



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 06:10 AM EDT

PDB ID : 7T0R  
Title : Crystal structure of the anti-CD4 adnectin 6940\_B01 as a complex with the extracellular domains of CD4 and ibalizumab fAb  
Authors : Williams, S.P.; Concha, N.O.; Wensel, D.L.; Hong, X.  
Deposited on : 2021-11-30  
Resolution : 3.65 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

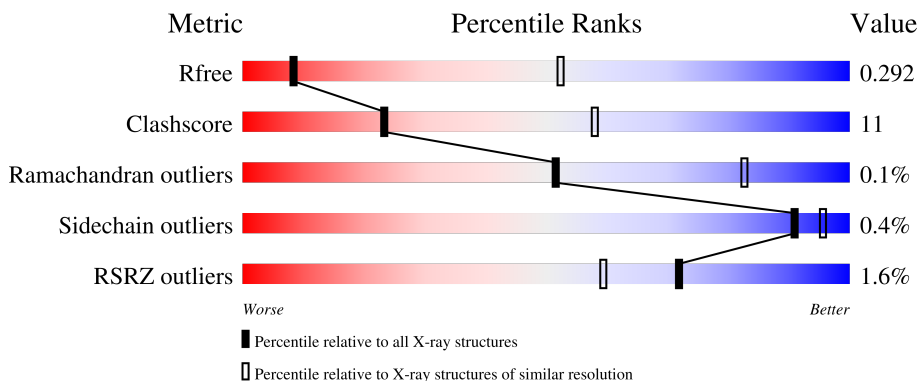
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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.



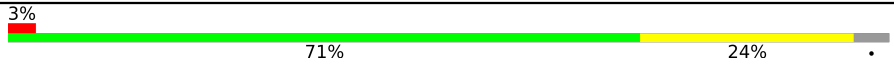

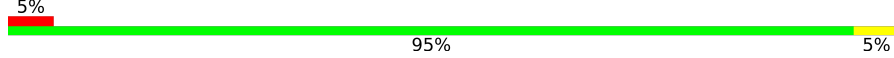
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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  $\geq 3$ , 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	219	 2% 75% 23%
1	L	219	 76% 22%
2	C	229	 2% 76% 21%
2	H	229	 79% 18%
3	A	373	 68% 27% 5%

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Mol	Chain	Length	Quality of chain
3	D	373	 <p>3% 71% 24%</p>
4	G	94	 <p>2% 72% 27%</p>
4	I	94	 <p>5% 95% 5%</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12963 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 Ibalizumab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	216	1664	1041	276	341	6	0	0	0
1	B	215	1521	960	247	308	6	0	0	0

- Molecule 2 is a protein called Ibalizumab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	221	1664	1050	270	337	7	0	0	0
2	C	222	1559	986	248	318	7	0	0	0

- Molecule 3 is a protein called T-cell surface glycoprotein CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	355	2557	1623	423	501	10	0	0	0
3	D	357	2554	1614	421	509	10	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	365	GLY	-	expression tag	UNP P01730
A	366	SER	-	expression tag	UNP P01730
A	367	HIS	-	expression tag	UNP P01730
A	368	HIS	-	expression tag	UNP P01730
A	369	HIS	-	expression tag	UNP P01730
A	370	HIS	-	expression tag	UNP P01730
A	371	HIS	-	expression tag	UNP P01730
A	372	HIS	-	expression tag	UNP P01730

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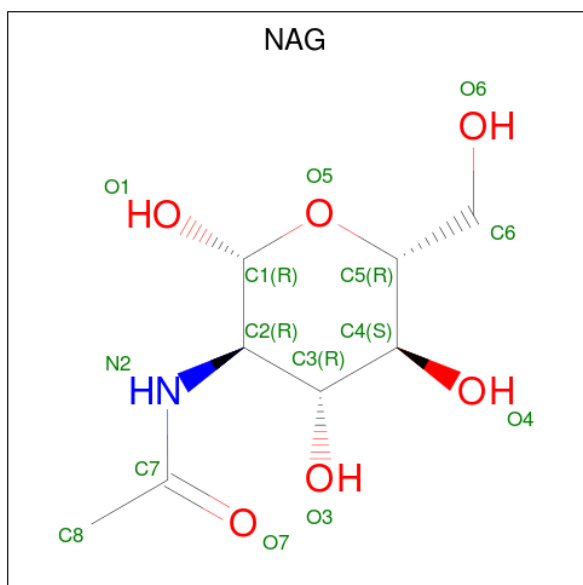
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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	HIS	-	expression tag	UNP P01730
D	365	GLY	-	expression tag	UNP P01730
D	366	SER	-	expression tag	UNP P01730
D	367	HIS	-	expression tag	UNP P01730
D	368	HIS	-	expression tag	UNP P01730
D	369	HIS	-	expression tag	UNP P01730
D	370	HIS	-	expression tag	UNP P01730
D	371	HIS	-	expression tag	UNP P01730
D	372	HIS	-	expression tag	UNP P01730
D	373	HIS	-	expression tag	UNP P01730

