



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 AM GMT

PDB ID : 3QIB  
Title : Crystal structure of the 2B4 TCR in complex with MCC/I-Ek  
Authors : Ely, L.K.; Newell, E.W.; Davis, M.M.; Garcia, K.C.  
Deposited on : 2011-01-26  
Resolution : 2.70 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

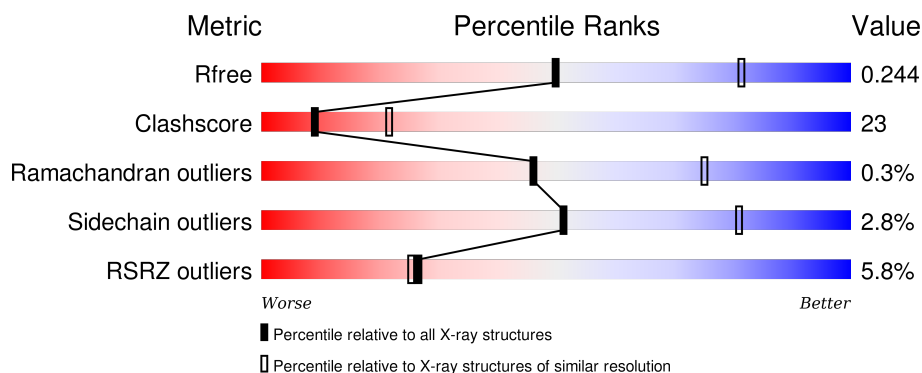
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	A	193	<div> <div>8%</div> <div>56%</div> <div>35%</div> <div>7%</div> </div>
2	B	202	<div> <div>10%</div> <div>48%</div> <div>32%</div> <div>18%</div> </div>
3	C	207	<div> <div>4%</div> <div>72%</div> <div>19%</div> <div>6%</div> </div>
4	D	270	<div> <div>63%</div> <div>26%</div> <div>10%</div> </div>
5	P	13	<div> <div>8%</div> <div>69%</div> <div>31%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	B	201	-	-	X	-
8	PEG	B	199	-	-	-	X
8	PEG	C	208	-	-	X	X
8	PEG	C	209	-	-	-	X
8	PEG	D	246	-	-	-	X

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 6465 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 H-2 class II histocompatibility antigen, E-K alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1440	932	237	267	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	192	SER	-	EXPRESSION TAG	UNP P04224
A	193	ARG	-	EXPRESSION TAG	UNP P04224

- Molecule 2 is a protein called MHC class II E-beta-k.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	165	Total	C	N	O	S	0	0	0
			1328	844	230	248	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	EXPRESSION TAG	UNP Q31163
B	-2	SER	-	EXPRESSION TAG	UNP Q31163
B	-1	GLY	-	EXPRESSION TAG	UNP Q31163
B	0	GLY	-	EXPRESSION TAG	UNP Q31163
B	1	GLY	-	EXPRESSION TAG	UNP Q31163
B	2	GLY	-	EXPRESSION TAG	UNP Q31163

- Molecule 3 is a protein called T-cell receptor alpha chain C region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	0	0
			1472	916	251	297	8			

- Molecule 4 is a protein called 2B4 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1914	1212	331	362	9			

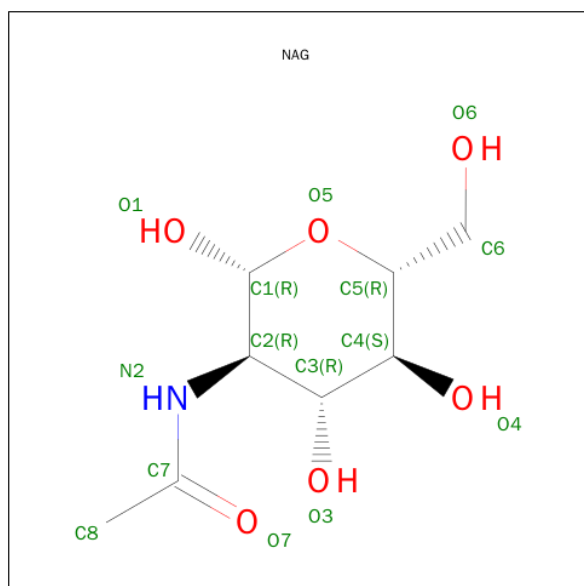
- Molecule 5 is a protein called MCC peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	P	13	Total	C	N	O	0	0	0
			97	63	16	18			

There is a discrepancy between the modelled and reference sequences:

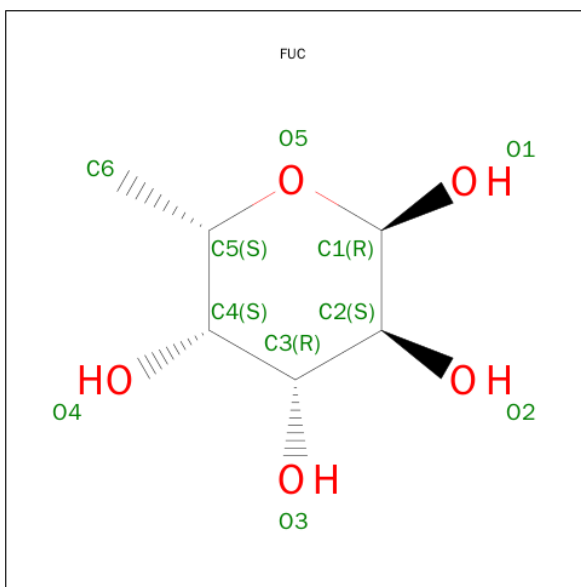
Chain	Residue	Modelled	Actual	Comment	Reference
P	14	GLY	-	EXPRESSION TAG	UNP P00039

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



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

- Molecule 7 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula:  $C_6H_{12}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		
7	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



