



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 23, 2022 – 10:06 AM EST

PDB ID : 7SU0
Title : Crystal structure of an acidic pH-selective Ipilimumab variant Ipi.105 in complex with CTLA-4
Authors : Lee, P.S.; Chau, B.; Strop, P.
Deposited on : 2021-11-15
Resolution : 2.41 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.26
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) : 2.26

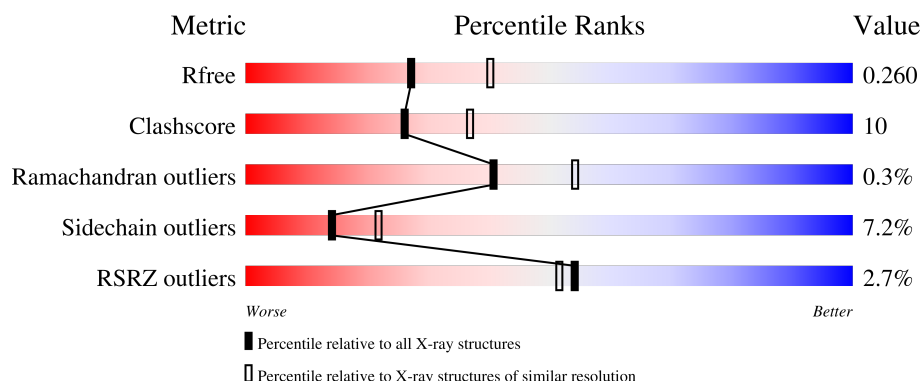
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 ≥ 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	C	125	<div> <div>5%</div> <div> <div>66%</div> <div>23%</div> <div>6%</div> </div> </div>
1	D	125	<div> <div>3%</div> <div> <div>66%</div> <div>22%</div> <div>7%</div> </div> </div>
2	H	229	<div> <div>71%</div> <div>21%</div> <div>7%</div> </div>
2	I	229	<div> <div>2%</div> <div> <div>68%</div> <div>24%</div> <div>8%</div> </div> </div>
3	L	215	<div> <div>80%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	215	<div><div></div><div>6%</div><div>70%</div><div>22%</div><div>6% ..</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8347 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 Cytotoxic T-lymphocyte protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	117	Total	C	N	O	S	0	0	0
			873	549	143	172	9			
1	D	116	Total	C	N	O	S	0	0	0
			865	545	142	169	9			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	119	GLY	-	expression tag	UNP P16410
C	120	HIS	-	expression tag	UNP P16410
C	121	HIS	-	expression tag	UNP P16410
C	122	HIS	-	expression tag	UNP P16410
C	123	HIS	-	expression tag	UNP P16410
C	124	HIS	-	expression tag	UNP P16410
C	125	HIS	-	expression tag	UNP P16410
D	119	GLY	-	expression tag	UNP P16410
D	120	HIS	-	expression tag	UNP P16410
D	121	HIS	-	expression tag	UNP P16410
D	122	HIS	-	expression tag	UNP P16410
D	123	HIS	-	expression tag	UNP P16410
D	124	HIS	-	expression tag	UNP P16410
D	125	HIS	-	expression tag	UNP P16410

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1619	1029	275	309	6			
2	I	210	Total	C	N	O	S	0	0	0
			1607	1023	273	305	6			

- Molecule 3 is a protein called Fab light chain.

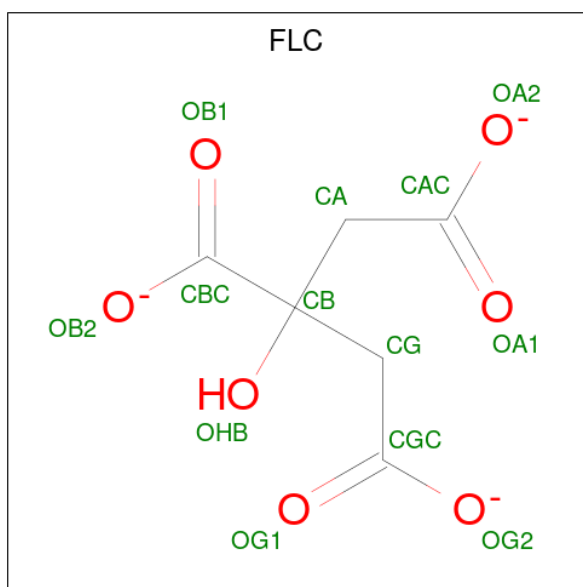
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1649	1033	278	334	4			
3	M	212	Total	C	N	O	S	0	0	0
			1636	1026	276	330	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total	C	O	0	0
			13	6	7		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			7	4	3		

