



# Full wwPDB X-ray Structure Validation 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
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

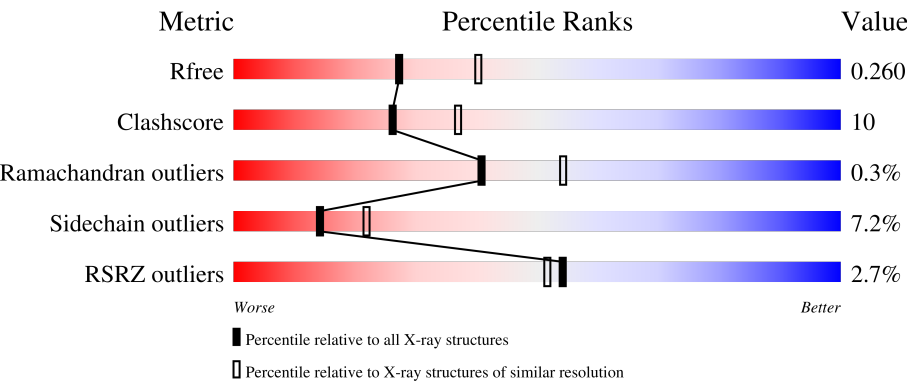
# 1 Overall quality at a glance i

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 <sub>free</sub>	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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	125	<div><div>5%</div><div><div></div><div>66%</div><div>23%</div><div>• • 6%</div></div></div>
1	D	125	<div><div>3%</div><div><div></div><div>66%</div><div>22%</div><div>• • 7%</div></div></div>
2	H	229	<div><div></div><div><div></div><div>71%</div><div>21%</div><div>7%</div></div></div>
2	I	229	<div><div>2%</div><div><div></div><div>68%</div><div>24%</div><div>8%</div></div></div>
3	L	215	<div><div></div><div><div></div><div>80%</div><div>18%</div><div>•</div></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.

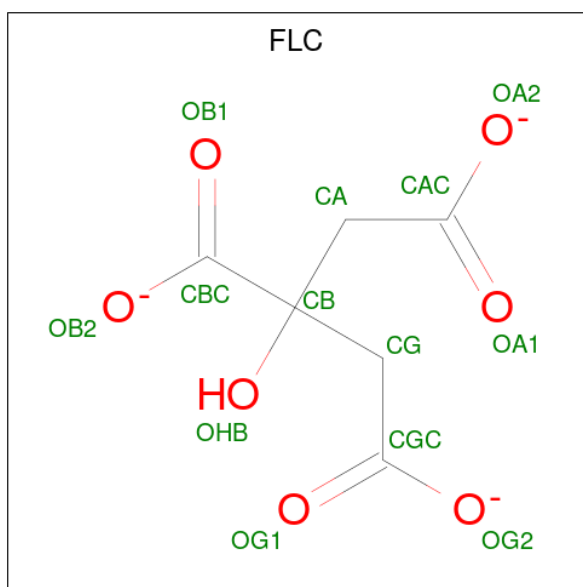
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1649	1033	278	334	4			
3	M	212	Total	C	N	O	S	0	0	0
			1636	1026	276	330	4			

- 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:  $C_4H_{10}O_3$ ).



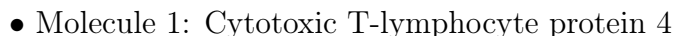
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	M	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is water.

