



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:06 PM GMT

PDB ID : 1NFD
Title : AN ALPHA-BETA T CELL RECEPTOR (TCR) HETERODIMER IN COMPLEX WITH AN ANTI-TCR FAB FRAGMENT DERIVED FROM A MITOGENIC ANTIBODY
Authors : Wang, J.-H.; Lim, K.; Smolyar, A.; Teng, M.-K.; Sacchittini, J.; Reinherz, E.L.
Deposited on : 1997-08-04
Resolution : 2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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

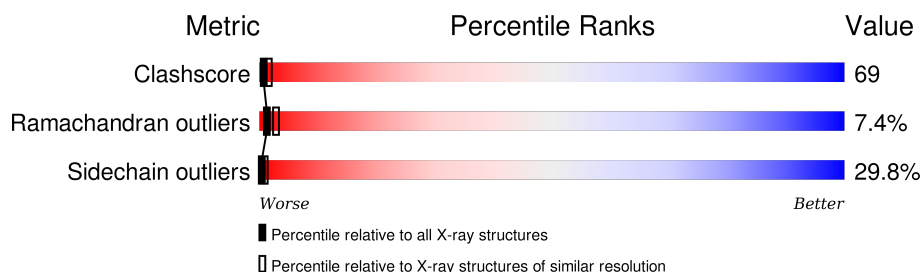
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

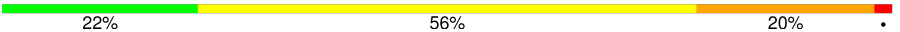
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey 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	203	
1	C	203	
2	B	239	
2	D	239	
3	E	212	
3	G	212	
4	F	222	

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Mol	Chain	Length	Quality of chain
4	H	222	

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
5	NAG	C	216	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13884 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 N15 ALPHA-BETA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1589	1002	259	320	8			
1	C	203	Total	C	N	O	S	0	0	0
			1589	1002	259	320	8			

- Molecule 2 is a protein called N15 ALPHA-BETA T-CELL RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	239	Total	C	N	O	S	0	0	0
			1926	1218	338	362	8			
2	D	239	Total	C	N	O	S	0	0	0
			1926	1218	338	362	8			

- Molecule 3 is a protein called H57 FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	212	Total	C	N	O	S	0	0	0
			1618	1012	269	330	7			
3	G	212	Total	C	N	O	S	0	0	0
			1618	1012	269	330	7			

- Molecule 4 is a protein called H57 FAB.

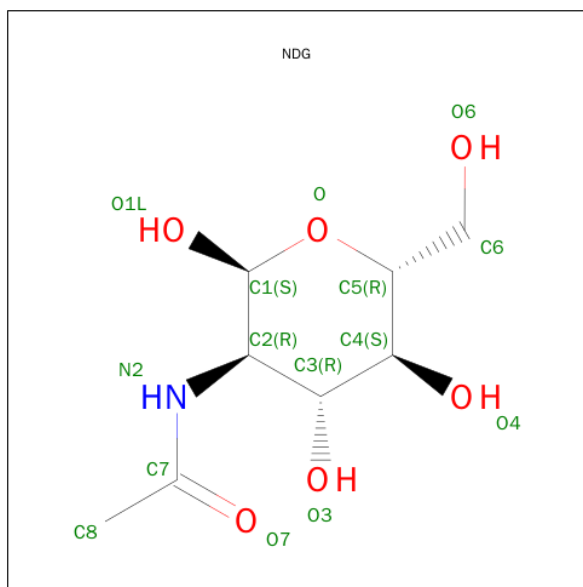
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	222	Total	C	N	O	S	0	0	0
			1711	1081	289	333	8			
4	H	222	Total	C	N	O	S	0	0	0
			1711	1081	289	333	8			

