



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 10:31 AM EDT

PDB ID : 2OL3  
Title : crystal structure of BM3.3 ScFV TCR in complex with PBM8-H-2KBM8 MHC class I molecule  
Authors : Mazza, C.; Auphan-Anezin, N.; Gregoire, C.; Guimezanes, A.; Kellenberger, C.; Roussel, A.; Kearney, A.; Van der Merwe, P.A.; Schmitt-Verhulst, A.M.; Malissen, B.  
Deposited on : 2007-01-18  
Resolution : 2.90 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  
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

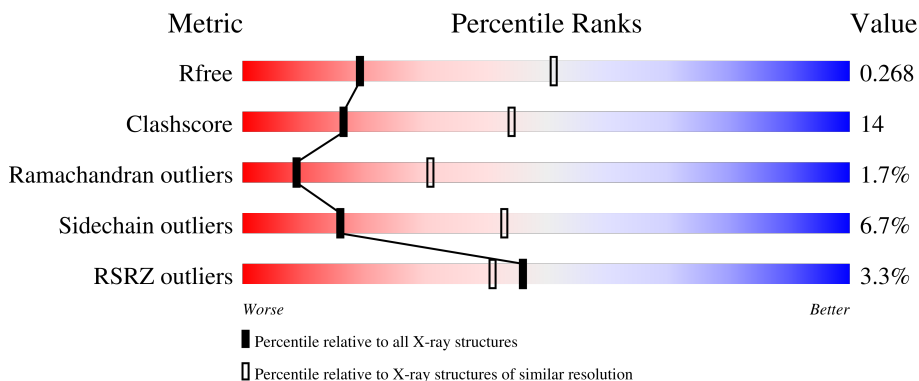
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	A	142	 6% 53% 26% 17%
2	B	113	 67% 29%
3	H	279	 3% 70% 27%
4	L	100	 5% 64% 30% 5%

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Mol	Chain	Length	Quality of chain
5	P	8	 62% 38%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5073 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 BM3.3 T-CELL RECEPTOR ALPHA-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	118	918	584	147	182	5	0	0	0

- Molecule 2 is a protein called BM3.3 T-CELL RECEPTOR BETA-CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	113	918	580	166	167	5	0	0	0

- Molecule 3 is a protein called ALLOGENEIC H-2KBM8 MHC CLASS I MOLECULE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	276	2243	1417	396	422	8	0	0	0

- Molecule 4 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	L	100	829	529	139	153	8	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	0	MET	-	initiating methionine	UNP P01887

- Molecule 5 is a protein called NATURALLY PROCESSED OCTAPEPTIDE PBM8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	P	8	74	48	10	16	0	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

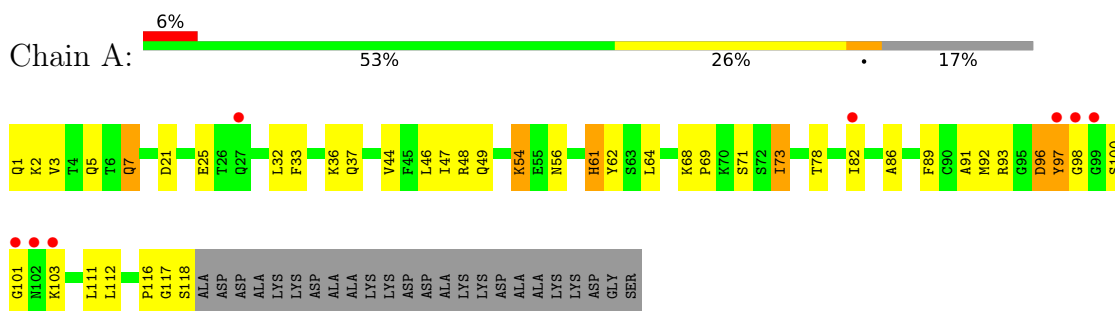
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	20	Total	O	0	0
			20	20		
7	H	35	Total	O	0	0
			35	35		
7	L	11	Total	O	0	0
			11	11		