- Molecule 4 is a protein called Adnectin 6940\_B01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	93	Total	C	N	O	S	0	0	0
			702	452	115	134	1			
4	I	94	Total	C	N	O	S	0	0	0
			709	456	118	134	1			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



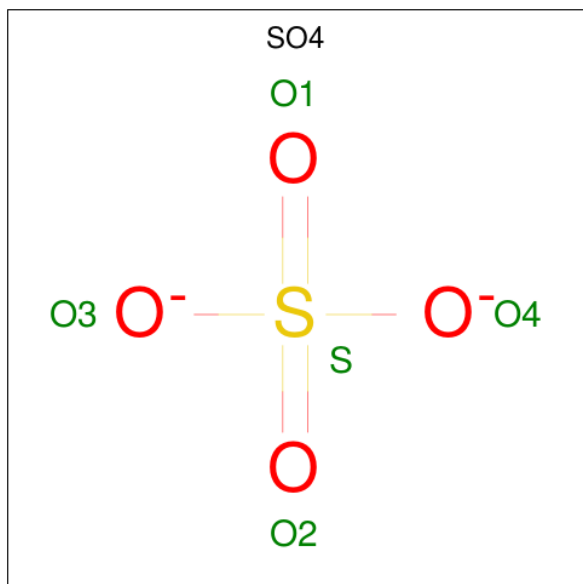
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

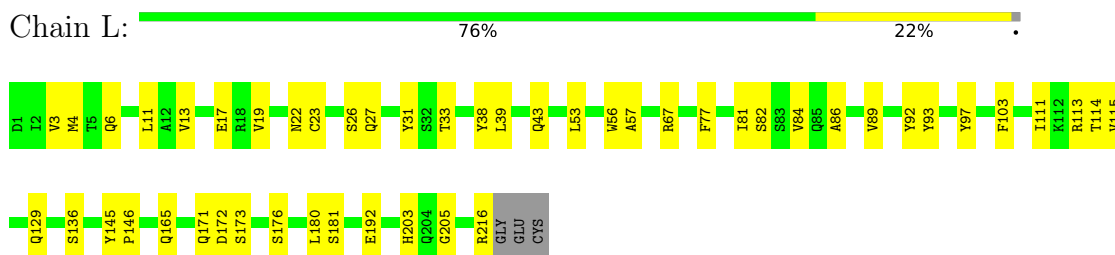


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
6	A	1	5	4	1	0	0

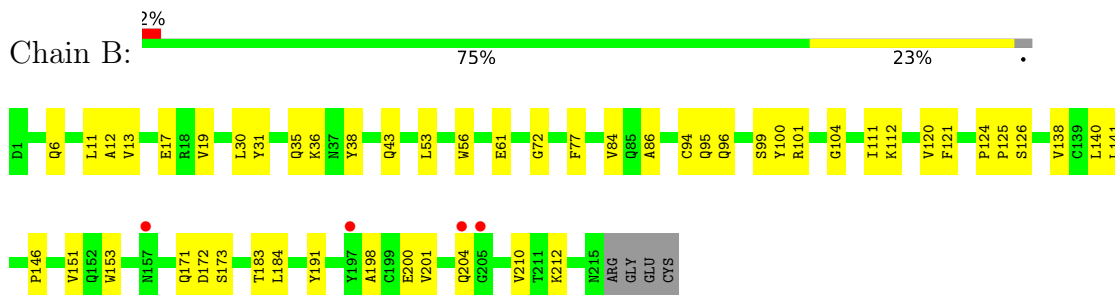
### 3 Residue-property plots [i](#)

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.

