



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:22 PM GMT

PDB ID : 1TCR  
Title : MURINE T-CELL ANTIGEN RECEPTOR 2C CLONE  
Authors : Garcia, K.C.; Degano, M.; Stanfield, R.L.; Wilson, I.A.  
Deposited on : 1996-09-12  
Resolution : 2.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

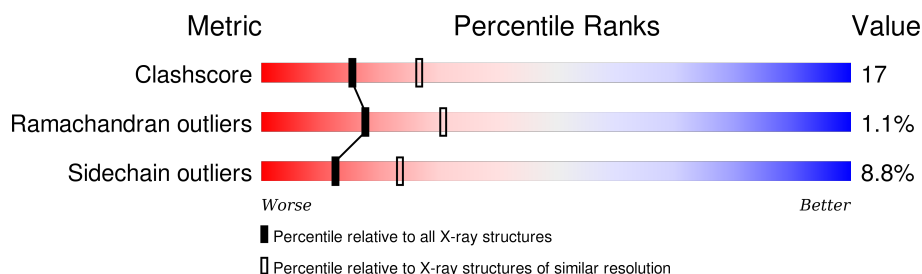
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	202	
2	B	237	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3589 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 ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2 \;VA3JA58CA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1570	999	253	310	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	ALA	GLN	CONFLICT	EMBL X01134
A	165	ALA	LYS	CONFLICT	EMBL X01134

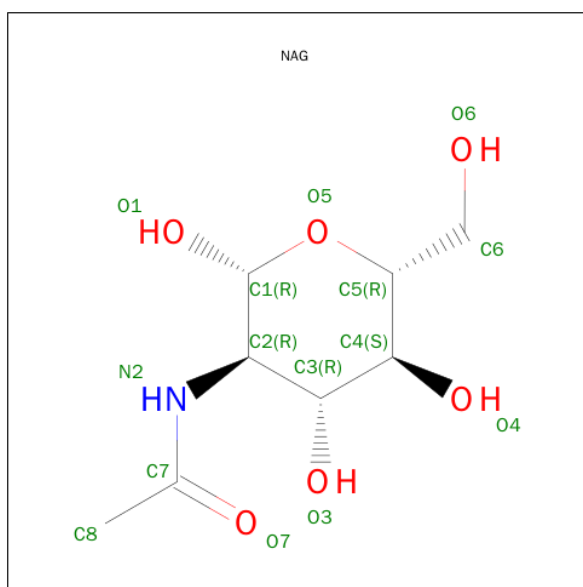
- Molecule 2 is a protein called ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2 \;VA3JA58CA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1853	1160	331	355	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	97	GLY	GLN	CONFLICT	GB 1791255
B	?	-	ARG	DELETION	GB 1791255
B	?	-	ALA	DELETION	GB 1791255
B	105	THR	GLU	CONFLICT	GB 1791255
B	106	LEU	GLN	CONFLICT	GB 1791255
B	107	TYR	PHE	CONFLICT	GB 1791255
B	110	ALA	PRO	CONFLICT	GB 1791255
B	115	SER	THR	CONFLICT	GB 1791255

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	4	Total	C	N	O	0	0
			49	28	2	19		

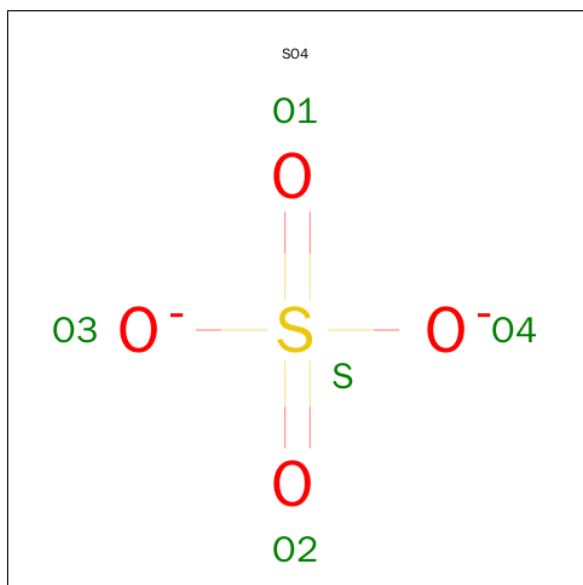
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