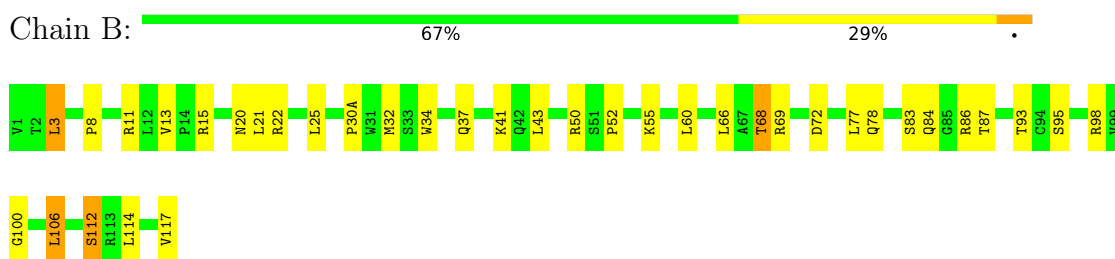
### 3 Residue-property plots

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.

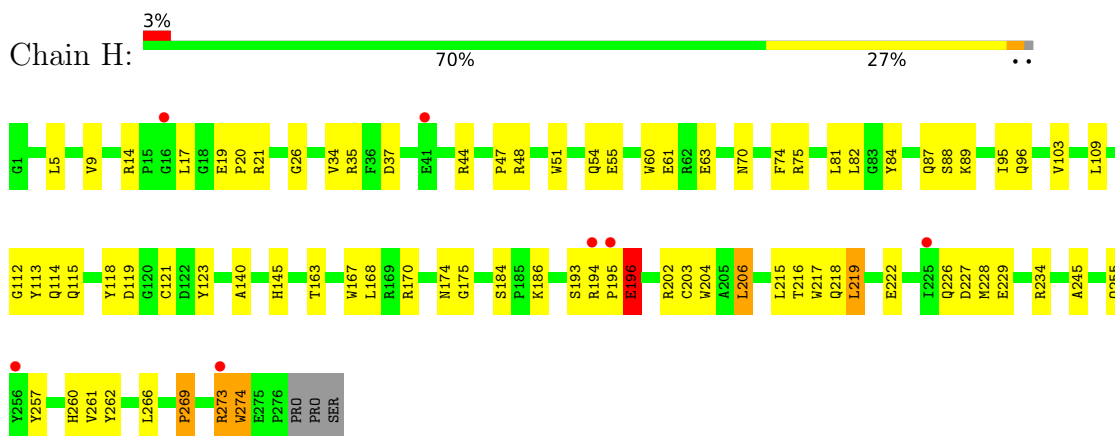
- Molecule 1: BM3.3 T-CELL RECEPTOR ALPHA-CHAIN



- Molecule 2: BM3.3 T-CELL RECEPTOR BETA-CHAIN

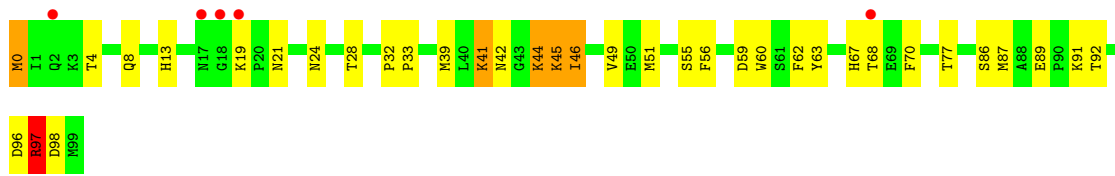


- Molecule 3: ALLOGENEIC H-2KBM8 MHC CLASS I MOLECULE



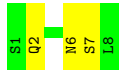
- Molecule 4: Beta-2-microglobulin





- Molecule 5: NATURALLY PROCESSED OCTAPEPTIDE PBM8

Chain P: 62% 38%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.52Å 102.52Å 198.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.90 24.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.00-2.90) 98.1 (24.87-2.90)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.89Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.224 , 0.284 0.214 , 0.268	Depositor DCC
$R_{free}$ test set	1214 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.7	Xtrriage
Anisotropy	0.006	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: 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	A	0.57	0/935	0.69	1/1262 (0.1%)
2	B	0.57	0/937	0.68	0/1271
3	H	0.54	0/2305	0.63	0/3132
4	L	0.50	0/855	0.56	0/1158
5	P	0.76	0/76	0.70	0/101
All	All	0.55	0/5108	0.64	1/6924 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	N-CA-C	-8.91	86.93	111.00

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	A	918	0	908	35	0
2	B	918	0	923	29	0
3	H	2243	0	2141	52	0
4	L	829	0	805	30	0
5	P	74	0	64	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	14	0	13	5	0
7	A	11	0	0	2	0
7	B	20	0	0	3	0
7	H	35	0	0	1	0
7	L	11	0	0	0	0
All	All	5073	0	4854	140	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 14.