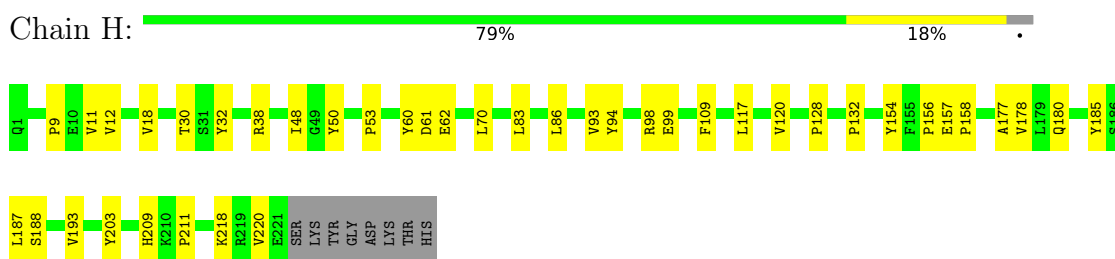
- Molecule 1: Ibalizumab Light Chain



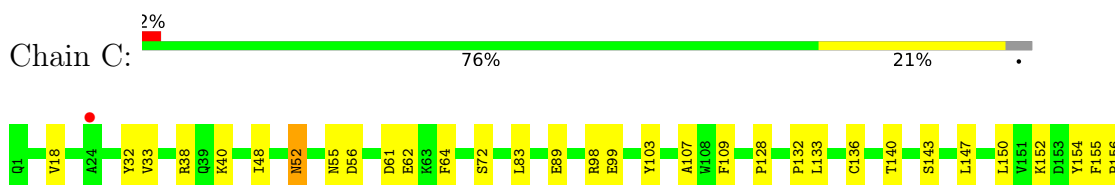
- Molecule 1: Ibalizumab Light Chain



- Molecule 2: Ibalizumab Heavy Chain



- Molecule 2: Ibalizumab Heavy Chain









## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.51Å 164.01Å 167.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.53 – 3.65 29.53 – 3.65	Depositor EDS
% Data completeness (in resolution range)	86.0 (29.53-3.65) 86.0 (29.53-3.65)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 3.65Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.226 , 0.292 0.225 , 0.292	Depositor DCC
$R_{free}$ test set	1587 reflections (7.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.9	Xtrriage
Anisotropy	0.551	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.035 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	12963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.13% 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, 0.333 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: SO4, 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	0.30	0/1554	0.58	0/2137
1	L	0.31	0/1700	0.57	0/2314
2	C	0.28	0/1600	0.55	0/2207
2	H	0.31	0/1707	0.55	0/2332
3	A	0.29	0/2602	0.56	0/3559
3	D	0.28	0/2598	0.57	0/3558
4	G	0.29	0/722	0.56	0/990
4	I	0.29	0/730	0.56	0/1002
All	All	0.29	0/13213	0.56	0/18099

There are no bond length outliers.

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	1521	0	1357	37	0
1	L	1664	0	1579	37	0
2	C	1559	0	1393	38	0
2	H	1664	0	1592	28	0
3	A	2557	0	2407	85	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2554	0	2373	63	0
4	G	702	0	665	15	0
4	I	709	0	673	4	0
5	A	14	0	13	0	0
5	D	14	0	13	0	0
6	A	5	0	0	0	0
All	All	12963	0	12065	282	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 11.