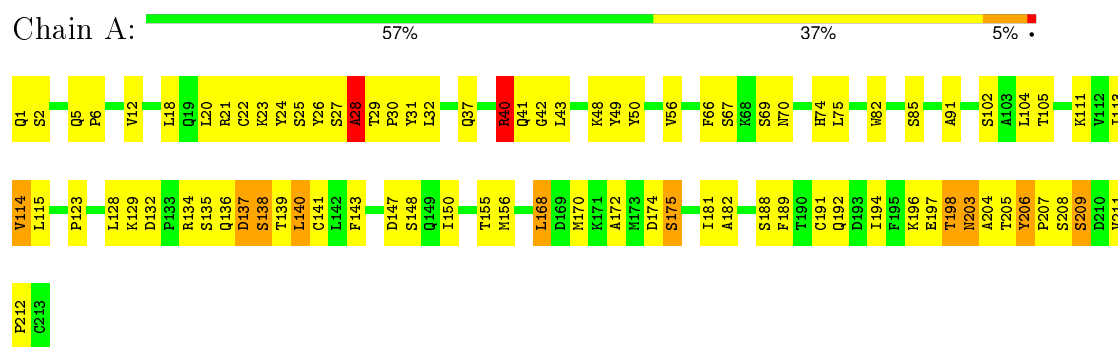
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	9	Total	O	0	0
			9	9		
8	B	13	Total	O	0	0
			13	13		

### 3 Residue-property plots

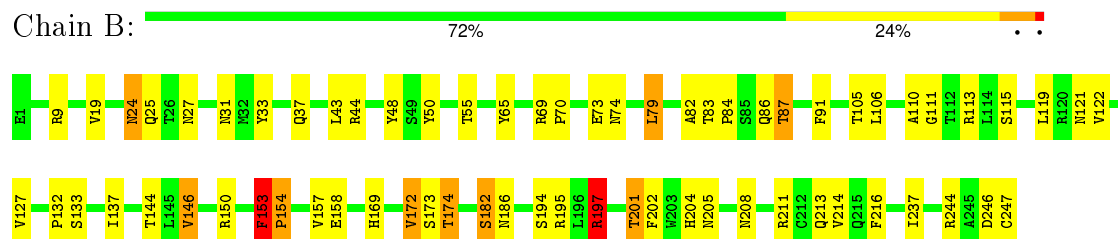
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

- Molecule 1: ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2\;VA3JA58CA)



- Molecule 2: ALPHA, BETA T-CELL RECEPTOR (VB8.2DB2JB2.4CB2\;VA3JA58CA)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.00 Å   72.90 Å   57.30 Å 90.00°   101.20°   90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	93.4 ((Not available)-2.50)	Depositor
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.208 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUC, BMA, 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	A	0.73	3/1611 (0.2%)	0.94	4/2193 (0.2%)
2	B	0.63	0/1904	0.90	5/2586 (0.2%)
All	All	0.67	3/3515 (0.1%)	0.92	9/4779 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	ALA	C-N	-7.29	1.17	1.34
1	A	29	THR	N-CA	-7.05	1.32	1.46
1	A	29	THR	C-N	-5.63	1.23	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	153	PHE	O-C-N	-9.66	102.75	121.10
1	A	40	ARG	NE-CZ-NH2	8.57	124.59	120.30
2	B	197	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	21	ARG	NE-CZ-NH2	6.76	123.68	120.30
2	B	44	ARG	NE-CZ-NH2	6.69	123.65	120.30
2	B	195	ARG	NE-CZ-NH2	6.65	123.63	120.30
2	B	153	PHE	CA-C-N	6.23	134.54	117.10
1	A	140	LEU	CA-CB-CG	5.92	128.91	115.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	209	SER	N-CA-C	-5.37	96.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	153	PHE	Peptide