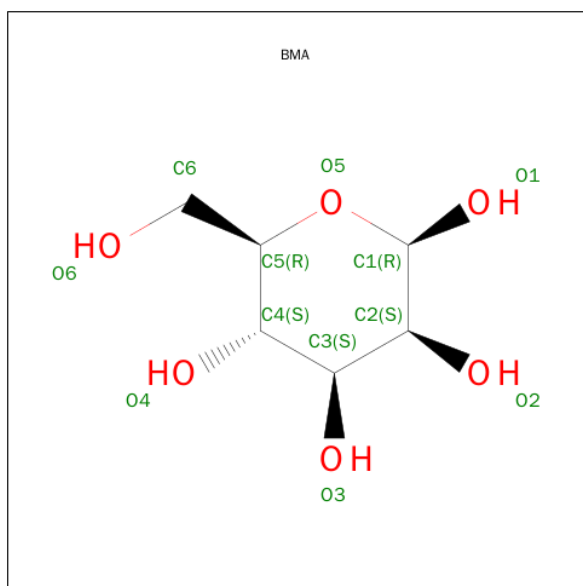
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		
8	C	1	Total	C	O	0	0
			7	4	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			7	4	3		
8	C	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	12	Total	O	0	0
			12	12		
10	B	17	Total	O	0	0
			17	17		
10	C	45	Total	O	0	0
			45	45		

*Continued on next page...*

*Continued from previous page...*

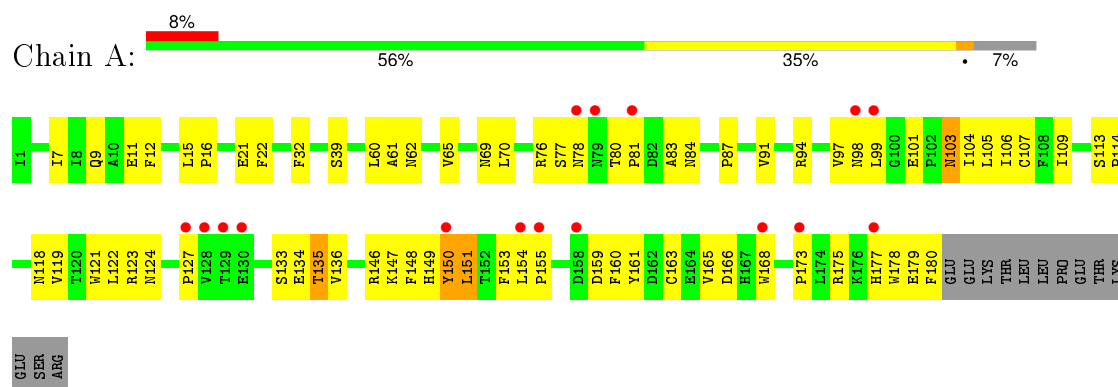
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	31	Total 31	O 31	0	0
10	P	1	Total 1	O 1	0	0



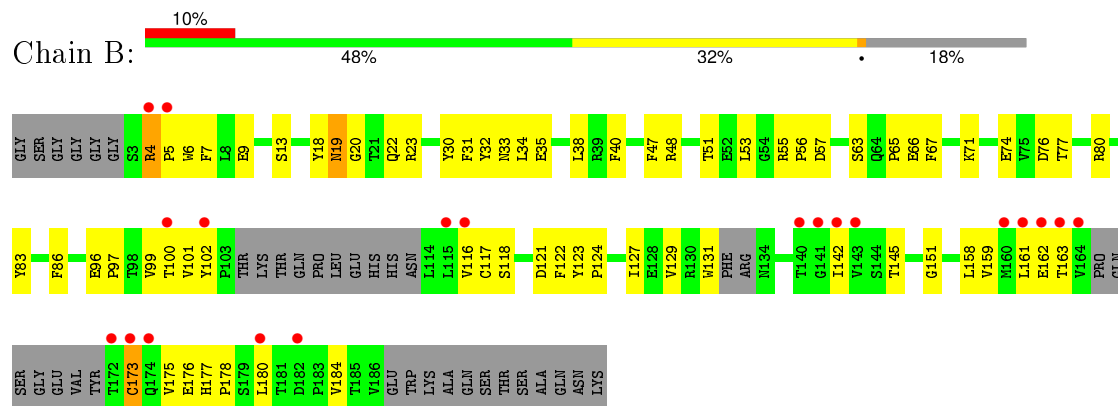
### 3 Residue-property plots [i](#)

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.

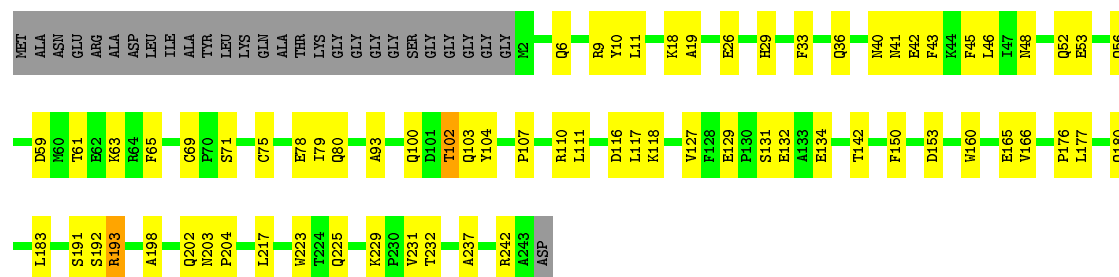
- Molecule 1: H-2 class II histocompatibility antigen, E-K alpha chain