All (140) 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:A:56:ASN:HD21	6:A:201:NAG:C1	1.62	1.12
1:A:56:ASN:ND2	6:A:201:NAG:C1	2.27	0.97
3:H:195:PRO:O	3:H:196:GLU:HB2	1.79	0.80
1:A:98:GLY:HA3	7:A:212:HOH:O	1.88	0.74
3:H:219:LEU:O	3:H:222:GLU:HG2	1.88	0.72
3:H:273:ARG:O	3:H:274:TRP:HB3	1.90	0.71
1:A:100:SER:HA	1:A:103:LYS:HB3	1.72	0.70
2:B:25:LEU:HB2	2:B:32:MET:CE	2.22	0.69
4:L:41:LYS:HB3	4:L:44:LYS:HB2	1.73	0.69
3:H:20:PRO:HD2	3:H:75:ARG:HD2	1.75	0.69
4:L:13:HIS:HB2	4:L:21:ASN:HD21	1.58	0.69
3:H:47:PRO:HB3	3:H:60:TRP:CH2	2.27	0.68
2:B:87:THR:HG21	7:B:132:HOH:O	1.94	0.68
2:B:25:LEU:HB2	2:B:32:MET:HE1	1.77	0.66
4:L:4:THR:HG22	4:L:86:SER:HB2	1.77	0.66
1:A:54:LYS:H	1:A:54:LYS:NZ	1.95	0.65
2:B:21:LEU:HD12	2:B:77:LEU:HD23	1.79	0.65
4:L:49:VAL:HG12	4:L:68:THR:HB	1.78	0.64
1:A:54:LYS:H	1:A:54:LYS:HZ2	1.43	0.64
1:A:47:ILE:HD13	1:A:64:LEU:HG	1.78	0.64
1:A:93:ARG:HD2	1:A:101:GLY:O	1.98	0.64
4:L:87:MET:HE1	4:L:91:LYS:HB2	1.81	0.63
1:A:56:ASN:HD21	6:A:201:NAG:C2	2.12	0.63
3:H:87:GLN:HE22	3:H:118:TYR:HE2	1.47	0.62
2:B:106:LEU:HD12	2:B:106:LEU:O	1.99	0.62
1:A:96:ASP:HB3	1:A:100:SER:HB3	1.82	0.61
1:A:56:ASN:HB3	1:A:64:LEU:O	2.01	0.61
2:B:20:ASN:OD1	2:B:78:GLN:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:35:ARG:HB3	3:H:48:ARG:HD3	1.83	0.60
1:A:93:ARG:HH22	1:A:97:TYR:HE2	1.50	0.60
3:H:54:GLN:OE1	3:H:174:ASN:HB3	2.02	0.60
4:L:42:ASN:HA	4:L:77:THR:HB	1.82	0.60
3:H:81:LEU:HD23	3:H:84:TYR:HD1	1.67	0.59
1:A:61:HIS:CD2	1:A:61:HIS:H	2.21	0.59
1:A:117:GLY:O	1:A:118:SER:HB2	2.03	0.59
1:A:36:LYS:HE2	1:A:46:LEU:HD11	1.84	0.58
1:A:54:LYS:O	6:A:201:NAG:H81	2.05	0.57
4:L:41:LYS:HD3	4:L:44:LYS:HE3	1.88	0.55
2:B:32:MET:HA	2:B:93:THR:O	2.06	0.55
1:A:78:THR:HA	7:A:203:HOH:O	2.06	0.55
3:H:9:VAL:O	3:H:96:GLN:HA	2.06	0.55
3:H:63:GLU:OE1	5:P:2:GLN:HG3	2.07	0.55
3:H:234:ARG:CD	4:L:8:GLN:HE21	2.20	0.54
2:B:34:TRP:CE2	2:B:77:LEU:HB2	2.42	0.54
3:H:194:ARG:HH11	3:H:194:ARG:HG3	1.72	0.54
4:L:24:ASN:HD22	4:L:67:HIS:HB3	1.71	0.54
2:B:95:SER:OG	2:B:100:GLY:HA2	2.08	0.53
1:A:61:HIS:H	1:A:61:HIS:HD2	1.56	0.53
3:H:55:GLU:OE1	3:H:170:ARG:NH2	2.41	0.53
1:A:37:GLN:O	1:A:86:ALA:HB1	2.08	0.53
1:A:111:LEU:HD12	1:A:112:LEU:N	2.24	0.53
4:L:39:MET:SD	4:L:68:THR:HG22	2.49	0.53
2:B:3:LEU:HD22	2:B:3:LEU:H	1.74	0.53
1:A:44:VAL:O	1:A:46:LEU:HD13	2.10	0.52
3:H:145:HIS:HB3	7:H:289:HOH:O	2.10	0.52
1:A:56:ASN:OD1	6:A:201:NAG:H82	2.10	0.52
2:B:52:PRO:HA	2:B:69:ARG:O	2.10	0.52
1:A:2:LYS:H	1:A:25:GLU:HB2	1.76	0.51
3:H:26:GLY:HA3	3:H:34:VAL:HG23	1.92	0.51
3:H:121:CYS:SG	4:L:0:MET:N	2.84	0.51
2:B:3:LEU:HD22	2:B:3:LEU:N	2.26	0.50
2:B:11:ARG:NH2	7:B:124:HOH:O	2.44	0.50
4:L:28:THR:HG22	4:L:63:TYR:HB2	1.93	0.50
4:L:45:LYS:O	4:L:46:ILE:C	2.50	0.50
4:L:89:GLU:O	4:L:91:LYS:HD2	2.12	0.50
3:H:229:GLU:O	3:H:245:ALA:HA	2.12	0.50
3:H:215:LEU:CD2	3:H:261:VAL:HG22	2.41	0.50
4:L:41:LYS:HD3	4:L:44:LYS:CE	2.41	0.49
5:P:6:ASN:CG	5:P:7:SER:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:118:TYR:O	3:H:119:ASP:HB2	2.12	0.49
1:A:32:LEU:HD13	1:A:73:ILE:HG21	1.95	0.48
3:H:184:SER:HB3	3:H:266:LEU:HD23	1.94	0.48
2:B:21:LEU:HD22	2:B:112:SER:CB	2.44	0.48
3:H:123:TYR:CZ	3:H:140:ALA:HA	2.49	0.48
3:H:204:TRP:HB3	3:H:206:LEU:HD21	1.96	0.48