## 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	1570	0	1502	72	0
2	B	1853	0	1762	59	0
3	A	14	0	13	0	0
4	A	49	0	43	2	0
5	B	28	0	25	0	0
6	A	38	0	34	2	0
7	B	15	0	0	1	0
8	A	9	0	0	0	0
8	B	13	0	0	0	0
All	All	3589	0	3379	119	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 17.

All (119) 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:26:TYR:CE2	1:A:28:ALA:HB3	1.75	1.20
2:B:153:PHE:O	2:B:154:PRO:O	1.72	1.08
1:A:27:SER:O	1:A:28:ALA:HB2	1.55	1.04
1:A:123:PRO:O	1:A:204:ALA:HB3	1.65	0.97
1:A:27:SER:O	1:A:28:ALA:CB	2.10	0.93
2:B:153:PHE:O	2:B:154:PRO:C	1.98	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:MET:HB2	1:A:175:SER:HB3	1.55	0.88
1:A:40:ARG:HD3	1:A:40:ARG:O	1.73	0.87
2:B:84:PRO:O	2:B:87:THR:HG23	1.79	0.82
1:A:28:ALA:O	1:A:30:PRO:HD3	1.79	0.81
1:A:91:ALA:HB1	1:A:104:LEU:HD22	1.60	0.81
2:B:174:THR:HB	2:B:194:SER:HB2	1.62	0.80
1:A:192:GLN:HG3	1:A:205:THR:HG21	1.69	0.75
1:A:26:TYR:CE2	1:A:28:ALA:CB	2.64	0.74
2:B:87:THR:HB	2:B:115:SER:HA	1.70	0.71
1:A:26:TYR:CD2	1:A:28:ALA:HB3	2.26	0.70
1:A:143:PHE:CZ	1:A:198:THR:HG21	2.26	0.70
1:A:67:SER:HB3	6:A:218:NAG:H82	1.73	0.70
2:B:205:ASN:HB3	2:B:208:ASN:ND2	2.06	0.69
1:A:128:LEU:HD12	2:B:146:VAL:HG13	1.75	0.68
2:B:133:SER:O	2:B:137:ILE:HG13	1.94	0.66
1:A:49:TYR:HB2	1:A:56:VAL:HG21	1.77	0.66
1:A:22:CYS:H	1:A:74:HIS:HD2	1.43	0.66
1:A:170:MET:HB2	1:A:175:SER:CB	2.26	0.66
2:B:127:VAL:HG13	2:B:237:ILE:HG22	1.77	0.65
2:B:174:THR:HB	2:B:194:SER:CB	2.26	0.65
2:B:246:ASP:O	2:B:247:CYS:HB2	1.97	0.65
2:B:37:GLN:HB2	2:B:43:LEU:CD2	2.26	0.65
1:A:48:LYS:O	1:A:56:VAL:HG11	1.96	0.65
1:A:172:ALA:HB3	1:A:175:SER:OG	1.98	0.64
1:A:132:ASP:HB3	1:A:138:SER:HB3	1.79	0.64
2:B:65:TYR:HD1	2:B:79:LEU:HD22	1.63	0.62
2:B:24:ASN:HA	2:B:73:GLU:O	2.00	0.62
1:A:22:CYS:H	1:A:74:HIS:CD2	2.19	0.60
2:B:169:HIS:O	2:B:172:VAL:HG13	2.02	0.60
1:A:42:GLY:HA2	2:B:91:PHE:CE2	2.36	0.60
2:B:83:THR:H	2:B:86:GLN:HE21	1.49	0.59
2:B:82:ALA:HA	2:B:86:GLN:NE2	2.17	0.59