All (282) 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)
3:A:313:LEU:HD13	3:A:347:LEU:HG	1.54	0.88
3:A:151:LEU:HD12	3:A:184:SER:HB2	1.56	0.86
3:A:313:LEU:HD13	3:A:347:LEU:CG	2.10	0.80
3:D:1:LYS:N	3:D:92:GLU:OE2	2.17	0.77
3:A:54:ARG:NH1	3:A:78:ASP:OD2	2.17	0.75
2:C:38:ARG:HB2	2:C:48:ILE:HD11	1.72	0.72
1:B:101:ARG:HH21	2:C:107:ALA:HB1	1.56	0.71
2:C:156:PRO:HG2	2:C:211:PRO:HG2	1.72	0.71
1:B:140:LEU:HD22	2:C:190:VAL:HG21	1.71	0.71
3:A:205:GLU:HG2	3:A:253:LEU:HD21	1.73	0.71
3:A:309:THR:HB	3:A:313:LEU:HD21	1.73	0.70
3:D:160:THR:HG22	3:D:169:GLU:HG2	1.72	0.70
3:A:234:LYS:HB3	3:A:253:LEU:HD22	1.72	0.69
2:H:209:HIS:CD2	2:H:211:PRO:HD2	2.28	0.69
3:A:151:LEU:HD23	3:A:176:VAL:HG23	1.74	0.69
3:A:263:LEU:HB2	3:A:266:TYR:HD2	1.56	0.68
1:B:151:VAL:HG22	1:B:201:VAL:HG22	1.75	0.68
1:B:36:LYS:HD3	1:B:56:TRP:CD2	2.29	0.67
2:C:56:ASP:OD1	2:C:72:SER:OG	2.12	0.67
1:L:13:VAL:HG21	1:L:19:VAL:HG22	1.76	0.67
3:A:80:ASP:OD1	3:A:81:THR:N	2.26	0.66
3:A:227:ILE:HG22	3:A:241:VAL:HA	1.78	0.66
3:D:73:ASN:ND2	4:I:11:VAL:O	2.29	0.66
3:D:151:LEU:HD12	3:D:184:SER:HB2	1.76	0.65
3:A:5:LEU:HD22	3:A:96:LEU:HB2	1.79	0.65
3:A:101:THR:HG22	4:G:88:ILE:HG22	1.79	0.65
3:D:25:GLN:NE2	3:D:39:ASN:OD1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:171:GLN:HE21	1:L:176:SER:HB3	1.63	0.64
4:G:29:VAL:HG11	4:G:32:TYR:CE1	2.31	0.64
3:D:227:ILE:HG22	3:D:241:VAL:HA	1.79	0.64
2:H:60:TYR:HE1	2:H:70:LEU:HG	1.62	0.64
3:A:14:LEU:HD12	3:A:69:LEU:HD23	1.79	0.64
3:A:175:VAL:HG21	4:G:42:TYR:CD2	2.34	0.63
3:A:79:SER:HB2	3:A:96:LEU:HA	1.80	0.63
3:D:14:LEU:HD12	3:D:69:LEU:HD23	1.82	0.62
3:A:118:LEU:HD22	3:A:128:VAL:HG21	1.80	0.62
1:B:101:ARG:HD3	2:C:109:PHE:CE1	2.35	0.62
3:D:140:GLY:HA3	3:D:144:LEU:HD21	1.82	0.62
1:B:121:PHE:CE1	1:B:140:LEU:HD11	2.35	0.62
3:A:185:ILE:HG13	3:A:288:ASN:HB2	1.82	0.61
3:A:207:LEU:HD11	3:A:278:ALA:HB2	1.83	0.61
1:B:124:PRO:HG3	2:C:136:CYS:HB2	1.82	0.61
3:A:268:GLY:HA2	3:A:308:PRO:HD3	1.81	0.61
3:A:259:LEU:HD23	3:A:260:PRO:HD2	1.83	0.61
3:A:151:LEU:HA	3:A:176:VAL:HG21	1.83	0.60
3:D:74:LEU:HD22	3:D:97:VAL:HG21	1.81	0.60
1:L:203:HIS:CD2	1:L:205:GLY:H	2.19	0.60
2:H:117:LEU:HD23	2:H:158:PRO:HD3	1.82	0.60
3:A:81:THR:OG1	3:A:94:GLN:HG2	2.01	0.60
1:B:43:GLN:HB2	1:B:53:LEU:HD11	1.83	0.59
2:C:194:PRO:HG2	2:C:197:SER:HB3	1.83	0.59
3:D:21:LYS:HA	3:D:65:GLY:HA3	1.85	0.59
3:D:187:TYR:HB3	3:D:355:LEU:HG	1.84	0.59
2:H:61:ASP:OD1	2:H:62:GLU:N	2.36	0.59
3:A:263:LEU:HD12	3:A:266:TYR:HE2	1.67	0.58
3:A:162:LEU:HD12	3:A:167:LYS:HB3	1.84	0.58
2:C:98:ARG:NH1	2:C:99:GLU:O	2.36	0.58
2:C:143:SER:O	2:C:195:SER:N	2.32	0.58
2:H:32:TYR:CB	2:H:98:ARG:HD3	2.34	0.58
3:D:194:VAL:HB	3:D:259:LEU:HB2	1.86	0.58
3:A:205:GLU:OE1	4:G:45:TYR:OH	2.18	0.57
3:A:313:LEU:HD13	3:A:347:LEU:CD2	2.33	0.57
3:A:37:LEU:HD13	3:A:44:LEU:HD11	1.87	0.57
1:L:111:ILE:O	1:L:171:GLN:NE2	2.37	0.57
2:H:12:VAL:HG21	2:H:18:VAL:HB	1.86	0.57
2:C:172:VAL:HG22	2:C:191:VAL:HG23	1.86	0.57
3:A:138:ILE:HG22	3:A:144:LEU:HD22	1.86	0.57
1:B:111:ILE:O	1:B:171:GLN:NE2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:263:LEU:HD12	3:D:266:TYR:HE2	1.70	0.56
1:L:6:GLN:HE22	1:L:93:TYR:HA	1.71	0.56
3:A:26:PHE:CE2	3:A:67:PHE:HB3	2.40	0.56
3:D:162:LEU:HD13	3:D:167:LYS:HB3	1.88	0.56
1:L:17:GLU:O	1:L:84:VAL:HG23	2.06	0.56
2:C:48:ILE:HA	2:C:64:PHE:HD2	1.71	0.56
1:L:89:VAL:HG11	1:L:171:GLN:HB3	1.87	0.56
3:D:319:LEU:HD23	3:D:319:LEU:H	1.71	0.56
2:H:30:THR:HA	2:H:53:PRO:HB2	1.87	0.55
2:H:98:ARG:HD2	2:H:99:GLU:O	2.05	0.55
3:D:268:GLY:HA2	3:D:308:PRO:HD3	1.88	0.55
1:B:13:VAL:HG11	1:B:84:VAL:HG21	1.89	0.55
2:C:103:TYR:CE1	3:D:164:ASN:HB2	2.42	0.55
3:A:305:VAL:HG11	3:A:347:LEU:HD13	1.88	0.55
3:A:192:GLU:O	3:A:262:ALA:N	2.35	0.55
1:L:31:TYR:CE2	1:L:33:THR:HB	2.42	0.55
3:A:17:THR:HG22	3:A:66:ASN:HA	1.89	0.55
3:A:349:ASP:OD1	3:A:350:SER:N	2.38	0.54
1:B:138:VAL:HG22	1:B:183:THR:HG23	1.88	0.54
1:B:100:TYR:O	1:B:101:ARG:HG3	2.08	0.54
1:B:126:SER:HB3	2:C:132:PRO:O	2.06	0.54
4:G:10:VAL:HG22	4:G:20:ILE:HG22	1.90	0.54
2:H:86:LEU:HD13	2:H:120:VAL:HG22	1.90	0.54
1:B:11:LEU:HD23	1:B:19:VAL:HG13	1.90	0.54
1:B:121:PHE:CZ	1:B:140:LEU:HD11	2.43	0.54
3:A:341:GLY:O	3:A:361:VAL:HG22	2.08	0.53
2:H:38:ARG:HB2	2:H:48:ILE:HD11	1.89	0.53
2:C:155:PHE:HB3	2:C:156:PRO:HD3	1.91	0.53
1:B:120:VAL:HG22	1:B:141:LEU:HG	1.90	0.53