3:H:218:GLN:O	3:H:257:TYR:HA	2.13	0.48
2:B:30(A):PRO:HB2	2:B:50:ARG:CZ	2.44	0.47
2:B:32:MET:HG3	2:B:69:ARG:NH1	2.28	0.47
3:H:202:ARG:HG2	3:H:204:TRP:NE1	2.29	0.47
3:H:219:LEU:HG	3:H:257:TYR:CZ	2.50	0.47
1:A:68:LYS:N	1:A:69:PRO:HD2	2.29	0.47
3:H:215:LEU:HD22	3:H:261:VAL:HG22	1.96	0.47
3:H:234:ARG:HD3	4:L:8:GLN:HE21	1.80	0.47
4:L:87:MET:CE	4:L:91:LYS:HB2	2.44	0.47
3:H:81:LEU:HD12	3:H:95:ILE:HD11	1.98	0.46
3:H:82:LEU:HD21	3:H:89:LYS:HA	1.97	0.46
3:H:89:LYS:H	3:H:89:LYS:HE2	1.79	0.46
3:H:5:LEU:HB2	3:H:168:LEU:HD13	1.98	0.46
2:B:66:LEU:C	2:B:66:LEU:HD23	2.36	0.46
3:H:186:LYS:N	3:H:186:LYS:HD2	2.30	0.46
4:L:32:PRO:HB2	4:L:33:PRO:HD2	1.97	0.46
4:L:24:ASN:ND2	4:L:67:HIS:HB3	2.31	0.45
1:A:32:LEU:HD23	1:A:92:MET:HG3	1.98	0.45
2:B:55:LYS:HE2	2:B:68:THR:HG21	1.98	0.45
2:B:21:LEU:HD21	2:B:114:LEU:HD21	1.99	0.45
3:H:21:ARG:NH2	3:H:37:ASP:OD1	2.43	0.45
3:H:204:TRP:HZ2	4:L:98:ASP:O	2.00	0.45
4:L:41:LYS:HB3	4:L:44:LYS:HE3	1.99	0.45
1:A:82:ILE:HD11	1:A:116:PRO:HB3	1.98	0.45
2:B:25:LEU:HB2	2:B:32:MET:HE3	1.97	0.44
3:H:234:ARG:HD2	4:L:8:GLN:HE21	1.82	0.44
1:A:5:GLN:HE22	1:A:89:PHE:HA	1.83	0.44
1:A:54:LYS:NZ	1:A:54:LYS:N	2.63	0.44
1:A:1:GLN:HA	1:A:25:GLU:O	2.18	0.44
1:A:46:LEU:HG	1:A:62:TYR:CE1	2.52	0.44
2:B:52:PRO:HG2	2:B:72:ASP:OD1	2.17	0.44
3:H:203:CYS:HB2	3:H:217:TRP:CZ2	2.53	0.44
1:A:48:ARG:HG2	1:A:49:GLN:N	2.32	0.44
2:B:8:PRO:HD2	2:B:21:LEU:HD23	2.00	0.44
3:H:51:TRP:CD2	3:H:175:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD13	1:A:73:ILE:HD11	1.99	0.43
3:H:216:THR:HG23	3:H:260:HIS:HB2	2.00	0.43
4:L:97:ARG:HD2	4:L:97:ARG:H	1.82	0.43
3:H:26:GLY:HA3	3:H:34:VAL:CG2	2.48	0.43
3:H:87:GLN:NE2	3:H:118:TYR:HE2	2.13	0.43
4:L:59:ASP:O	4:L:60:TRP:HB2	2.18	0.43
4:L:56:PHE:HB3	4:L:62:PHE:CD2	2.53	0.43
2:B:84:GLN:HB2	7:B:122:HOH:O	2.18	0.43
2:B:11:ARG:HB3	2:B:114:LEU:HD22	2.01	0.43
4:L:96:ASP:O	4:L:98:ASP:N	2.52	0.42
1:A:33:PHE:N	1:A:91:ALA:O	2.51	0.42
2:B:13:VAL:C	2:B:117:VAL:HG12	2.40	0.42
3:H:70:ASN:O	3:H:74:PHE:HD2	2.03	0.42
3:H:112:GLY:O	3:H:113:TYR:HB3	2.20	0.42
3:H:234:ARG:HD3	4:L:8:GLN:NE2	2.33	0.41
3:H:273:ARG:O	3:H:274:TRP:CB	2.65	0.41
3:H:51:TRP:HB2	3:H:174:ASN:O	2.21	0.41
3:H:121:CYS:HG	4:L:0:MET:CE	2.32	0.41
2:B:37:GLN:HB2	2:B:43:LEU:HD13	2.02	0.41
2:B:60:LEU:HD23	2:B:60:LEU:N	2.35	0.41
3:H:115:GLN:HE21	3:H:115:GLN:HB3	1.61	0.41
4:L:24:ASN:HD22	4:L:67:HIS:CB	2.33	0.41
3:H:163:THR:O	3:H:167:TRP:HD1	2.04	0.41
3:H:44:ARG:NH1	3:H:61:GLU:OE2	2.54	0.40
3:H:262:TYR:CD1	3:H:269:PRO:HB3	2.57	0.40
2:B:15:ARG:HG3	2:B:83:SER:HA	2.03	0.40
2:B:25:LEU:HD13	2:B:32:MET:HE3	2.02	0.40
1:A:7:GLN:H	1:A:7:GLN:HE21	1.69	0.40
3:H:19:GLU:HA	3:H:19:GLU:OE2	2.22	0.40
4:L:46:ILE:H	4:L:46:ILE:HG13	1.77	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	A	116/142 (82%)	101 (87%)	13 (11%)	2 (2%)	9	31
2	B	111/113 (98%)	103 (93%)	8 (7%)	0	100	100
3	H	274/279 (98%)	252 (92%)	18 (7%)	4 (2%)	10	34
4	L	98/100 (98%)	84 (86%)	10 (10%)	4 (4%)	3	11
5	P	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
All	All	605/642 (94%)	545 (90%)	50 (8%)	10 (2%)	9	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	196	GLU
3	H	227	ASP
4	L	44	LYS
3	H	193	SER
4	L	97	ARG
1	A	71	SER
1	A	73	ILE
4	L	41	LYS
3	H	269	PRO
4	L	46	ILE