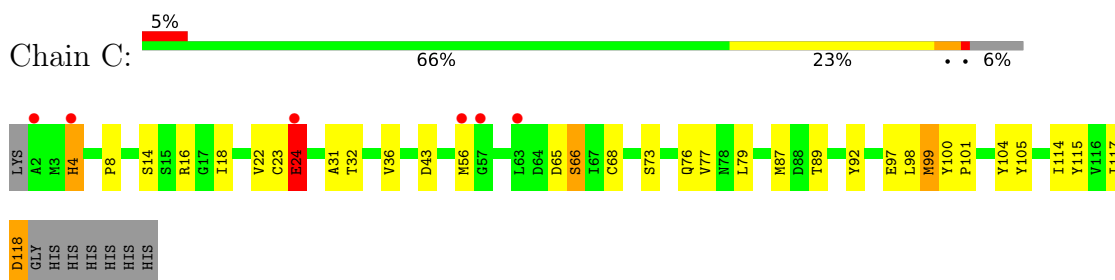
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	O 1	0	0
7	H	7	Total 7	O 7	0	0
7	L	15	Total 15	O 15	0	0
7	I	7	Total 7	O 7	0	0
7	M	6	Total 6	O 6	0	0

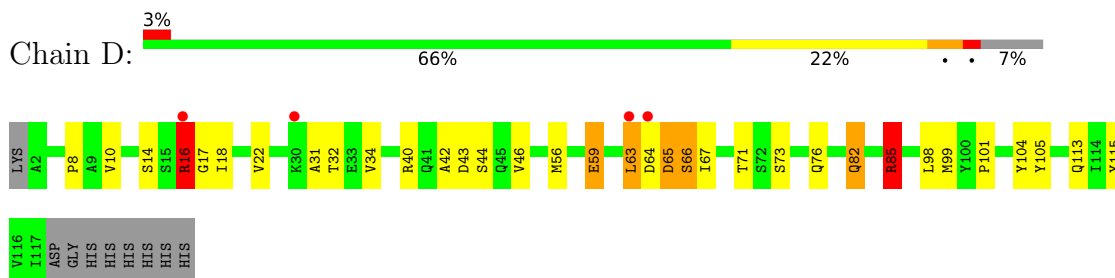
3 Residue-property plots

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.

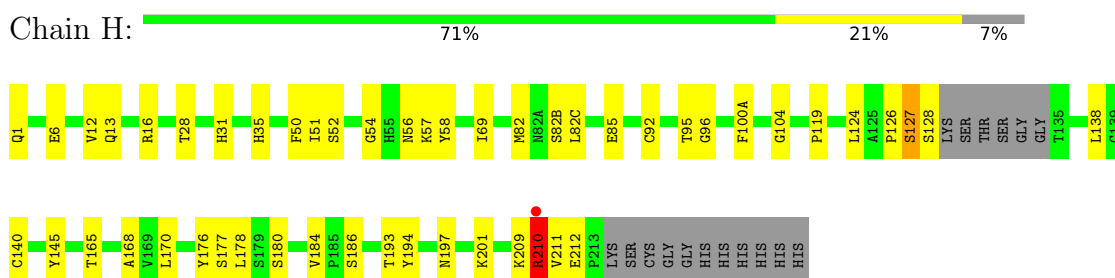
• Molecule 1: Cytotoxic T-lymphocyte protein 4



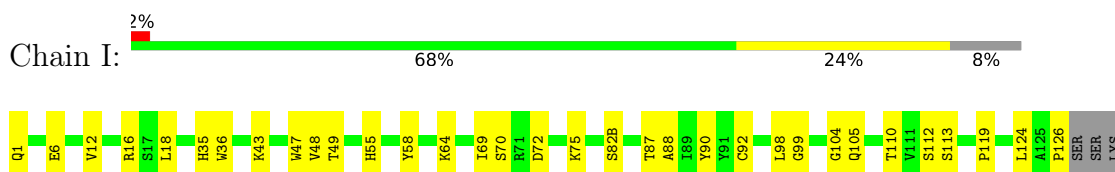
• Molecule 1: Cytotoxic T-lymphocyte protein 4