2:C:128:PRO:HB3	2:C:154:TYR:HB3	1.90	0.53
3:D:234:LYS:HA	3:D:253:LEU:HD13	1.89	0.53
4:G:34:ILE:HG13	4:G:72:VAL:HG22	1.90	0.53
1:B:38:TYR:CE2	3:D:122:PRO:HB2	2.43	0.53
3:D:305:VAL:HG21	3:D:347:LEU:HD12	1.91	0.52
3:A:335:VAL:HG21	3:A:343:TRP:HZ3	1.74	0.52
2:C:32:TYR:HB2	2:C:98:ARG:HD2	1.91	0.52
3:A:214:TRP:CD1	3:A:225:SER:HB2	2.44	0.52
2:C:48:ILE:HG12	2:C:64:PHE:CE2	2.45	0.52
3:D:231:LEU:HD13	3:D:236:VAL:HG22	1.92	0.52
3:A:313:LEU:HD22	3:A:347:LEU:HD21	1.92	0.52
3:A:12:VAL:HG22	3:A:74:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:172:ASP:OD1	1:L:173:SER:N	2.44	0.51
2:C:33:VAL:HG21	3:D:125:SER:OG	2.11	0.51
3:A:195:GLU:OE1	3:A:256:HIS:NE2	2.44	0.51
3:D:213:LEU:HD12	3:D:271:ASN:O	2.11	0.51
2:H:50:TYR:OH	3:A:126:PRO:O	2.27	0.51
3:A:154:SER:HB2	3:A:176:VAL:HG22	1.93	0.51
3:D:304:GLU:OE2	3:D:306:TRP:NE1	2.40	0.50
1:B:30:LEU:HD11	1:B:35:GLN:HA	1.94	0.50
1:L:192:GLU:OE1	1:L:216:ARG:NH2	2.44	0.50
1:B:146:PRO:HG3	1:B:204:GLN:HG2	1.94	0.50
3:D:187:TYR:HB3	3:D:355:LEU:CG	2.41	0.50
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.94	0.50
3:A:133:PRO:HD3	3:A:157:TRP:CD1	2.47	0.50
1:B:31:TYR:CD1	3:D:122:PRO:HG2	2.46	0.49
1:L:38:TYR:CE2	3:A:122:PRO:HB2	2.47	0.49
2:C:209:HIS:CD2	2:C:211:PRO:HD2	2.47	0.49
3:D:213:LEU:HD13	3:D:272:LEU:HB2	1.93	0.49
4:G:75:GLU:HB3	4:G:83:MET:SD	2.52	0.49
3:D:118:LEU:HD22	3:D:128:VAL:HG21	1.94	0.49
1:L:146:PRO:HD2	1:L:203:HIS:NE2	2.28	0.49
1:L:165:GLN:HB3	2:H:178:VAL:HG11	1.94	0.49
3:D:244:ASP:HB3	3:D:245:PRO:CD	2.43	0.49
2:C:55:ASN:HD22	3:D:162:LEU:HD23	1.77	0.49
2:C:61:ASP:OD1	2:C:62:GLU:N	2.46	0.49
1:B:101:ARG:HD3	2:C:109:PHE:HE1	1.75	0.48
3:A:151:LEU:CD1	3:A:184:SER:HB2	2.38	0.48
2:H:132:PRO:HD3	2:H:218:LYS:HE2	1.96	0.48
3:A:173:ASP:OD2	4:G:40:GLY:N	2.39	0.48
3:A:264:PRO:HG2	3:A:293:ARG:NH2	2.28	0.48
3:A:215:TRP:CE3	3:A:270:GLY:HA3	2.49	0.48
3:A:313:LEU:HD13	3:A:347:LEU:HD21	1.95	0.48
1:B:121:PHE:CE1	1:B:140:LEU:CD1	2.96	0.48
2:H:177:ALA:HB2	2:H:187:LEU:HD12	1.96	0.48
3:A:226:TRP:HE3	3:A:247:LEU:HD11	1.79	0.48
3:D:12:VAL:HG22	3:D:74:LEU:HD11	1.94	0.48
3:A:263:LEU:HD12	3:A:266:TYR:CE2	2.49	0.47
1:L:129:GLN:HE22	1:L:136:SER:HB2	1.79	0.47
3:A:319:LEU:HG	3:A:321:ASN:H	1.78	0.47
3:A:74:LEU:HD13	3:A:97:VAL:HG22	1.96	0.47
3:D:301:LEU:HB2	3:D:338:PRO:HG3	1.96	0.47
1:L:11:LEU:HG	1:L:13:VAL:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:TYR:HB3	2:H:98:ARG:HD3	1.96	0.47
1:B:12:ALA:HB1	1:B:112:LYS:CB	2.44	0.47
3:D:200:LEU:HD22	3:D:204:VAL:HG21	1.95	0.47
1:L:19:VAL:HB	1:L:81:ILE:HB	1.95	0.47
3:A:157:TRP:CE2	3:A:174:ILE:HD12	2.50	0.47
3:D:318:LYS:CB	3:D:324:ALA:HA	2.44	0.47
2:H:11:VAL:CG2	2:H:156:PRO:HG3	2.44	0.47
3:A:214:TRP:HA	3:A:225:SER:HA	1.96	0.47
1:B:153:TRP:CE2	1:B:184:LEU:HD13	2.50	0.47
2:C:174:THR:HG22	2:C:189:SER:OG	2.15	0.46
1:L:4:MET:HB2	1:L:103:PHE:O	2.15	0.46
3:D:51:LEU:HG	3:D:55:ALA:HB2	1.98	0.46
1:L:22:ASN:OD1	1:L:23:CYS:N	2.49	0.46
1:L:113:ARG:HG2	1:L:114:THR:N	2.30	0.46
1:L:115:VAL:HG13	1:L:146:PRO:HG2	1.98	0.46
3:D:28:TRP:CH2	3:D:84:CYS:HB2	2.50	0.46
1:L:13:VAL:HG11	1:L:84:VAL:HG21	1.96	0.46
3:A:227:ILE:HG23	3:A:247:LEU:HD12	1.96	0.46
2:C:205:CYS:O	2:C:217:ASP:HA	2.16	0.46
3:D:274:LEU:O	3:D:283:LEU:HB2	2.15	0.46
1:L:56:TRP:O	1:L:57:ALA:HB3	2.16	0.46
2:C:52:ASN:C	2:C:52:ASN:HD22	2.19	0.46
1:L:43:GLN:HB2	1:L:53:LEU:HD11	1.98	0.46
4:G:5:PRO:HG3	4:G:74:ALA:HB2	1.98	0.46
3:A:313:LEU:HD11	3:A:347:LEU:HD11	1.97	0.45
3:D:73:ASN:ND2	4:I:10:VAL:O	2.48	0.45
3:D:226:TRP:HA	3:D:242:THR:CG2	2.46	0.45
2:C:133:LEU:HD11	2:C:150:LEU:HB2	1.97	0.45
3:A:186:VAL:O	3:A:289:LEU:HD12	2.15	0.45
1:B:125:PRO:HG3	1:B:191:TYR:CZ	2.51	0.45
1:L:13:VAL:O	1:L:111:ILE:HA	2.17	0.45
3:D:218:GLU:N	3:D:218:GLU:OE1	2.50	0.45
3:D:226:TRP:HA	3:D:242:THR:HG23	1.98	0.45
1:L:3:VAL:H	1:L:26:SER:HB3	1.81	0.45
2:C:40:LYS:HE3	2:C:89:GLU:O	2.17	0.45
3:A:157:TRP:CD1	3:A:174:ILE:HD12	2.52	0.45
1:B:200:GLU:HA	1:B:210:VAL:O	2.17	0.45
3:D:263:LEU:HB2	3:D:266:TYR:CD2	2.52	0.45
3:A:226:TRP:CE3	3:A:247:LEU:HD11	2.52	0.45
3:A:295:THR:HA	3:A:359:ILE:HD12	1.98	0.45
3:A:98:PHE:CD2	3:A:161:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:335:VAL:HG21	3:D:343:TRP:CZ3	2.52	0.45
1:L:39:LEU:HD13	1:L:77:PHE:CD2	2.52	0.44
3:D:244:ASP:HB3	3:D:245:PRO:HD3	1.98	0.44
4:G:62:LEU:HD22	4:G:68:TYR:CZ	2.53	0.44