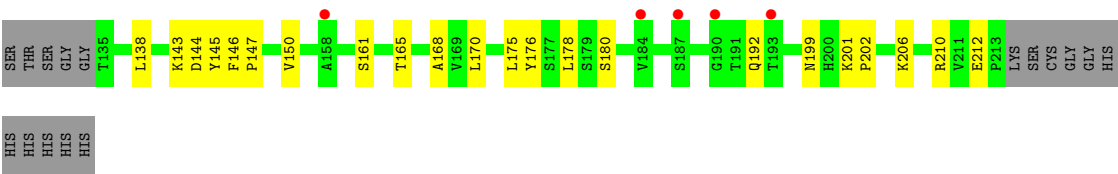
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	O 1	0	0
7	H	7	Total 7	O 7	0	0
7	L	15	Total 15	O 15	0	0
7	I	7	Total 7	O 7	0	0
7	M	6	Total 6	O 6	0	0



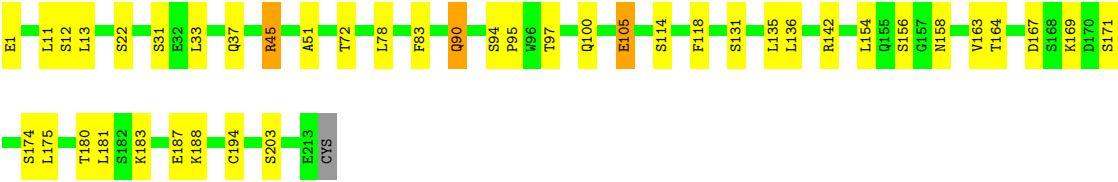
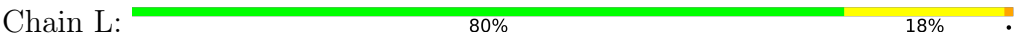
- Molecule 1: Cytotoxic T-lymphocyte protein 4



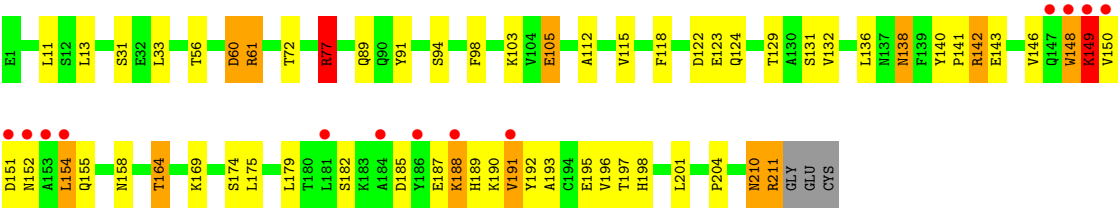




● Molecule 3: Fab light chain



● 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	48.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 29.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 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

All (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
3	L	154	LEU	CA-CB-CG	6.71	130.73	115.30
3	M	154	LEU	CB-CG-CD2	-6.49	99.96	111.00
2	H	210	ARG	CB-CG-CD	6.29	127.96	111.60
1	C	4	HIS	CB-CA-C	-6.17	98.06	110.40
1	D	16	ARG	CB-CG-CD	6.13	127.54	111.60
1	C	4	HIS	N-CA-CB	5.94	121.29	110.60
1	C	24	GLU	OE1-CD-OE2	-5.61	116.56	123.30
2	H	210	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	99	MET	CA-CB-CG	-5.19	104.48	113.30

There are no chirality outliers.