- Molecule 2: MHC class II E-beta-k



Chain D:  63% 26% • 10%



- Molecule 5: MCC peptide

Chain P: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	146.75Å 167.18Å 259.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.97 – 2.70 35.14 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.97-2.70) 99.0 (35.14-2.69)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.52 (at 2.68Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.2_432)	Depositor
R, $R_{free}$	0.221 , 0.246 0.220 , 0.244	Depositor DCC
$R_{free}$ test set	2196 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.3	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 55.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 43816 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6465	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: FUC, PEG, BMA, 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	0.46	2/1483 (0.1%)	0.55	0/2021
2	B	0.46	0/1361	0.61	0/1855
3	C	0.55	0/1499	0.66	1/2033 (0.0%)
4	D	0.59	2/1966 (0.1%)	0.61	0/2679
5	P	0.53	0/97	0.60	0/129
All	All	0.53	4/6406 (0.1%)	0.61	1/8717 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	53	GLU	CG-CD	7.96	1.63	1.51
1	A	150	TYR	CD1-CE1	5.47	1.47	1.39
4	D	53	GLU	CD-OE1	5.43	1.31	1.25
1	A	150	TYR	CE1-CZ	5.08	1.45	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	111	ASP	CB-CG-OD1	5.22	123.00	118.30

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	1440	0	1349	94	0
2	B	1328	0	1225	85	0
3	C	1472	0	1377	59	0
4	D	1914	0	1804	74	0
5	P	97	0	104	6	0
6	B	14	0	13	8	0
6	C	14	0	13	0	0
7	B	10	0	10	2	0
7	C	10	0	10	4	0
8	B	7	0	10	0	0
8	C	21	0	30	8	0
8	D	21	0	30	1	0
9	C	11	0	10	0	0
10	A	12	0	0	0	0
10	B	17	0	0	0	0
10	C	45	0	0	2	0
10	D	31	0	0	1	0
10	P	1	0	0	0	0
All	All	6465	0	5985	285	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 23.