2:B:204:HIS:HA	2:B:244:ARG:O	2.02	0.59
1:A:182:ALA:HB1	1:A:194:ILE:CD1	2.32	0.59
1:A:2:SER:HB3	1:A:25:SER:HB3	1.85	0.58
1:A:26:TYR:HE2	1:A:28:ALA:HB3	1.57	0.57
2:B:65:TYR:CD1	2:B:79:LEU:HD22	2.37	0.57
2:B:9:ARG:NH1	2:B:110:ALA:HB3	2.20	0.57
1:A:18:LEU:HD11	1:A:20:LEU:HD21	1.86	0.57
1:A:168:LEU:HB3	2:B:173:SER:CB	2.36	0.56
1:A:129:LYS:HG2	1:A:139:THR:HG22	1.89	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:ARG:HD2	2:B:74:ASN:O	2.05	0.55
1:A:82:TRP:HA	1:A:114:VAL:HG22	1.89	0.55
1:A:40:ARG:O	1:A:40:ARG:CD	2.49	0.54
1:A:67:SER:CB	6:A:218:NAG:H82	2.35	0.54
1:A:128:LEU:HD12	2:B:146:VAL:CG1	2.38	0.54
1:A:182:ALA:HB1	1:A:194:ILE:HD11	1.90	0.53
1:A:12:VAL:O	1:A:114:VAL:HA	2.08	0.53
1:A:111:LYS:HD3	1:A:113:ILE:HD11	1.89	0.53
2:B:82:ALA:HA	2:B:86:GLN:HE22	1.73	0.52
1:A:115:LEU:HB3	1:A:148:SER:HB3	1.89	0.52
1:A:147:ASP:O	1:A:150:ILE:HG22	2.09	0.52
2:B:48:TYR:HE2	2:B:50:TYR:CE2	2.27	0.52
1:A:28:ALA:O	1:A:30:PRO:CD	2.54	0.52
2:B:119:LEU:O	2:B:122:VAL:HG23	2.10	0.51
1:A:168:LEU:HD12	1:A:168:LEU:C	2.30	0.51
2:B:132:PRO:HB2	2:B:137:ILE:HD11	1.91	0.51
1:A:42:GLY:HA2	2:B:91:PHE:HE2	1.73	0.51
2:B:121:ASN:O	2:B:153:PHE:CB	2.58	0.51
2:B:37:GLN:CB	2:B:43:LEU:HD23	2.41	0.51
1:A:31:TYR:O	1:A:32:LEU:HD23	2.11	0.51
2:B:144:THR:OG1	2:B:197:ARG:HD3	2.12	0.50
1:A:192:GLN:CG	1:A:205:THR:HG21	2.41	0.50
1:A:141:CYS:HG	1:A:191:CYS:CB	2.18	0.50
1:A:203:ASN:OD1	1:A:203:ASN:N	2.44	0.50
1:A:43:LEU:HD11	2:B:43:LEU:HD12	1.94	0.49
1:A:43:LEU:HD11	2:B:43:LEU:CD1	2.41	0.49
1:A:70:ASN:OD1	1:A:70:ASN:N	2.45	0.49
2:B:84:PRO:O	2:B:87:THR:CG2	2.57	0.49
2:B:37:GLN:HB2	2:B:43:LEU:HD23	1.93	0.49
2:B:9:ARG:NH1	2:B:111:GLY:O	2.46	0.49
1:A:212:PRO:HB3	2:B:247:CYS:O	2.14	0.48
2:B:121:ASN:O	2:B:153:PHE:HB3	2.14	0.47
1:A:168:LEU:CB	2:B:173:SER:HB2	2.45	0.47
1:A:182:ALA:HB1	1:A:194:ILE:HD13	1.97	0.47
1:A:168:LEU:HB3	2:B:173:SER:HB3	1.96	0.47
4:A:217:FUC:H5	2:B:150:ARG:HH21	1.79	0.47
1:A:85:SER:OG	1:A:114:VAL:HG13	2.15	0.47