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

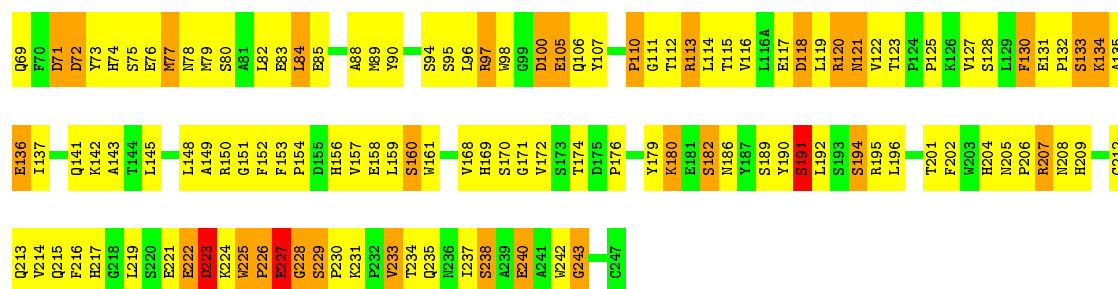


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1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

- Molecule 6 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).

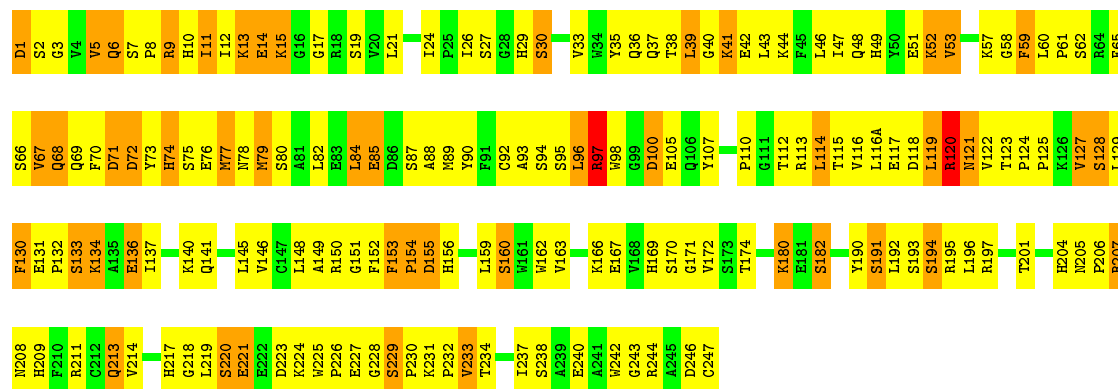


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		



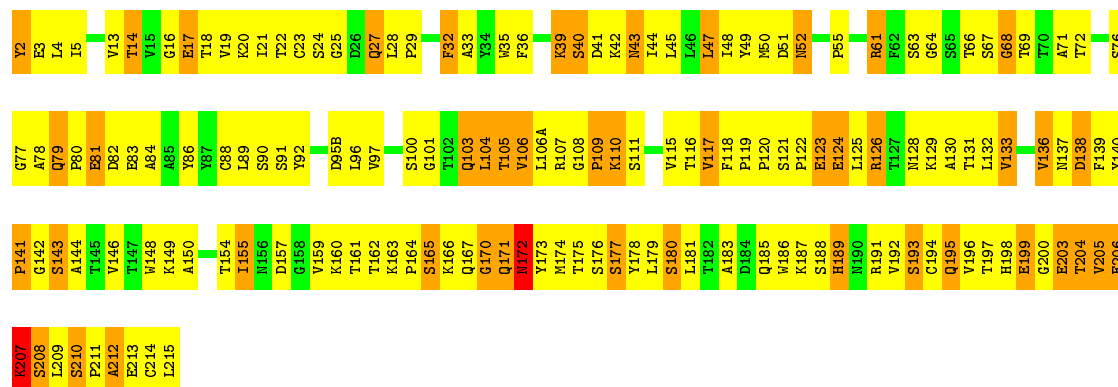
• Molecule 2: N15 ALPHA-BETA T-CELL RECEPTOR