All (285) 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:B:19:ASN:HD21	6:B:201:NAG:C1	1.61	1.11
2:B:19:ASN:HD21	6:B:201:NAG:C2	1.69	1.06
3:C:188:ASN:HD22	3:C:190:SER:H	1.11	0.98
3:C:113:GLN:HG3	7:C:206:FUC:O3	1.66	0.96
4:D:48:ASN:HD22	4:D:56:GLN:HB2	1.29	0.95
2:B:4:ARG:CG	2:B:4:ARG:HH11	1.83	0.91
3:C:113:GLN:CG	7:C:206:FUC:O3	2.22	0.87
1:A:114:PRO:HG3	2:B:6:TRP:CD2	2.08	0.87
2:B:19:ASN:ND2	6:B:201:NAG:C1	2.37	0.86
1:A:105:LEU:HB3	1:A:151:LEU:CD1	2.05	0.86
4:D:100:GLN:HE22	4:D:102:THR:HG22	1.40	0.86
3:C:190:SER:HA	3:C:191:ILE:HG12	1.58	0.85
2:B:129:VAL:HG11	2:B:159:VAL:HG21	1.58	0.84
1:A:16:PRO:HD2	2:B:4:ARG:HH22	1.42	0.84
3:C:188:ASN:ND2	3:C:190:SER:H	1.75	0.83
2:B:57:ASP:OD2	5:P:13:LYS:HE2	1.77	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:CZ3	2:B:4:ARG:HD3	2.14	0.83
4:D:100:GLN:NE2	4:D:102:THR:HG22	1.94	0.82
1:A:105:LEU:HB3	1:A:151:LEU:HD11	1.61	0.82
1:A:105:LEU:HD12	1:A:121:TRP:CZ3	2.15	0.81
3:C:182:ALA:H	3:C:185:ASN:ND2	1.78	0.80
4:D:153:ASP:HB2	4:D:176:PRO:HG2	1.63	0.78
2:B:102:TYR:CZ	2:B:116:VAL:HG11	2.19	0.77
4:D:65:PHE:CE1	4:D:79:ILE:HG12	2.21	0.76
2:B:99:VAL:HA	2:B:118:SER:O	1.84	0.76
4:D:134:GLU:OE2	4:D:142:THR:HG22	1.85	0.76
1:A:105:LEU:HD12	1:A:151:LEU:HD11	1.68	0.75
1:A:16:PRO:HD2	2:B:4:ARG:NH2	2.02	0.74
2:B:19:ASN:HD21	6:B:201:NAG:H2	1.50	0.74
2:B:4:ARG:HG2	2:B:4:ARG:HH11	1.51	0.73
3:C:182:ALA:O	3:C:185:ASN:ND2	2.21	0.73
3:C:23:ASN:HB3	8:C:209:PEG:H31	1.69	0.73
1:A:118:ASN:HB2	1:A:166:ASP:HB3	1.70	0.73
4:D:176:PRO:HD3	8:D:246:PEG:H32	1.70	0.73
2:B:19:ASN:ND2	6:B:201:NAG:C2	2.50	0.73
1:A:121:TRP:CZ2	1:A:151:LEU:HD12	2.26	0.71
1:A:151:LEU:HD13	1:A:151:LEU:H	1.55	0.70
8:C:208:PEG:H12	4:D:41:ASN:O	1.92	0.70
1:A:103:ASN:HB3	1:A:153:PHE:CZ	2.27	0.70
3:C:97:LYS:HD2	4:D:45:PHE:HB3	1.73	0.70
1:A:121:TRP:CH2	1:A:151:LEU:HD12	2.28	0.69
1:A:99:LEU:HA	1:A:155:PRO:HB2	1.74	0.68
2:B:4:ARG:HG3	2:B:4:ARG:HH11	1.56	0.68
1:A:107:CYS:HB2	1:A:121:TRP:CH2	2.28	0.68
4:D:198:ALA:O	4:D:202:GLN:HG3	1.93	0.67
2:B:102:TYR:O	2:B:116:VAL:HB	1.95	0.67
4:D:134:GLU:CD	4:D:142:THR:HG22	2.14	0.67
1:A:160:PHE:HD2	1:A:177:HIS:HE1	1.44	0.66
1:A:104:ILE:C	1:A:153:PHE:HE1	1.99	0.65
1:A:61:ALA:O	1:A:65:VAL:HG23	1.95	0.65
3:C:130:LYS:HB3	3:C:130:LYS:HZ2	1.61	0.65
4:D:100:GLN:OE1	4:D:102:THR:HG22	1.97	0.65
2:B:101:VAL:HG13	2:B:116:VAL:O	1.96	0.65
4:D:127:VAL:HG23	4:D:237:ALA:HB3	1.78	0.65
1:A:119:VAL:HG22	1:A:165:VAL:HG22	1.79	0.64
4:D:150:PHE:HE1	4:D:153:ASP:HA	1.62	0.64
3:C:190:SER:HA	3:C:191:ILE:CG1	2.28	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:26:GLU:HB2	4:D:29:HIS:CE1	2.34	0.63
2:B:129:VAL:CG1	2:B:159:VAL:HG21	2.26	0.63
2:B:32:TYR:CD2	2:B:53:LEU:HD21	2.33	0.63
1:A:151:LEU:H	1:A:151:LEU:CD1	2.11	0.63
1:A:105:LEU:HB2	1:A:153:PHE:CD1	2.34	0.63
4:D:116:ASP:OD1	4:D:118:LYS:HG2	1.99	0.62
2:B:4:ARG:HG2	2:B:4:ARG:NH1	2.15	0.62
4:D:100:GLN:CD	4:D:102:THR:HG22	2.19	0.62
4:D:117:LEU:HD13	4:D:217:LEU:HD22	1.81	0.62
3:C:127:SER:HB2	3:C:129:ASP:OD1	2.01	0.61
4:D:183:LEU:HD23	4:D:183:LEU:N	2.15	0.61
2:B:80:ARG:HD2	3:C:65:LYS:HD3	1.82	0.61
4:D:26:GLU:HB2	4:D:29:HIS:ND1	2.16	0.61
3:C:127:SER:CB	3:C:129:ASP:OD1	2.48	0.61
4:D:61:THR:HG23	4:D:65:PHE:HB2	1.83	0.61
2:B:66:GLU:OE2	4:D:102:THR:HG21	2.01	0.60
3:C:122:LEU:HB3	4:D:129:GLU:O	2.02	0.60
1:A:124:ASN:HA	1:A:160:PHE:CE1	2.36	0.60
1:A:109:ILE:HD12	1:A:109:ILE:N	2.16	0.60
2:B:100:THR:O	2:B:118:SER:HB3	2.03	0.59
2:B:19:ASN:ND2	6:B:201:NAG:H2	2.15	0.59
1:A:91:VAL:HG13	1:A:105:LEU:HD11	1.83	0.59
1:A:105:LEU:HB3	1:A:151:LEU:HD13	1.82	0.59
1:A:91:VAL:CG1	1:A:105:LEU:HD11	2.33	0.59
3:C:188:ASN:ND2	3:C:190:SER:N	2.49	0.58
8:C:208:PEG:H12	4:D:42:GLU:HA	1.85	0.58
4:D:36:GLN:HG3	4:D:46:LEU:HD11	1.84	0.58
2:B:67:PHE:CE1	2:B:71:LYS:HD3	2.38	0.57
3:C:10:LEU:HD22	3:C:12:LEU:HD13	1.86	0.57
4:D:61:THR:CG2	4:D:65:PHE:HB2	2.34	0.57
4:D:6:GLN:HB2	4:D:107:PRO:HD2	1.86	0.57
4:D:202:GLN:HA	4:D:242:ARG:O	2.04	0.57
4:D:59:ASP:OD2	4:D:63:LYS:HE3	2.04	0.57
1:A:122:LEU:HD23	1:A:127:PRO:HA	1.86	0.57
4:D:223:TRP:HB2	4:D:229:LYS:HD2	1.87	0.57
4:D:48:ASN:ND2	4:D:56:GLN:HB2	2.10	0.57
1:A:151:LEU:N	1:A:151:LEU:CD1	2.68	0.57
2:B:76:ASP:OD2	2:B:80:ARG:HD3	2.04	0.57
1:A:133:SER:HB2	1:A:150:TYR:HB2	1.86	0.57
3:C:106:LEU:HD12	3:C:107:SER:N	2.20	0.57
3:C:188:ASN:HD22	3:C:188:ASN:C	2.09	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ASN:ND2	1:A:168:TRP:HB2	2.20	0.57
1:A:21:GLU:OE1	1:A:136:VAL:HB	2.04	0.57
1:A:114:PRO:HG3	2:B:6:TRP:CE3	2.39	0.56
3:C:130:LYS:HB3	3:C:130:LYS:NZ	2.19	0.56
2:B:127:ILE:CD1	2:B:177:HIS:HB2	2.35	0.56
4:D:134:GLU:OE1	4:D:142:THR:HG22	2.05	0.56
1:A:104:ILE:C	1:A:153:PHE:CE1	2.79	0.56
1:A:109:ILE:HD12	1:A:109:ILE:H	1.69	0.56
2:B:9:GLU:OE2	5:P:13:LYS:NZ	2.38	0.55
1:A:84:ASN:HD22	1:A:168:TRP:HB2	1.71	0.55
3:C:29:ARG:NH2	5:P:7:TYR:O	2.39	0.55
2:B:129:VAL:HG11	2:B:159:VAL:CG2	2.32	0.55
4:D:100:GLN:OE1	4:D:102:THR:CG2	2.55	0.55
4:D:132:GLU:HA	4:D:132:GLU:OE1	2.06	0.55
3:C:98:LEU:HD23	4:D:103:GLN:CD	2.27	0.55
1:A:168:TRP:CH2	2:B:4:ARG:HD3	2.42	0.55
3:C:78:LEU:H	3:C:78:LEU:CD1	2.20	0.55
3:C:182:ALA:H	3:C:185:ASN:HD21	1.55	0.54
1:A:163:CYS:O	1:A:175:ARG:HA	2.07	0.54
3:C:78:LEU:HD12	3:C:78:LEU:N	2.21	0.54
1:A:160:PHE:HD2	1:A:177:HIS:CE1	2.24	0.54
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.90	0.54
2:B:18:TYR:CD2	2:B:23:ARG:HG3	2.43	0.54
3:C:44:ASN:ND2	10:C:214:HOH:O	2.42	0.53
1:A:83:ALA:O	2:B:34:LEU:HD11	2.08	0.53
3:C:78:LEU:HD12	3:C:78:LEU:H	1.73	0.53
3:C:39:ARG:NH1	3:C:39:ARG:HG2	2.24	0.53
4:D:18:LYS:HG2	4:D:80:GLN:O	2.08	0.53
8:C:208:PEG:H41	4:D:43:PHE:O	2.09	0.53
4:D:9:ARG:HG2	4:D:10:TYR:CE1	2.44	0.53
1:A:12:PHE:CE2	1:A:21:GLU:HB3	2.43	0.53
3:C:97:LYS:HD2	4:D:45:PHE:CB	2.37	0.52
1:A:84:ASN:ND2	1:A:168:TRP:CB	2.73	0.52
2:B:142:ILE:HD11	2:B:161:LEU:HD13	1.91	0.52
4:D:223:TRP:CG	4:D:229:LYS:HG3	2.45	0.52
4:D:10:TYR:CE2	4:D:110:ARG:HD2	2.44	0.52
3:C:199:PRO:O	3:C:201:PRO:HD3	2.09	0.52
3:C:184:ALA:HA	3:C:198:PHE:CE2	2.44	0.52
1:A:94:ARG:HD3	1:A:104:ILE:HD13	1.91	0.52
1:A:106:ILE:HG12	1:A:150:TYR:CD1	2.45	0.52
8:C:208:PEG:C1	4:D:41:ASN:O	2.57	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:197:PHE:CE2	3:C:199:PRO:HG3	2.45	0.51
2:B:180:LEU:HD13	2:B:184:VAL:HG23	1.93	0.51
1:A:97:VAL:HG21	1:A:178:TRP:HZ2	1.74	0.51
3:C:10:LEU:CD2	3:C:12:LEU:HD13	2.40	0.51