1:L:146:PRO:O	1:L:203:HIS:HE1	2.01	0.44
4:G:39:LEU:HD13	4:G:69:GLN:NE2	2.31	0.44
1:L:146:PRO:HB2	1:L:203:HIS:CE1	2.53	0.44
3:A:317:LEU:HB2	3:A:326:VAL:HG12	2.00	0.44
1:B:198:ALA:HA	1:B:212:LYS:O	2.18	0.44
3:A:335:VAL:HG11	3:A:343:TRP:CH2	2.52	0.44
1:B:72:GLY:HA3	1:B:77:PHE:HA	2.00	0.44
3:D:179:PHE:HD2	3:D:200:LEU:HD21	1.83	0.44
4:G:71:ARG:NH2	4:G:87:GLN:OE1	2.41	0.44
3:A:295:THR:HA	3:A:359:ILE:CD1	2.48	0.43
1:B:101:ARG:NH2	2:C:107:ALA:HB1	2.30	0.43
3:A:238:VAL:HG11	3:A:241:VAL:HG23	2.00	0.43
3:D:301:LEU:O	3:D:335:VAL:N	2.35	0.43
1:L:171:GLN:NE2	1:L:176:SER:HB3	2.32	0.43
2:H:157:GLU:HG3	2:H:185:TYR:CE2	2.53	0.43
2:H:193:VAL:HG11	2:H:203:TYR:CE1	2.53	0.43
3:D:309:THR:HB	3:D:313:LEU:HD21	1.99	0.43
3:D:313:LEU:HD22	3:D:347:LEU:HD21	2.00	0.43
1:B:6:GLN:NE2	1:B:94:CYS:SG	2.91	0.43
1:B:61:GLU:OE1	1:B:61:GLU:HA	2.17	0.43
1:L:31:TYR:CD1	3:A:122:PRO:HG2	2.54	0.43
1:L:67:ARG:HB2	1:L:82:SER:HB3	2.01	0.43
3:A:132:SER:HB2	3:A:133:PRO:HD2	2.00	0.43
3:A:266:TYR:O	3:A:289:LEU:HD23	2.18	0.43
3:D:205:GLU:HB3	3:D:253:LEU:HD21	2.00	0.43
3:A:315:LEU:HA	3:A:346:LEU:O	2.18	0.43
3:A:9:GLY:N	3:A:74:LEU:O	2.46	0.43
3:D:247:LEU:HD22	3:D:257:LEU:HD21	2.01	0.43
1:L:86:ALA:HA	1:L:111:ILE:HD13	2.01	0.42
3:A:244:ASP:HB3	3:A:245:PRO:CD	2.48	0.42
3:D:295:THR:HA	3:D:359:ILE:HD12	2.01	0.42
2:H:9:PRO:HG2	2:H:211:PRO:HD3	2.02	0.42
2:H:38:ARG:HG3	2:H:94:TYR:CE2	2.54	0.42
2:C:152:LYS:HA	2:C:186:SER:HA	2.00	0.42
2:H:12:VAL:HG11	2:H:86:LEU:HD12	2.01	0.42
2:H:93:VAL:HG22	2:H:117:LEU:HD13	2.02	0.42
3:A:335:VAL:HG11	3:A:343:TRP:CZ3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:204:THR:HG22	2:C:219:ARG:HA	2.01	0.42
3:A:128:VAL:HG22	3:A:161:VAL:HG22	2.01	0.42
2:H:132:PRO:HB3	2:H:220:VAL:HG22	2.02	0.42
1:B:96:GLN:NE2	1:B:99:SER:O	2.50	0.42
2:C:55:ASN:ND2	3:D:162:LEU:HD23	2.35	0.42
3:D:66:ASN:C	3:D:68:PRO:HD3	2.40	0.42
3:D:248:GLN:HB3	3:D:258:THR:OG1	2.19	0.42
4:I:3:ASP:OD1	4:I:3:ASP:N	2.53	0.42
3:A:137:ASN:O	3:A:138:ILE:HD13	2.20	0.42
3:A:207:LEU:HD12	3:A:208:THR:H	1.84	0.42
2:C:18:VAL:HG12	2:C:83:LEU:HB2	2.02	0.41
3:D:133:PRO:HG3	3:D:155:GLY:HA3	2.01	0.41
3:A:56:ASP:OD1	3:A:57:SER:N	2.52	0.41
2:C:48:ILE:HG12	2:C:64:PHE:CD2	2.55	0.41
1:L:145:TYR:HB3	1:L:146:PRO:HD3	2.02	0.41
3:A:51:LEU:HG	3:A:55:ALA:HB2	2.01	0.41
3:A:313:LEU:CD2	3:A:347:LEU:HD21	2.50	0.41
1:L:26:SER:OG	1:L:27:GLN:N	2.53	0.41
3:D:229:PHE:CD2	3:D:249:MET:HE1	2.56	0.41
1:B:38:TYR:N	1:B:38:TYR:CD1	2.89	0.41
2:C:103:TYR:CD2	3:D:3:VAL:HG21	2.55	0.41
4:G:18:LEU:HG	4:G:62:LEU:CD1	2.51	0.41
1:L:43:GLN:HG3	1:L:92:TYR:CE2	2.56	0.41
1:B:17:GLU:O	1:B:84:VAL:HG23	2.21	0.41
2:C:109:PHE:N	2:C:109:PHE:CD1	2.88	0.41
2:H:187:LEU:HD23	2:H:188:SER:N	2.36	0.41
3:D:132:SER:OG	3:D:136:LYS:N	2.52	0.41
3:D:318:LYS:O	3:D:344:GLN:HB3	2.21	0.41
2:H:83:LEU:HD11	2:H:94:TYR:CE2	2.56	0.41
3:A:5:LEU:HA	3:A:96:LEU:O	2.21	0.41
3:A:38:GLY:O	3:A:44:LEU:HD12	2.21	0.41
3:A:44:LEU:HD13	3:A:62:TRP:CH2	2.56	0.41
3:D:214:TRP:CD1	3:D:225:SER:HB2	2.55	0.41
4:I:15:PRO:HA	4:I:92:THR:HB	2.02	0.41
1:L:180:LEU:HD23	1:L:181:SER:N	2.36	0.41
1:B:172:ASP:OD1	1:B:173:SER:N	2.54	0.41
3:A:9:GLY:O	3:A:73:ASN:HA	2.21	0.40
3:A:151:LEU:HD23	3:A:176:VAL:CG2	2.48	0.40
2:C:147:LEU:HD13	2:C:220:VAL:HG23	2.01	0.40
4:G:67:GLU:HG2	4:G:91:ARG:NH2	2.36	0.40
1:L:165:GLN:HE22	2:H:180:GLN:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:175:PHE:N	2:C:175:PHE:CD1	2.90	0.40
3:D:266:TYR:O	3:D:289:LEU:HD23	2.21	0.40
4:G:27:VAL:HG21	4:G:76:THR:HG21	2.03	0.40
2:H:109:PHE:N	2:H:109:PHE:CD1	2.88	0.40
3:A:234:LYS:HD2	3:A:253:LEU:HD22	2.02	0.40
1:B:6:GLN:HE21	1:B:104:GLY:HA3	1.86	0.40
1:B:86:ALA:HA	1:B:111:ILE:CD1	2.52	0.40
3:D:301:LEU:HB3	3:D:335:VAL:HB	2.03	0.40
3:D:310:SER:O	3:D:313:LEU:HG	2.22	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	213/219 (97%)	203 (95%)	10 (5%)	0	100	100
1	L	214/219 (98%)	205 (96%)	9 (4%)	0	100	100
2	C	220/229 (96%)	214 (97%)	5 (2%)	1 (0%)	29	66
2	H	219/229 (96%)	214 (98%)	5 (2%)	0	100	100
3	A	351/373 (94%)	336 (96%)	15 (4%)	0	100	100
3	D	353/373 (95%)	338 (96%)	15 (4%)	0	100	100
4	G	89/94 (95%)	85 (96%)	4 (4%)	0	100	100
4	I	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
All	All	1751/1830 (96%)	1683 (96%)	67 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	140	THR