### 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	A	103/119 (87%)	97 (94%)	6 (6%)	20	50
2	B	101/101 (100%)	93 (92%)	8 (8%)	12	34
3	H	234/237 (99%)	220 (94%)	14 (6%)	19	49
4	L	95/95 (100%)	87 (92%)	8 (8%)	11	31
5	P	8/8 (100%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	541/560 (97%)	505 (93%)	36 (7%)	16 43

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	7	GLN
1	A	21	ASP
1	A	54	LYS
1	A	61	HIS
1	A	97	TYR
2	B	3	LEU
2	B	22	ARG
2	B	41	LYS
2	B	68	THR
2	B	86	ARG
2	B	98	ARG
2	B	106	LEU
2	B	112	SER
3	H	14	ARG
3	H	17	LEU
3	H	88	SER
3	H	103	VAL
3	H	109	LEU
3	H	114	GLN
3	H	196	GLU
3	H	206	LEU
3	H	219	LEU
3	H	226	GLN
3	H	228	MET
3	H	255	GLN
3	H	273	ARG
3	H	274	TRP
4	L	0	MET
4	L	19	LYS
4	L	45	LYS
4	L	51	MET
4	L	55	SER
4	L	70	PHE
4	L	92	THR
4	L	97	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	37	GLN
1	A	56	ASN
1	A	65	ASN
2	B	17	GLN
2	B	29	GLN
2	B	37	GLN
2	B	42	GLN
2	B	44	GLN
3	H	115	GLN
3	H	127	ASN
3	H	174	ASN
3	H	192	HIS
3	H	218	GLN
3	H	255	GLN
3	H	260	HIS
4	L	8	GLN
4	L	24	ASN
4	L	38	GLN
5	P	2	GLN