3:C:190:SER:N	3:C:191:ILE:HA	2.25	0.51
2:B:30:TYR:HB2	2:B:38:LEU:HB3	1.93	0.51
8:C:208:PEG:H32	4:D:43:PHE:HB2	1.90	0.51
1:A:84:ASN:HD22	1:A:168:TRP:CB	2.23	0.51
2:B:131:TRP:CZ3	2:B:173:CYS:HB3	2.46	0.51
2:B:74:GLU:HA	2:B:77:THR:OG1	2.11	0.51
2:B:63:SER:O	2:B:65:PRO:HD3	2.11	0.50
1:A:168:TRP:CE3	2:B:4:ARG:HD3	2.47	0.50
1:A:121:TRP:CH2	1:A:151:LEU:CD1	2.94	0.50
2:B:96:GLU:OE1	2:B:180:LEU:HD21	2.11	0.50
2:B:20:GLY:HA3	7:B:203:FUC:O4	2.11	0.50
3:C:39:ARG:HH11	3:C:39:ARG:HG2	1.76	0.50
2:B:102:TYR:CE1	2:B:116:VAL:HG11	2.46	0.49
1:A:151:LEU:HD22	1:A:151:LEU:O	2.11	0.49
3:C:134:LEU:HD21	4:D:142:THR:HG21	1.93	0.49
4:D:11:LEU:O	4:D:111:LEU:HD12	2.12	0.49
2:B:40:PHE:HB2	2:B:47:PHE:CE2	2.48	0.49
2:B:31:PHE:CD1	2:B:31:PHE:N	2.80	0.49
3:C:99:THR:HG23	8:C:208:PEG:O4	2.13	0.49
2:B:127:ILE:HD11	2:B:175:VAL:CG1	2.42	0.49
2:B:142:ILE:CD1	2:B:161:LEU:HD13	2.42	0.49
4:D:19:ALA:O	4:D:78:GLU:HA	2.13	0.49
1:A:7:ILE:HD13	2:B:86:PHE:CD2	2.48	0.49
3:C:188:ASN:ND2	3:C:190:SER:HB2	2.27	0.49
4:D:9:ARG:HG2	4:D:10:TYR:CD1	2.47	0.49
2:B:161:LEU:HD12	2:B:162:GLU:H	1.77	0.49
1:A:87:PRO:HB3	1:A:109:ILE:CG2	2.43	0.48
1:A:11:GLU:HA	1:A:21:GLU:O	2.14	0.48
3:C:134:LEU:CD2	4:D:142:THR:HG21	2.44	0.48
1:A:39:SER:HB2	1:A:60:LEU:HD11	1.95	0.48
2:B:145:THR:HG23	2:B:158:LEU:HB2	1.95	0.48
1:A:103:ASN:HB3	1:A:153:PHE:CE2	2.49	0.48
2:B:161:LEU:HD11	2:B:163:THR:HG23	1.95	0.48
3:C:182:ALA:N	3:C:185:ASN:ND2	2.55	0.48
2:B:20:GLY:HA2	2:B:83:TYR:CZ	2.49	0.48
2:B:4:ARG:CG	2:B:4:ARG:NH1	2.53	0.47
3:C:127:SER:OG	3:C:129:ASP:OD1	2.28	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:ASN:HD22	4:D:56:GLN:CB	2.15	0.47
1:A:135:THR:HB	1:A:148:PHE:O	2.15	0.47
4:D:192:SER:C	4:D:193:ARG:HD3	2.35	0.47
3:C:188:ASN:HD21	3:C:190:SER:HB2	1.80	0.47
1:A:154:LEU:HD22	1:A:155:PRO:HD2	1.95	0.47
4:D:52:GLN:NE2	4:D:71:SER:HB3	2.30	0.47
3:C:113:GLN:HG2	7:C:206:FUC:O3	2.13	0.47
4:D:48:ASN:ND2	4:D:56:GLN:OE1	2.47	0.47
1:A:97:VAL:HG21	1:A:178:TRP:CZ2	2.50	0.47
1:A:105:LEU:CD1	1:A:151:LEU:HD11	2.42	0.47
1:A:69:ASN:HB3	5:P:13:LYS:HD2	1.96	0.47
2:B:102:TYR:CE1	2:B:116:VAL:HG21	2.50	0.47
2:B:102:TYR:CE2	2:B:116:VAL:HG11	2.49	0.47
4:D:52:GLN:HA	4:D:69:CYS:O	2.14	0.47
1:A:180:PHE:C	1:A:180:PHE:CD2	2.89	0.47
1:A:114:PRO:HG3	2:B:6:TRP:CE2	2.50	0.46
2:B:131:TRP:CE3	2:B:173:CYS:HB3	2.50	0.46
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.50	0.46
4:D:117:LEU:HD13	4:D:217:LEU:CD2	2.44	0.46
2:B:145:THR:CG2	2:B:158:LEU:HB2	2.45	0.46
1:A:32:PHE:C	1:A:32:PHE:CD1	2.88	0.46
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.51	0.46
4:D:127:VAL:HG23	4:D:237:ALA:CB	2.43	0.46
2:B:99:VAL:HG21	2:B:175:VAL:HG21	1.98	0.46
1:A:7:ILE:CD1	2:B:86:PHE:HD2	2.28	0.46
1:A:179:GLU:O	1:A:180:PHE:C	2.54	0.46
1:A:119:VAL:HG11	1:A:149:HIS:CD2	2.51	0.45
2:B:127:ILE:HD12	2:B:176:GLU:O	2.16	0.45
2:B:161:LEU:HD12	2:B:162:GLU:N	2.31	0.45
4:D:116:ASP:OD1	4:D:118:LYS:CG	2.64	0.45
3:C:197:PHE:HE2	3:C:199:PRO:HG3	1.81	0.45
1:A:91:VAL:HG13	1:A:105:LEU:CD1	2.46	0.45
3:C:155:THR:HG21	4:D:191:SER:OG	2.16	0.45
3:C:78:LEU:N	3:C:78:LEU:CD1	2.80	0.45
4:D:160:TRP:CZ3	4:D:165:GLU:HB2	2.52	0.45
3:C:6:SER:HB2	3:C:7:PRO:HA	1.97	0.45
3:C:89:LEU:HD22	3:C:90:ARG:O	2.17	0.45
1:A:105:LEU:HD12	1:A:121:TRP:CH2	2.51	0.45
2:B:48:ARG:HA	2:B:48:ARG:HD3	1.83	0.45
1:A:104:ILE:N	1:A:104:ILE:HD12	2.32	0.45
2:B:55:ARG:N	2:B:56:PRO:CD	2.80	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HD3	2:B:56:PRO:HG2	1.98	0.44
1:A:9:GLN:OE1	5:P:7:TYR:HB2	2.17	0.44
4:D:80:GLN:HA	4:D:80:GLN:OE1	2.16	0.44
1:A:103:ASN:ND2	1:A:104:ILE:H	2.14	0.44
1:A:123:ARG:HG3	1:A:161:TYR:CE2	2.52	0.44
1:A:124:ASN:HA	1:A:160:PHE:CZ	2.53	0.44
4:D:93:ALA:HA	4:D:104:TYR:O	2.18	0.44
1:A:98:ASN:O	1:A:155:PRO:HG2	2.17	0.44
4:D:193:ARG:N	4:D:193:ARG:HD3	2.33	0.44
5:P:10:GLN:HE21	5:P:11:ALA:H	1.65	0.44
4:D:61:THR:HG23	4:D:65:PHE:CB	2.46	0.44
1:A:160:PHE:CD2	1:A:177:HIS:HE1	2.29	0.44
1:A:121:TRP:CZ3	1:A:151:LEU:CD1	3.02	0.43
1:A:134:GLU:HG2	1:A:147:LYS:HZ1	1.83	0.43
1:A:113:SER:HB3	2:B:34:LEU:CD2	2.48	0.43
2:B:22:GLN:HG2	7:B:203:FUC:H63	2.00	0.43
1:A:101:GLU:O	1:A:155:PRO:CD	2.66	0.43
2:B:35:GLU:OE2	2:B:51:THR:HG21	2.18	0.43
4:D:40:ASN:O	4:D:41:ASN:HB2	2.18	0.43
1:A:135:THR:HG22	1:A:136:VAL:O	2.19	0.43
1:A:9:GLN:HB3	2:B:13:SER:HB2	2.00	0.43
2:B:123:TYR:CG	2:B:124:PRO:HA	2.54	0.43
3:C:39:ARG:HB3	4:D:9:ARG:HH22	1.83	0.43
1:A:150:TYR:OH	2:B:151:GLY:HA3	2.19	0.43
3:C:168:LYS:NZ	7:C:206:FUC:H62	2.34	0.43
2:B:129:VAL:CB	2:B:159:VAL:HG21	2.49	0.43
1:A:105:LEU:O	1:A:151:LEU:HD13	2.19	0.42
2:B:4:ARG:NH1	2:B:5:PRO:O	2.52	0.42
3:C:160:LEU:HD23	10:C:218:HOH:O	2.18	0.42
4:D:177:LEU:HD12	4:D:177:LEU:C	2.40	0.42
4:D:231:VAL:O	4:D:232:THR:C	2.56	0.42
1:A:105:LEU:CB	1:A:151:LEU:HD11	2.42	0.42
2:B:32:TYR:O	2:B:33:ASN:HB2	2.19	0.42
1:A:70:LEU:HD11	2:B:7:PHE:HB3	2.01	0.42
3:C:124:ASP:HB3	3:C:127:SER:O	2.20	0.42
1:A:22:PHE:HE2	1:A:62:ASN:HD22	1.68	0.42
1:A:124:ASN:OD1	1:A:159:ASP:HA	2.20	0.42
2:B:96:GLU:CG	2:B:180:LEU:HD21	2.50	0.41
3:C:39:ARG:HH11	3:C:39:ARG:CG	2.33	0.41
3:C:130:LYS:CB	3:C:130:LYS:NZ	2.81	0.41
3:C:87:ALA:HA	3:C:99:THR:O	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:208:PEG:C1	4:D:43:PHE:HD2	2.33	0.41
2:B:19:ASN:CG	6:B:201:NAG:C1	2.88	0.41
3:C:96:ASN:O	4:D:33:PHE:HE1	2.03	0.41
2:B:19:ASN:OD1	6:B:201:NAG:C1	2.69	0.41
1:A:103:ASN:HD22	1:A:104:ILE:H	1.69	0.41
1:A:107:CYS:HB3	1:A:149:HIS:HB2	2.03	0.41
2:B:127:ILE:HD12	2:B:177:HIS:HB2	2.02	0.41
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.56	0.41
1:A:87:PRO:HB3	1:A:109:ILE:HG23	2.03	0.41
2:B:161:LEU:CD1	2:B:163:THR:HG23	2.50	0.41
1:A:77:SER:O	1:A:78:ASN:HB3	2.20	0.41
4:D:118:LYS:CD	4:D:225:GLN:NE2	2.84	0.41
3:C:122:LEU:HD12	3:C:122:LEU:N	2.36	0.41
4:D:52:GLN:CD	4:D:71:SER:HB3	2.42	0.41
3:C:146:GLN:NE2	3:C:154:ILE:O	2.53	0.41
4:D:116:ASP:CG	4:D:118:LYS:HG2	2.41	0.40
4:D:203:ASN:HA	4:D:204:PRO:HD3	1.86	0.40
1:A:80:THR:HA	1:A:81:PRO:HD3	1.76	0.40
4:D:75:CYS:HB3	10:D:252:HOH:O	2.20	0.40
3:C:120:TYR:HB3	4:D:131:SER:OG	2.20	0.40
1:A:15:LEU:HD23	1:A:15:LEU:HA	1.94	0.40
1:A:154:LEU:C	1:A:154:LEU:HD13	2.41	0.40
1:A:134:GLU:HG2	1:A:147:LYS:NZ	2.36	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	178/193 (92%)	169 (95%)	8 (4%)	1 (1%)	30	59
2	B	157/202 (78%)	148 (94%)	8 (5%)	1 (1%)	30	59

