN:ND2	1:B:82:SER:OG	2.38	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
2:A:1450:PHE:HA	2:A:1464:LEU:HD13	1.98	0.46
1:B:373:VAL:HG22	1:B:418:ALA:HB3	1.98	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
1:B:352:TYR:HE1	1:B:383:VAL:HG11	1.80	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
2:A:975:ARG:HA	2:A:1362:THR:O	2.16	0.45
1:B:477:LEU:HB2	1:B:480:GLU:HG3	1.98	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:981:GLY:HA3	2:A:1333:PHE:CD2	2.51	0.45
2:A:1386:ILE:HA	2:A:1386:ILE:HD12	1.83	0.45
2:A:934:VAL:HG22	2:A:1492:THR:HG21	1.99	0.45
1:B:570:GLN:O	1:B:594:THR:HA	2.17	0.45
2:A:968:VAL:HG22	2:A:1368:THR:HG22	1.97	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
1:B:331:GLU:OE2	1:B:333:THR:OG1	2.22	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
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
1:B:422:LEU:HD12	1:B:422:LEU:HA	1.83	0.44
1:B:460:LEU:HD12	1:B:460:LEU:HA	1.70	0.44
2:A:691:LYS:HE2	2:A:757:LEU:HD13	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:1129:LEU:HA	2:A:1129:LEU:HD23	1.84	0.43
2:A:823:VAL:HG21	2:A:853:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1037:ASP:OD2	2:A:1040:ILE:HG13	2.17	0.43
1:B:311:SER:O	1:B:313:TYR:N	2.51	0.43
1:B:43:VAL:HG23	1:B:79:PHE:HB3	2.00	0.43
2:A:1015:VAL:HG22	2:A:1049:LEU:HD12	2.00	0.43
1:B:496:ILE:O	1:B:517:LYS:HD3	2.18	0.43
1:B:132:LYS:HD2	1:B:609:VAL:HG11	1.99	0.43
2:A:1319:HIS:N	2:A:1344:ASP:OD2	2.49	0.43
1:B:268:THR:OG1	1:B:326:ALA:HB3	2.17	0.43
3:C:47:ARG:NH1	3:C:160:GLN:OE1	2.48	0.43
4:D:46:ASP:N	4:D:46:ASP:OD1	2.50	0.43
1:B:144:ARG:HG2	2:A:775:TRP:CZ2	2.53	0.43
2:A:988:LEU:HD23	2:A:1021:VAL:HG22	2.00	0.43
2:A:765:ILE:HG13	2:A:767:SER:H	1.84	0.43
1:B:627:LEU:HA	1:B:627:LEU:HD12	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:1187:THR:HA	2:A:1190:ILE:HG22	2.01	0.42
2:A:973:ILE:HG23	2:A:1365:VAL:HG12	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
2:A:1654:CYS:HB2	2:A:1657:CYS:HB3	1.95	0.42
1:B:94:GLY:HA2	4:D:26:ARG:NH2	2.34	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
2:A:1031:TRP:HB3	2:A:1038:PRO:HB3	2.01	0.42
2:A:688:ALA:HA	2:A:691:LYS:HD2	2.02	0.42
2:A:781:PRO:C	2:A:783:ARG:H	2.23	0.42
2:A:860:SER:HB3	2:A:911:ASN:H	1.85	0.42
1:B:263:ALA:HB3	1:B:292:LEU:HB3	2.01	0.42
2:A:1554:LYS:HB3	2:A:1557:ILE:HG12	2.01	0.41
2:A:701:ASP:HA	2:A:704:CYS:SG	2.60	0.41
1:B:267:ILE:HD13	1:B:299:VAL:HG21	2.01	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
2:A:1423:VAL:O	2:A:1495:VAL:HA	2.20	0.41
2:A:872:VAL:HG22	2:A:881:SER:O	2.21	0.41
1:B:202:LYS:HE3	1:B:214:THR:OG1	2.21	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:HB3	2:A:1044:LYS:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1229:LYS:NZ	2:A:1236:ASP:O	2.54	0.40
2:A:1451:THR:HG22	2:A:1463:GLN:C	2.42	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:1663:ASN:O	2:A:1666:GLU:HB2	2.22	0.40
2:A:987:ILE:HG13	2:A:987:ILE:H	1.53	0.40
2:A:1438:ASP:OD1	2:A:1438:ASP:N	2.55	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
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%)	56	89
3	C	146/165 (88%)	138 (94%)	8 (6%)	0	100	100
4	D	47/80 (59%)	43 (92%)	3 (6%)	1 (2%)	9	38
All	All	1811/1899 (95%)	1720 (95%)	89 (5%)	2 (0%)	56	89

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%)	559 (97%)	15 (3%)	54	84
2	A	872/885 (98%)	848 (97%)	24 (3%)	51	83
3	C	128/143 (90%)	125 (98%)	3 (2%)	58	87
4	D	42/71 (59%)	36 (86%)	6 (14%)	4	17
All	All	1616/1680 (96%)	1568 (97%)	48 (3%)	48	82