### 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](#)

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	NAG	A	201	-	14,14,15	0.55	0	17,19,21	0.94	1 (5%)

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	NAG	A	201	-	-	4/6/23/26	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(°)
6	A	201	NAG	C4-C3-C2	-2.35	107.57	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	201	NAG	O7-C7-N2-C2
6	A	201	NAG	C8-C7-N2-C2
6	A	201	NAG	C4-C5-C6-O6
6	A	201	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	201	NAG	5	0

## 5.7 Other polymers [i](#)

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	A	118/142 (83%)	0.13	8 (6%) 17 13	2, 27, 48, 54	0
2	B	113/113 (100%)	-0.30	0 100 100	2, 8, 24, 30	0
3	H	276/279 (98%)	-0.28	7 (2%) 57 55	2, 18, 50, 56	0
4	L	100/100 (100%)	0.08	5 (5%) 28 25	8, 45, 53, 55	0
5	P	8/8 (100%)	-1.05	0 100 100	4, 11, 22, 29	0
All	All	615/642 (95%)	-0.16	20 (3%) 46 41	2, 20, 51, 56	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	GLY	4.9
1	A	102	ASN	4.3
1	A	101	GLY	4.3
3	H	195	PRO	3.8
3	H	225	ILE	3.4
1	A	99	GLY	3.4
3	H	16	GLY	3.3
4	L	18	GLY	3.1
1	A	97	TYR	3.1
4	L	19	LYS	3.0
3	H	41	GLU	2.9
1	A	82	ILE	2.7
1	A	103	LYS	2.6
4	L	2	GLN	2.6
3	H	273	ARG	2.4
1	A	27	GLN	2.4
3	H	256	TYR	2.2
4	L	68	THR	2.2
4	L	17	ASN	2.1
3	H	194	ARG	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 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
6	NAG	A	201	14/15	0.84	0.24	51,56,60,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.