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	188/207 (91%)	181 (96%)	7 (4%)	0	100	100
4	D	240/270 (89%)	232 (97%)	8 (3%)	0	100	100
5	P	11/13 (85%)	11 (100%)	0	0	100	100
All	All	774/885 (88%)	741 (96%)	31 (4%)	2 (0%)	46	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	19	ASN
1	A	173	PRO

### 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	A	153/176 (87%)	149 (97%)	4 (3%)	54	83
2	B	143/183 (78%)	140 (98%)	3 (2%)	61	87
3	C	162/182 (89%)	154 (95%)	8 (5%)	31	61
4	D	207/230 (90%)	203 (98%)	4 (2%)	65	88
5	P	9/9 (100%)	9 (100%)	0	100	100
All	All	674/780 (86%)	655 (97%)	19 (3%)	51	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	135	THR
1	A	146	ARG
1	A	151	LEU
2	B	4	ARG
2	B	121	ASP
2	B	173	CYS
3	C	10	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	12	LEU
3	C	45	LEU
3	C	89	LEU
3	C	98	LEU
3	C	130	LYS
3	C	158	CYS
3	C	188	ASN
4	D	102	THR
4	D	166	VAL
4	D	180	GLN
4	D	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	149	HIS
1	A	177	HIS
2	B	19	ASN
3	C	44	ASN
3	C	185	ASN
3	C	188	ASN
4	D	15	GLN
4	D	48	ASN
4	D	52	GLN
4	D	56	GLN
4	D	225	GLN
5	P	10	GLN