### 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	153/194 (79%)	152 (99%)	1 (1%)	84	91
1	L	187/194 (96%)	186 (100%)	1 (0%)	88	94
2	C	159/196 (81%)	158 (99%)	1 (1%)	86	93
2	H	186/196 (95%)	186 (100%)	0	100	100
3	A	263/333 (79%)	262 (100%)	1 (0%)	91	95
3	D	262/333 (79%)	261 (100%)	1 (0%)	91	95
4	G	72/78 (92%)	72 (100%)	0	100	100
4	I	72/78 (92%)	72 (100%)	0	100	100
All	All	1354/1602 (84%)	1349 (100%)	5 (0%)	91	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	97	TYR
3	A	202	PHE
1	B	95	GLN
2	C	52	ASN
3	D	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	203	HIS
1	B	6	GLN
2	C	52	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](#)

There are no monosaccharides 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
6	SO4	A	402	-	4,4,4	0.15	0	6,6,6	0.05	0
5	NAG	A	401	3	14,14,15	0.29	0	17,19,21	0.50	0
5	NAG	D	401	3	14,14,15	0.30	0	17,19,21	0.58	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	401	3	-	4/6/23/26	0/1/1/1
5	NAG	D	401	3	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	401	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	401	NAG	C8-C7-N2-C2
5	A	401	NAG	O7-C7-N2-C2
5	A	401	NAG	O5-C5-C6-O6
5	D	401	NAG	C4-C5-C6-O6
5	A	401	NAG	C4-C5-C6-O6