Chain D: 27% 52% 20%



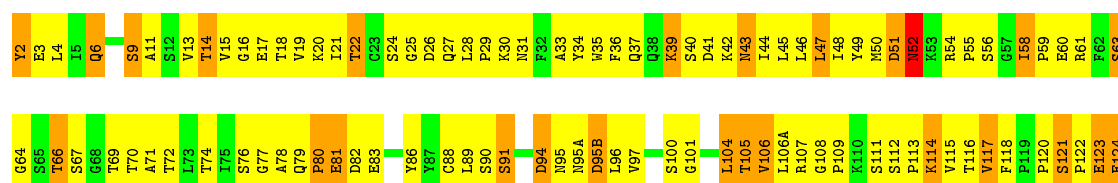
• Molecule 3: H57 FAB

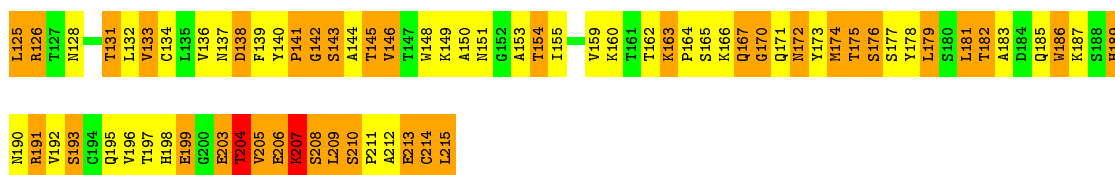
Chain E: 25% 53% 22%



• Molecule 3: H57 FAB

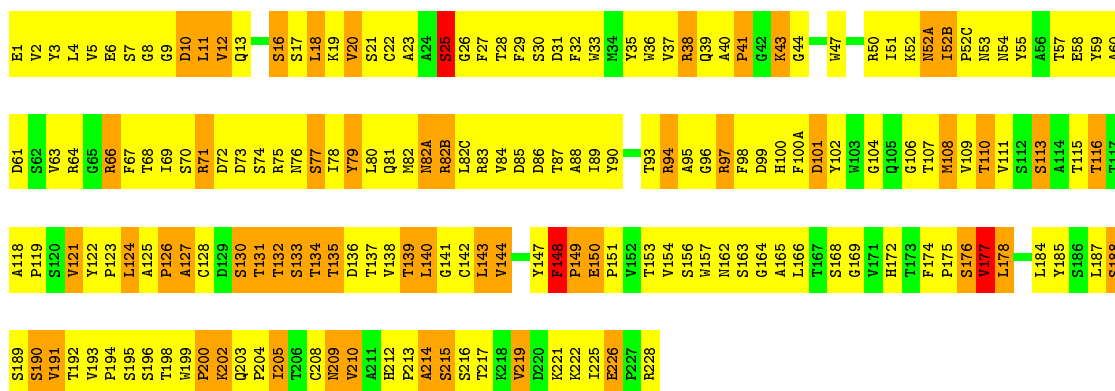
Chain G: 19% 51% 28%





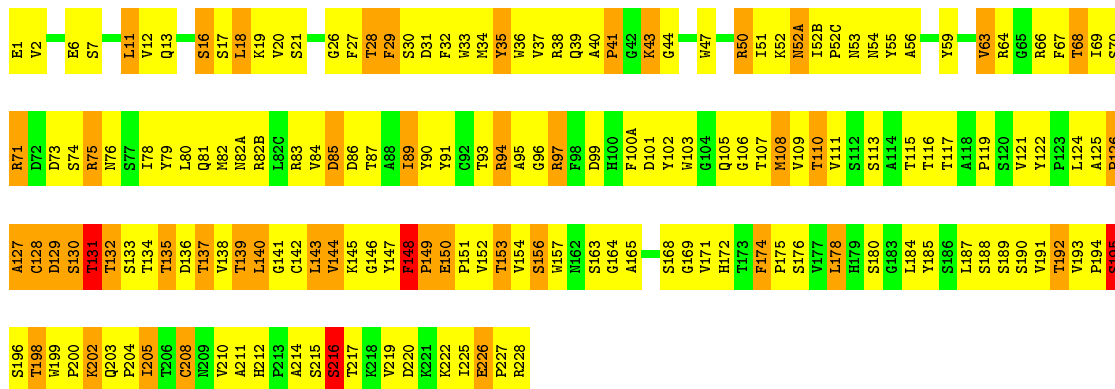
• Molecule 4: H57 FAB

Chain F: 16% 58% 24%



• Molecule 4: H57 FAB

Chain H: 22% 56% 20%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.74Å 122.30Å 115.84Å 90.00° 107.95° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	73.5 (15.00-2.80)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.243 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