### 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

12 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$
8	PEG	B	199	-	6,6,6	0.44	0	5,5,5	0.92	0
6	NAG	B	201	-	14,14,15	0.79	0	15,19,21	2.84	4 (26%)
7	FUC	B	203	-	10,10,11	0.99	1 (10%)	14,14,16	2.93	4 (28%)
6	NAG	C	205	-	14,14,15	0.78	0	15,19,21	3.40	4 (26%)
7	FUC	C	206	-	10,10,11	1.16	0	14,14,16	3.48	5 (35%)
9	BMA	C	207	-	11,11,12	0.94	1 (9%)	14,15,17	2.64	5 (35%)
8	PEG	C	208	-	6,6,6	0.47	0	5,5,5	0.50	0
8	PEG	C	209	-	6,6,6	0.38	0	5,5,5	0.63	0
8	PEG	C	210	-	6,6,6	0.32	0	5,5,5	0.72	0
8	PEG	D	245	-	6,6,6	0.42	0	5,5,5	0.77	0
8	PEG	D	246	-	6,6,6	0.34	0	5,5,5	1.39	1 (20%)
8	PEG	D	247	-	6,6,6	0.56	0	5,5,5	0.29	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
8	PEG	B	199	-	-	0/4/4/4	0/0/0/0
6	NAG	B	201	-	-	0/6/23/26	0/1/1/1
7	FUC	B	203	-	-	0/0/17/20	0/1/1/1
6	NAG	C	205	-	-	0/6/23/26	0/1/1/1
7	FUC	C	206	-	-	0/0/17/20	0/1/1/1
9	BMA	C	207	-	-	0/2/19/22	0/1/1/1
8	PEG	C	208	-	-	0/4/4/4	0/0/0/0
8	PEG	C	209	-	-	0/4/4/4	0/0/0/0
8	PEG	C	210	-	-	0/4/4/4	0/0/0/0
8	PEG	D	245	-	-	0/4/4/4	0/0/0/0
8	PEG	D	246	-	-	0/4/4/4	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	D	247	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	207	BMA	O5-C1	-2.52	1.39	1.43
7	B	203	FUC	O5-C1	-2.46	1.39	1.43