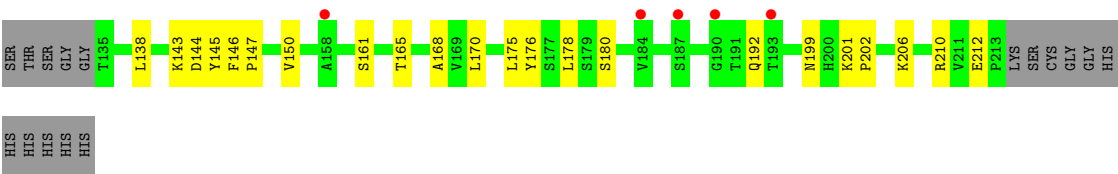


• Molecule 2: Fab heavy chain

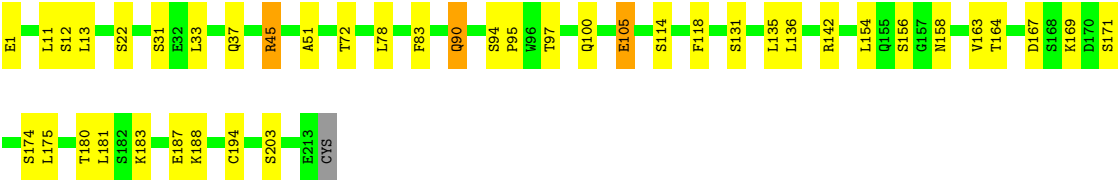
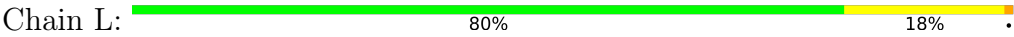


• Molecule 2: Fab heavy chain

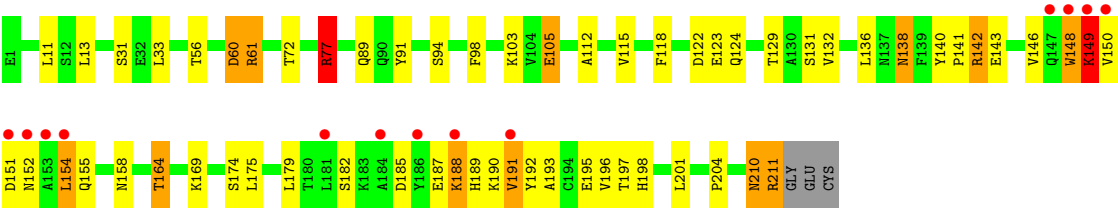




● Molecule 3: Fab light chain



● Molecule 3: Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	96.73Å 197.84Å 146.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.36 – 2.41 36.36 – 2.41	Depositor EDS
% Data completeness (in resolution range)	69.9 (36.36-2.41) 69.9 (36.36-2.41)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.206 , 0.264 0.203 , 0.260	Depositor DCC
R_{free} test set	1906 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 29.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8347	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PCA, FLC, 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	C	0.59	1/887 (0.1%)	0.80	4/1208 (0.3%)
1	D	0.49	0/879	0.84	2/1197 (0.2%)
2	H	0.53	1/1656 (0.1%)	0.79	4/2260 (0.2%)
2	I	0.43	0/1644	0.67	0/2244
3	L	0.53	1/1686 (0.1%)	0.70	1/2289 (0.0%)
3	M	0.52	0/1673	0.79	3/2272 (0.1%)
All	All	0.51	3/8425 (0.0%)	0.76	14/11470 (0.1%)

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
1	C	0	1
1	D	0	2
2	H	0	1
3	M	0	3
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	210	ARG	CG-CD	-8.81	1.29	1.51
1	C	24	GLU	CD-OE2	7.02	1.33	1.25
3	L	194	CYS	CB-SG	-6.20	1.71	1.82

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	210	ARG	CA-CB-CG	-14.10	82.38	113.40
2	H	210	ARG	CG-CD-NE	10.21	133.25	111.80
1	D	16	ARG	CG-CD-NE	-9.58	91.69	111.80
3	M	149	LYS	CA-CB-CG	7.30	129.46	113.40
3	M	149	LYS	CD-CE-NZ	-6.92	95.78	111.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	24	GLU	Sidechain
1	D	16	ARG	Sidechain
1	D	85	ARG	Sidechain
2	H	210	ARG	Sidechain
3	M	77	ARG	Sidechain

5.2 Too-close contacts

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	C	873	0	860	20	0
1	D	865	0	857	18	0
2	H	1619	0	1570	35	0
2	I	1607	0	1560	33	0
3	L	1649	0	1593	23	0
3	M	1636	0	1584	49	0
4	C	28	0	26	2	0
4	D	14	0	13	0	0
5	I	13	0	5	2	0
6	M	7	0	10	0	0
7	C	1	0	0	0	0
7	H	7	0	0	0	0
7	I	7	0	0	0	0
7	L	15	0	0	1	0
7	M	6	0	0	0	0
All	All	8347	0	8078	170	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 10.