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, NDG

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	0.37	0/1625	0.66	0/2208
1	C	0.37	0/1625	0.64	2/2208 (0.1%)
2	B	0.74	1/1981 (0.1%)	0.60	0/2683
2	D	0.77	1/1981 (0.1%)	0.62	0/2683
3	E	0.32	0/1653	0.57	0/2249
3	G	0.29	0/1653	0.55	0/2249
4	F	0.30	0/1759	0.56	0/2404
4	H	0.31	0/1759	0.60	0/2404
All	All	0.49	2/14036 (0.0%)	0.60	2/19088 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	191	SER	CB-OG	30.51	1.81	1.42
2	B	191	SER	CB-OG	28.96	1.79	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	ASN	N-CA-CB	5.92	121.26	110.60
1	C	203	ASN	CB-CG-ND2	5.45	129.78	116.70

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	1589	0	1526	241	1
1	C	1589	0	1525	163	0
2	B	1926	0	1835	249	2
2	D	1926	0	1836	257	1
3	E	1618	0	1576	269	0
3	G	1618	0	1576	258	0
4	F	1711	0	1647	294	0
4	H	1711	0	1647	283	2
5	A	42	0	39	4	0
5	B	42	0	39	4	0
5	C	14	0	11	3	0
5	D	56	0	52	3	0
6	B	14	0	13	3	0
6	C	28	0	26	2	0
All	All	13884	0	13348	1890	3

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 69.

The worst 5 of 1890 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:E:117:VAL:HG22	3:E:209:LEU:CD2	1.55	1.35
1:A:34:TRP:HD1	1:A:73:PHE:CE1	1.44	1.34
3:E:165:SER:HB2	3:E:173:TYR:CD1	1.66	1.30
1:A:34:TRP:CD1	1:A:73:PHE:HE1	1.49	1.29
1:A:34:TRP:CD1	1:A:73:PHE:CE1	2.21	1.29

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:CYS:O	2:D:57:LYS:NZ[2_546]	2.01	0.19
2:B:53:VAL:O	4:H:70:SER:OG[2_656]	2.09	0.11
2:B:55:ARG:NH2	4:H:19:LYS:NZ[2_656]	2.16	0.04

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	201/203 (99%)	156 (78%)	33 (16%)	12 (6%)	2	5
1	C	201/203 (99%)	162 (81%)	23 (11%)	16 (8%)	1	2
2	B	237/239 (99%)	198 (84%)	25 (10%)	14 (6%)	2	5
2	D	237/239 (99%)	195 (82%)	30 (13%)	12 (5%)	2	8
3	E	210/212 (99%)	159 (76%)	35 (17%)	16 (8%)	1	2
3	G	210/212 (99%)	158 (75%)	33 (16%)	19 (9%)	1	2
4	F	220/222 (99%)	160 (73%)	39 (18%)	21 (10%)	1	1
4	H	220/222 (99%)	170 (77%)	32 (14%)	18 (8%)	1	2
All	All	1736/1752 (99%)	1358 (78%)	250 (14%)	128 (7%)	1	3

5 of 128 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	134	ARG
1	A	204	ALA
2	B	39	LEU
1	C	53	ASN

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	181/181 (100%)	127 (70%)	54 (30%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	181/181 (100%)	118 (65%)	63 (35%)	0	0
2	B	212/212 (100%)	151 (71%)	61 (29%)	0	1
2	D	212/212 (100%)	147 (69%)	65 (31%)	0	1
3	E	185/185 (100%)	137 (74%)	48 (26%)	0	2
3	G	185/185 (100%)	122 (66%)	63 (34%)	0	0
4	F	192/192 (100%)	135 (70%)	57 (30%)	0	1
4	H	192/192 (100%)	144 (75%)	48 (25%)	1	2
All	All	1540/1540 (100%)	1081 (70%)	459 (30%)	0	1