1:A:205:THR:O	1:A:207:PRO:HD3	2.15	0.46
1:A:197:GLU:O	1:A:198:THR:HG23	2.16	0.46
1:A:155:THR:HG22	1:A:156:MET:N	2.31	0.46
1:A:20:LEU:HD12	1:A:75:LEU:HD23	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:N	1:A:128:LEU:HD23	2.31	0.45
2:B:201:THR:HG22	2:B:202:PHE:N	2.31	0.45
1:A:136:GLN:HE21	1:A:137:ASP:H	1.64	0.45
1:A:5:GLN:HA	1:A:6:PRO:HD2	1.74	0.45
2:B:246:ASP:O	2:B:247:CYS:CB	2.65	0.45
2:B:25:GLN:OE1	2:B:27:ASN:HB2	2.17	0.44
1:A:37:GLN:HB2	1:A:43:LEU:HD22	1.99	0.44
1:A:48:LYS:HD2	1:A:50:TYR:CE2	2.53	0.43
1:A:168:LEU:HB3	2:B:173:SER:HB2	2.00	0.43
1:A:91:ALA:HA	1:A:105:THR:O	2.17	0.43
2:B:246:ASP:CG	2:B:247:CYS:N	2.71	0.43
2:B:31:ASN:OD1	2:B:50:TYR:CD1	2.72	0.43
2:B:19:VAL:HB	2:B:79:LEU:HG	2.00	0.42
1:A:170:MET:CB	1:A:175:SER:HB3	2.39	0.42
4:A:217:FUC:O3	2:B:182:SER:HB3	2.19	0.42
2:B:113:ARG:NH2	2:B:158:GLU:OE2	2.53	0.41
2:B:157:VAL:HG12	2:B:216:PHE:HA	2.02	0.41
1:A:26:TYR:CD2	1:A:30:PRO:HB3	2.56	0.41
2:B:79:LEU:N	2:B:79:LEU:HD23	2.35	0.41
1:A:188:SER:C	1:A:189:PHE:HD1	2.24	0.41
1:A:24:TYR:C	1:A:24:TYR:CD1	2.93	0.41
2:B:174:THR:HA	2:B:194:SER:HA	2.02	0.41
1:A:32:LEU:HD12	1:A:66:PHE:CD1	2.55	0.41
2:B:211:ARG:HD3	7:B:251:SO4:O3	2.20	0.41
1:A:196:LYS:HG2	1:A:196:LYS:O	2.20	0.41
2:B:205:ASN:HB3	2:B:208:ASN:HD22	1.81	0.41
1:A:104:LEU:HD12	2:B:106:LEU:HG	2.03	0.40
1:A:206:TYR:HA	1:A:207:PRO:HD2	1.90	0.40
2:B:70:PRO:HG2	2:B:74:ASN:HB2	2.02	0.40
2:B:213:GLN:HG2	2:B:214:VAL:N	2.35	0.40
1:A:141:CYS:SG	1:A:191:CYS:CB	3.09	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/202 (99%)	177 (88%)	20 (10%)	3 (2%)	13	22
2	B	235/237 (99%)	222 (94%)	11 (5%)	2 (1%)	21	37
All	All	435/439 (99%)	399 (92%)	31 (7%)	5 (1%)	17	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ALA
1	A	175	SER
2	B	153	PHE
1	A	135	SER
2	B	154	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	176/176 (100%)	156 (89%)	20 (11%)	7	13
2	B	200/200 (100%)	187 (94%)	13 (6%)	21	39
All	All	376/376 (100%)	343 (91%)	33 (9%)	12	23