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	215/219 (98%)	-0.07	4 (1%) 66 53	42, 84, 120, 136	0
1	L	216/219 (98%)	-0.40	0 100 100	27, 51, 72, 88	0
2	C	222/229 (96%)	0.04	5 (2%) 60 46	45, 74, 128, 145	0
2	H	221/229 (96%)	-0.47	0 100 100	29, 44, 77, 100	0
3	A	355/373 (95%)	-0.22	1 (0%) 94 90	35, 70, 111, 128	0
3	D	357/373 (95%)	-0.05	12 (3%) 45 33	36, 71, 140, 194	0
4	G	93/94 (98%)	-0.43	2 (2%) 62 48	34, 53, 100, 119	0
4	I	94/94 (100%)	-0.18	5 (5%) 26 18	45, 62, 102, 144	0
All	All	1773/1830 (96%)	-0.20	29 (1%) 72 59	27, 64, 121, 194	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	42	SER	12.3
3	D	43	PHE	8.2
4	I	0	GLY	4.7
3	A	321	ASN	4.6
3	D	46	LYS	4.2
1	B	205	GLY	4.0
3	D	41	GLY	3.9
2	C	158	PRO	3.3
3	D	45	THR	3.2
3	D	47	GLY	3.2
4	G	0	GLY	3.0
1	B	204	GLN	3.0
4	I	79	ALA	3.0
4	I	80	ASP	2.9
3	D	44	LEU	2.9
3	D	88	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	208	ASP	2.7
1	B	197	TYR	2.5
1	B	157	ASN	2.5
3	D	19	SER	2.4
3	D	48	PRO	2.4
2	C	212	SER	2.4
4	I	81	GLN	2.4
3	D	23	SER	2.3
2	C	213	ASN	2.3
4	G	81	GLN	2.3
3	D	18	ALA	2.2
4	I	1	VAL	2.1
2	C	24	ALA	2.1

## 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 monosaccharides 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	401	14/15	0.80	0.30	86,111,127,130	0
5	NAG	D	401	14/15	0.85	0.30	78,86,95,98	0
6	SO4	A	402	5/5	0.95	0.31	96,102,105,110	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.