5 of 459 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	87	SER
3	E	79	GLN
4	H	71	ARG
2	D	114	LEU
2	D	207	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 46 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	37	GLN
2	D	156	HIS
3	G	195	GLN
2	D	48	GLN
2	D	68	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	NAG	A	214	1	14,14,15	1.07	1 (7%)	15,19,21	1.14	1 (6%)
5	NAG	A	215	1	14,14,15	0.40	0	15,19,21	0.69	1 (6%)
5	NAG	A	216	1	14,14,15	0.52	0	15,19,21	0.79	1 (6%)
6	NDG	B	248	2	14,14,15	0.45	0	15,19,21	0.84	1 (6%)
5	NAG	B	249	2	14,14,15	0.35	0	15,19,21	0.88	0
5	NAG	B	250	2	14,14,15	0.39	0	15,19,21	0.91	1 (6%)
5	NAG	B	251	2	14,14,15	0.50	0	15,19,21	0.68	0
6	NDG	C	214	1	14,14,15	0.43	0	15,19,21	0.67	0
6	NDG	C	215	1	14,14,15	0.42	0	15,19,21	0.65	1 (6%)
5	NAG	C	216	1	14,14,15	4.44	6 (42%)	15,19,21	1.74	4 (26%)
5	NAG	D	248	2	14,14,15	0.38	0	15,19,21	0.58	0
5	NAG	D	249	2	14,14,15	0.52	0	15,19,21	0.71	0
5	NAG	D	250	2	14,14,15	0.42	0	15,19,21	0.63	0
5	NAG	D	251	2	14,14,15	0.49	0	15,19,21	0.71	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	214	1	-	0/6/23/26	0/1/1/1
5	NAG	A	215	1	-	0/6/23/26	0/1/1/1
5	NAG	A	216	1	-	0/6/23/26	0/1/1/1
6	NDG	B	248	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	249	2	-	0/6/23/26	0/1/1/1
5	NAG	B	250	2	-	0/6/23/26	0/1/1/1
5	NAG	B	251	2	-	0/6/23/26	0/1/1/1
6	NDG	C	214	1	-	0/6/23/26	0/1/1/1
6	NDG	C	215	1	-	0/6/23/26	0/1/1/1
5	NAG	C	216	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	D	248	2	-	0/6/23/26	0/1/1/1
5	NAG	D	249	2	-	0/6/23/26	0/1/1/1
5	NAG	D	250	2	-	0/6/23/26	0/1/1/1
5	NAG	D	251	2	-	0/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	216	NAG	C1-C2	-11.61	1.36	1.52
5	C	216	NAG	C4-C5	-5.59	1.41	1.53
5	C	216	NAG	C3-C2	-3.40	1.44	1.52
5	C	216	NAG	O7-C7	-2.69	1.17	1.23
5	A	214	NAG	O5-C1	2.87	1.48	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	214	NAG	C2-N2-C7	-3.44	118.62	123.04
5	C	216	NAG	C1-O5-C5	-2.85	108.63	112.25
5	B	250	NAG	C2-N2-C7	-2.84	119.39	123.04
6	B	248	NDG	C2-N2-C7	-2.59	119.71	123.04
5	A	215	NAG	C2-N2-C7	-2.38	119.98	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	C	216	NAG	C1

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	214	NAG	2	0
5	A	216	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	248	NDG	3	0
5	B	249	NAG	3	0
5	B	251	NAG	1	0
6	C	214	NDG	2	0
5	C	216	NAG	3	0
5	D	248	NAG	2	0
5	D	249	NAG	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 ⓘ

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

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

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

6.3 Carbohydrates ⓘ

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

6.4 Ligands ⓘ

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

6.5 Other polymers ⓘ

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