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	23	LYS
1	A	40	ARG
1	A	41	GLN
1	A	69	SER
1	A	102	SER
1	A	114	VAL
1	A	134	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	137	ASP
1	A	138	SER
1	A	140	LEU
1	A	168	LEU
1	A	174	ASP
1	A	181	ILE
1	A	198	THR
1	A	203	ASN
1	A	206	TYR
1	A	208	SER
1	A	209	SER
1	A	211	VAL
2	B	24	ASN
2	B	33	TYR
2	B	55	THR
2	B	79	LEU
2	B	87	THR
2	B	105	THR
2	B	146	VAL
2	B	172	VAL
2	B	174	THR
2	B	182	SER
2	B	186	ASN
2	B	197	ARG
2	B	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	60	ASN
1	A	74	HIS
1	A	136	GLN
2	B	74	ASN
2	B	86	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 ⓘ

9 carbohydrates 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$
4	NAG	A	214	1,4	14,14,15	0.84	1 (7%)	15,19,21	0.73	0
4	NAG	A	215	4	14,14,15	0.60	0	15,19,21	0.68	0
4	BMA	A	216	4	11,11,12	1.39	2 (18%)	14,15,17	0.84	0
4	FUC	A	217	4	10,10,11	1.00	1 (10%)	14,14,16	1.87	3 (21%)
6	NAG	A	218	1,6	14,14,15	1.08	1 (7%)	15,19,21	0.70	0
6	NAG	A	219	6	14,14,15	0.86	0	15,19,21	0.59	0
6	FUC	A	220	6	10,10,11	1.23	1 (10%)	14,14,16	1.46	2 (14%)
5	NAG	B	248	2,5	14,14,15	0.60	0	15,19,21	0.51	0
5	NAG	B	249	5	14,14,15	0.62	0	15,19,21	0.81	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
4	NAG	A	214	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	215	4	-	0/6/23/26	0/1/1/1
4	BMA	A	216	4	-	0/2/19/22	0/1/1/1
4	FUC	A	217	4	-	0/0/17/20	0/1/1/1
6	NAG	A	218	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	219	6	-	0/6/23/26	0/1/1/1
6	FUC	A	220	6	-	0/0/17/20	0/1/1/1
5	NAG	B	248	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	249	5	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	214	NAG	C1-C2	2.01	1.55	1.52
4	A	217	FUC	C4-C3	2.09	1.57	1.52
4	A	216	BMA	C1-C2	2.33	1.57	1.52
6	A	218	NAG	C1-C2	2.83	1.56	1.52
4	A	216	BMA	C2-C3	2.86	1.56	1.52
6	A	220	FUC	C2-C3	2.98	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	217	FUC	C1-O5-C5	2.04	115.54	112.38
6	A	220	FUC	C6-C5-C4	2.90	118.79	113.08
6	A	220	FUC	C1-C2-C3	3.62	113.82	109.54
4	A	217	FUC	C3-C4-C5	3.63	115.83	109.72
4	A	217	FUC	C6-C5-C4	4.55	122.04	113.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	217	FUC	2	0
6	A	218	NAG	2	0

## 5.6 Ligand geometry ⓘ

4 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	$\# Z  > 2$
3	NAG	A	200	1	14,14,15	1.18	2 (14%)	15,19,21	0.80	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	SO4	B	250	-	4,4,4	1.18	1 (25%)	6,6,6	0.96	1 (16%)
7	SO4	B	251	-	4,4,4	0.86	0	6,6,6	0.50	0
7	SO4	B	252	-	4,4,4	0.75	0	6,6,6	0.99	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
3	NAG	A	200	1	-	0/6/23/26	0/1/1/1
7	SO4	B	250	-	-	0/0/0/0	0/0/0/0
7	SO4	B	251	-	-	0/0/0/0	0/0/0/0
7	SO4	B	252	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	250	SO4	O2-S	-2.17	1.39	1.47
3	A	200	NAG	C3-C2	2.41	1.58	1.52
3	A	200	NAG	C1-C2	3.35	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	250	SO4	O2-S-O1	-2.23	102.42	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	251	SO4	1	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.