The worst 5 of 170 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:H:193:THR:HB	2:H:210:ARG:NH1	1.81	0.95
1:C:24:GLU:HB2	1:C:76:GLN:HA	1.44	0.94
2:H:13:GLN:OE1	2:H:16:ARG:NH1	2.05	0.88
1:C:24:GLU:OE1	1:C:76:GLN:HB2	1.76	0.86
3:L:164:THR:HG22	3:L:174:SER:H	1.43	0.84

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	C	115/125 (92%)	108 (94%)	5 (4%)	2 (2%)	9	11
1	D	114/125 (91%)	108 (95%)	5 (4%)	1 (1%)	17	24
2	H	208/229 (91%)	196 (94%)	12 (6%)	0	100	100
2	I	206/229 (90%)	197 (96%)	9 (4%)	0	100	100
3	L	212/215 (99%)	203 (96%)	9 (4%)	0	100	100
3	M	210/215 (98%)	196 (93%)	14 (7%)	0	100	100
All	All	1065/1138 (94%)	1008 (95%)	54 (5%)	3 (0%)	41	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	65	ASP
1	D	43	ASP
1	C	43	ASP

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	C	96/103 (93%)	89 (93%)	7 (7%)	14	21
1	D	95/103 (92%)	83 (87%)	12 (13%)	4	5
2	H	179/192 (93%)	171 (96%)	8 (4%)	27	42
2	I	177/192 (92%)	168 (95%)	9 (5%)	24	37
3	L	184/185 (100%)	172 (94%)	12 (6%)	17	26
3	M	183/185 (99%)	165 (90%)	18 (10%)	8	11
All	All	914/960 (95%)	848 (93%)	66 (7%)	14	22

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	M	138	ASN
3	M	149	LYS
3	M	210	ASN
3	L	131	SER
3	L	114	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	31	HIS
2	I	105	GLN
2	I	199	ASN
3	M	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
2	PCA	I	1	2	7,8,9	1.78	1 (14%)	9,10,12	2.28	5 (55%)
2	PCA	H	1	2	7,8,9	1.90	1 (14%)	9,10,12	2.10	4 (44%)

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
2	PCA	I	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	4.73	1.47	1.34
2	I	1	PCA	CD-N	4.49	1.46	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-3.51	101.57	113.58
2	I	1	PCA	CA-N-CD	-3.44	101.80	113.58
2	H	1	PCA	CB-CA-N	3.10	112.20	103.30
2	I	1	PCA	CB-CA-N	2.84	111.44	103.30
2	I	1	PCA	CB-CA-C	-2.83	108.81	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	FLC	I	301	-	3,12,12	1.13	0	3,17,17	2.02	1 (33%)
6	PEG	M	301	-	6,6,6	0.66	0	5,5,5	0.49	0
4	NAG	C	202	1	14,14,15	0.82	1 (7%)	17,19,21	0.51	0
4	NAG	C	201	1	14,14,15	0.98	1 (7%)	17,19,21	0.89	1 (5%)
4	NAG	D	201	1	14,14,15	0.48	0	17,19,21	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	FLC	I	301	-	-	3/6/16/16	-
6	PEG	M	301	-	-	2/4/4/4	-
4	NAG	C	202	1	-	0/6/23/26	0/1/1/1
4	NAG	C	201	1	-	2/6/23/26	0/1/1/1
4	NAG	D	201	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	NAG	O5-C1	3.47	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	202	NAG	O5-C1	2.27	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	301	FLC	CB-CG-CGC	-3.34	109.64	114.98
4	C	201	NAG	C1-O5-C5	2.62	115.74	112.19

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	NAG	C4-C5-C6-O6
4	D	201	NAG	O5-C5-C6-O6
4	C	201	NAG	O5-C5-C6-O6
4	D	201	NAG	C4-C5-C6-O6
6	M	301	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	301	FLC	2	0
4	C	202	NAG	2	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 [i](#)

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

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, 95th 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 ²)	Q<0.9
1	C	117/125 (93%)	0.11	6 (5%) 28 26	35, 50, 89, 110	0
1	D	116/125 (92%)	0.05	4 (3%) 45 43	30, 49, 80, 115	0
2	H	211/229 (92%)	-0.38	1 (0%) 91 89	27, 38, 56, 88	0
2	I	209/229 (91%)	-0.07	5 (2%) 59 56	26, 45, 71, 88	0
3	L	214/215 (99%)	-0.57	0 100 100	24, 35, 47, 59	0
3	M	212/215 (98%)	-0.02	13 (6%) 21 19	23, 47, 88, 108	0
All	All	1079/1138 (94%)	-0.19	29 (2%) 54 52	23, 41, 80, 115	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	154	LEU	7.7
3	M	149	LYS	6.0
1	D	63	LEU	4.8
1	C	63	LEU	4.3
2	I	187	SER	4.2

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
2	PCA	H	1	8/9	0.92	0.14	45,51,61,66	0
2	PCA	I	1	8/9	0.92	0.22	48,52,55,58	0

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, 95th 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(\AA^2)	Q<0.9
5	FLC	I	301	13/13	0.88	0.15	58,68,75,76	0
4	NAG	C	201	14/15	0.90	0.27	54,60,67,73	0
6	PEG	M	301	7/7	0.90	0.16	33,36,37,38	0
4	NAG	C	202	14/15	0.92	0.13	52,62,67,73	0
4	NAG	D	201	14/15	0.94	0.20	48,50,54,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.