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	61	ASP
1	B	103	TYR
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	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	1326	TYR
2	A	1370	THR
2	A	1515	LYS
2	A	1516	ILE

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Mol	Chain	Res	Type
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	1654	CYS
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	23	VAL
4	D	26	ARG
4	D	34	CYS
4	D	46	ASP
4	D	51	LEU
4	D	57	LEU

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

### 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 ⓘ

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	NAG	A	2001	2,5	14,14,15	0.27	0	15,19,21	0.49	0
5	NAG	A	2002	5	14,14,15	0.29	0	15,19,21	0.43	0
6	CYS	A	2003	2	3,5,6	0.76	0	3,5,7	1.19	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	A	2001	2,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2002	5	-	0/6/23/26	0/1/1/1
6	CYS	A	2003	2	-	0/1/4/6	0/0/0/0

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.

## 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, 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%)	0.69	36 (5%)	28 14	43, 68, 106, 155	0
2	A	981/998 (98%)	0.69	60 (6%)	25 12	39, 59, 148, 208	0
3	C	148/165 (89%)	0.33	2 (1%)	78 57	56, 78, 116, 178	0
4	D	49/80 (61%)	0.52	0	100 100	49, 69, 92, 173	0
All	All	1825/1899 (96%)	0.66	98 (5%)	29 15	39, 64, 134, 208	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	1518	LYS	14.8
2	A	1517	GLN	11.8
2	A	1588	GLY	9.4
2	A	1656	SER	5.4
1	B	96	GLN	5.3
2	A	758	LEU	5.2
2	A	1671	ILE	5.1
2	A	995	GLU	4.5
2	A	1521	GLU	4.4
2	A	1623	GLU	4.3
2	A	1516	ILE	4.3
3	C	21	GLU	4.2
2	A	1622	LYS	4.2
2	A	1621	GLY	4.1
1	B	474	LYS	4.1
2	A	1520	CYS	4.0
2	A	1541	LEU	4.0
1	B	469	TRP	3.9
2	A	1662	ALA	3.8
1	B	674	ARG	3.7
1	B	394	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	673	LEU	3.7
2	A	1655	SER	3.6
2	A	1514	ILE	3.4
1	B	623	VAL	3.4
1	B	97	ASN	3.3
1	B	548	GLY	3.3
2	A	996	GLY	3.1
2	A	1519	VAL	3.1
2	A	1635	TYR	3.1
1	B	413	VAL	3.0
2	A	1676	CYS	3.0
1	B	428	VAL	2.9
2	A	880	SER	2.9
1	B	334	GLY	2.9
2	A	1515	LYS	2.9
1	B	549	GLU	2.9
1	B	431	LEU	2.8
2	A	1271	ILE	2.8
1	B	520	ASP	2.8
1	B	473	HIS	2.7
2	A	1585	TYR	2.6
2	A	1557	ILE	2.6
2	A	1164	ILE	2.6
2	A	1642	LEU	2.6
2	A	1619	ILE	2.6
1	B	224	LEU	2.5
2	A	1352	PHE	2.5
1	B	368	PRO	2.5
2	A	1667	PHE	2.5
2	A	729	THR	2.5
2	A	1551	THR	2.5
2	A	686	ILE	2.4
2	A	1625	LEU	2.4
2	A	741	ASN	2.4
2	A	1524	ALA	2.4
2	A	1660	PHE	2.4
1	B	672	ILE	2.4
2	A	1627	ILE	2.3
2	A	1553	CYS	2.3
2	A	1589	GLU	2.3
2	A	750	GLY	2.3
2	A	1346	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	695	VAL	2.2
2	A	1650	ARG	2.2
1	B	388	VAL	2.2
2	A	1653	THR	2.2
2	A	1527	CYS	2.2
1	B	665	ASN	2.2
2	A	981	GLY	2.2
1	B	120	THR	2.2
1	B	426	SER	2.2
1	B	164	ILE	2.2
1	B	118	PRO	2.2
1	B	202	LYS	2.2
2	A	1628	LYS	2.1
1	B	40	VAL	2.1
2	A	1300	TYR	2.1
2	A	1522	GLY	2.1
1	B	356	LEU	2.1
1	B	640	LEU	2.1
2	A	819	VAL	2.1
2	A	1323	LEU	2.1
1	B	171	VAL	2.1
2	A	728	PHE	2.1
1	B	550	GLN	2.1
2	A	888	VAL	2.1
1	B	404	LEU	2.1
1	B	476	LEU	2.1
2	A	914	LEU	2.1
2	A	1598	ILE	2.0
2	A	1601	ILE	2.0
1	B	655	THR	2.0
1	B	143	VAL	2.0
2	A	1209	VAL	2.0
2	A	997	ILE	2.0
1	B	402	SER	2.0
3	C	91	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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
6	CYS	A	2003	6/7	0.87	0.21	-0.34	85,92,98,99	0
5	NAG	A	2001	14/15	0.92	0.16	-2.02	36,54,78,81	0
5	NAG	A	2002	14/15	0.87	0.23	-	76,91,102,112	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.