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	205	NAG	C1-O5-C5	-9.64	100.02	112.25
6	B	201	NAG	C1-O5-C5	-5.26	105.57	112.25
9	C	207	BMA	C1-O5-C5	-4.42	106.64	112.25
6	C	205	NAG	O4-C4-C5	-4.32	97.80	109.24
7	C	206	FUC	C1-C2-C3	-4.13	104.66	109.54
7	B	203	FUC	C1-C2-C3	-2.90	106.11	109.54
9	C	207	BMA	O5-C1-C2	-2.88	106.19	110.86
8	D	246	PEG	C3-O2-C2	-2.44	102.82	113.31
7	B	203	FUC	O3-C3-C2	2.07	113.74	110.00
9	C	207	BMA	O3-C3-C4	2.55	116.08	110.34
7	C	206	FUC	C6-C5-C4	2.70	118.40	113.08
7	C	206	FUC	O4-C4-C5	2.71	116.20	109.84
6	C	205	NAG	O3-C3-C4	2.93	116.93	110.34
7	C	206	FUC	O5-C5-C6	3.12	111.30	106.13
6	B	201	NAG	O3-C3-C2	3.60	116.24	109.11
7	B	203	FUC	O5-C5-C4	3.94	116.35	109.53
6	B	201	NAG	O5-C5-C6	4.73	117.58	107.35
9	C	207	BMA	O5-C5-C6	5.08	118.34	107.35
9	C	207	BMA	C1-C2-C3	5.47	116.01	109.54
6	B	201	NAG	C3-C4-C5	6.36	121.29	110.20
6	C	205	NAG	O5-C5-C6	6.73	121.92	107.35
7	B	203	FUC	C1-O5-C5	9.29	126.72	112.38
7	C	206	FUC	C1-O5-C5	10.62	128.78	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 23 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	201	NAG	8	0
7	B	203	FUC	2	0
7	C	206	FUC	4	0
8	C	208	PEG	7	0
8	C	209	PEG	1	0
8	D	246	PEG	1	0

## 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	A	180/193 (93%)	0.61	16 (8%) 12 9	33, 66, 106, 116	0
2	B	165/202 (81%)	0.56	20 (12%) 6 4	25, 59, 106, 118	0
3	C	194/207 (93%)	0.05	9 (4%) 36 35	18, 38, 83, 105	0
4	D	242/270 (89%)	-0.05	0 100 100	26, 47, 74, 93	0
5	P	13/13 (100%)	0.25	1 (7%) 16 14	28, 35, 64, 64	0
All	All	794/885 (89%)	0.26	46 (5%) 26 25	18, 51, 99, 118	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	161	LEU	7.4
2	B	143	VAL	4.8
2	B	140	THR	4.8
1	A	129	THR	4.7
2	B	163	THR	4.6
2	B	164	VAL	4.4
2	B	116	VAL	4.3
2	B	5	PRO	4.1
2	B	100	THR	3.9
3	C	200	SER	3.8
3	C	184	ALA	3.6
2	B	162	GLU	3.4
2	B	160	MET	3.3
2	B	102	TYR	3.1
3	C	129	ASP	3.0
1	A	168	TRP	2.9
2	B	173	CYS	2.9
1	A	173	PRO	2.9
2	B	141	GLY	2.9
3	C	201	PRO	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	78	ASN	2.9
2	B	172	THR	2.9
1	A	79	ASN	2.8
3	C	145	SER	2.8
2	B	142	ILE	2.8
1	A	127	PRO	2.7
1	A	177	HIS	2.7
1	A	81	PRO	2.7
1	A	155	PRO	2.7
3	C	183	CYS	2.6
2	B	4	ARG	2.5
1	A	128	VAL	2.5
3	C	195	ASP	2.4
3	C	186	ALA	2.4
1	A	154	LEU	2.3
2	B	182	ASP	2.3
1	A	130	GLU	2.3
5	P	2	ALA	2.3
1	A	98	ASN	2.3
2	B	180	LEU	2.3
2	B	174	GLN	2.3
1	A	158	ASP	2.2
3	C	198	PHE	2.2
1	A	99	LEU	2.1
1	A	150	TYR	2.1
2	B	115	LEU	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
8	PEG	C	209	7/7	0.81	0.38	9.52	46,48,60,63	0
8	PEG	D	246	7/7	0.87	0.33	5.72	45,54,59,63	0
8	PEG	C	208	7/7	0.94	0.38	5.30	32,37,42,46	0
8	PEG	B	199	7/7	0.76	0.31	4.22	56,58,64,70	0
8	PEG	D	247	7/7	0.95	0.19	1.52	30,41,42,45	0
8	PEG	D	245	7/7	0.95	0.17	1.03	34,43,44,47	0
7	FUC	B	203	10/11	0.88	0.20	0.53	42,46,52,53	0
7	FUC	C	206	10/11	0.91	0.25	0.40	44,52,56,60	0
8	PEG	C	210	7/7	0.86	0.23	0.21	61,64,70,72	0
6	NAG	C	205	14/15	0.92	0.19	-	48,58,63,67	0
9	BMA	C	207	11/12	0.69	0.31	-	62,75,82,83	0
6	NAG	B	201	14/15	0.95	0.18	-	37,43,52,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.