All (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	148	TRP	Peptide
3	M	211	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
3:M:150:VAL:HB	3:M:155:GLN:HE21	1.46	0.81
3:M:77:ARG:O	3:M:77:ARG:HG2	1.81	0.80
3:M:115:VAL:HG21	3:M:196:VAL:HG21	1.63	0.80
3:L:37:GLN:OE1	3:L:45:ARG:NH1	2.15	0.78
2:H:193:THR:HB	2:H:210:ARG:HH11	1.50	0.77
3:M:132:VAL:HG23	3:M:179:LEU:HB3	1.66	0.77
3:M:151:ASP:HA	3:M:191:VAL:HG23	1.68	0.74
3:M:187:GLU:O	3:M:211:ARG:NH2	2.21	0.74
3:L:163:VAL:HG22	3:L:175:LEU:HD12	1.68	0.73
1:D:31:ALA:HA	1:D:101:PRO:HD2	1.68	0.73
1:C:89:THR:HG23	1:C:115:TYR:HA	1.72	0.72
3:M:61:ARG:HG2	3:M:77:ARG:HH11	1.55	0.71
1:D:98:LEU:HD12	1:D:105:TYR:HB2	1.71	0.71
1:D:99:MET:O	2:I:58:TYR:OH	2.09	0.71
2:I:199:ASN:HD21	2:I:206:LYS:HE3	1.57	0.70
3:M:164:THR:HG22	3:M:174:SER:H	1.58	0.69
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.74	0.68
1:C:31:ALA:HA	1:C:101:PRO:HD2	1.74	0.68
2:H:210:ARG:CG	2:H:211:VAL:N	2.57	0.67
2:I:126:PRO:HG3	2:I:138:LEU:HB3	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:48:VAL:HG12	2:I:49:THR:HG22	1.78	0.66
3:L:167:ASP:OD1	3:L:169:LYS:HE3	1.97	0.65
2:I:199:ASN:ND2	2:I:206:LYS:HE3	2.10	0.65
5:I:301:FLC:OA1	3:M:56:THR:HG23	1.97	0.65
2:H:210:ARG:HG3	2:H:211:VAL:N	2.07	0.65
1:C:66:SER:HB3	1:C:68:CYS:H	1.61	0.64
3:M:211:ARG:HG3	3:M:211:ARG:HH11	1.64	0.63
3:M:182:SER:HB2	3:M:185:ASP:HB3	1.80	0.62
2:H:127:SER:OG	2:H:128:SER:N	2.32	0.62
3:M:11:LEU:HD13	3:M:13:LEU:HD11	1.80	0.62
1:D:85:ARG:HH21	1:D:85:ARG:HB2	1.65	0.61
2:I:119:PRO:HB3	2:I:145:TYR:HB3	1.81	0.61
1:C:14:SER:HB3	1:C:18:ILE:H	1.64	0.61
1:C:24:GLU:HB2	1:C:76:GLN:CA	2.27	0.61
1:C:77:VAL:HG12	1:C:79:LEU:HG	1.82	0.60
3:M:149:LYS:HB2	3:M:193:ALA:O	2.00	0.60
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.84	0.60
2:I:168:ALA:HA	2:I:178:LEU:HB3	1.83	0.59
1:C:92:TYR:CD1	1:C:114:ILE:HD12	2.38	0.59
1:C:24:GLU:OE1	1:C:76:GLN:NE2	2.37	0.58
3:M:103:LYS:HE2	3:M:105:GLU:HB3	1.85	0.58
1:C:32:THR:HA	1:C:56:MET:HB2	1.87	0.57
3:M:124:GLN:HG2	3:M:129:THR:O	2.04	0.57
1:C:99:MET:O	2:H:58:TYR:OH	2.22	0.57
2:H:12:VAL:HG11	2:H:82(C):LEU:HD12	1.87	0.56
1:D:64:ASP:HB2	1:D:66:SER:HB2	1.87	0.55
3:M:138:ASN:HD22	3:M:138:ASN:N	2.03	0.55
1:C:100:TYR:CD1	1:C:101:PRO:HA	2.42	0.55
2:H:35:HIS:CE1	2:H:50:PHE:HD2	2.24	0.55
3:L:142:ARG:HH11	3:L:142:ARG:HG2	1.70	0.54
2:H:210:ARG:NH2	2:H:212:GLU:HG2	2.23	0.54
2:I:36:TRP:HD1	2:I:69:ILE:HD12	1.73	0.54
2:H:85:GLU:OE1	2:H:85:GLU:N	2.40	0.54
2:I:210:ARG:HD3	2:I:212:GLU:OE2	2.08	0.54
2:I:12:VAL:HG13	2:I:16:ARG:HB3	1.90	0.53
1:D:8:PRO:HD3	1:D:22:VAL:O	2.08	0.53
2:H:57:LYS:HD3	2:H:69:ILE:O	2.08	0.53
2:H:52:SER:HB3	2:H:56:ASN:HB2	1.89	0.53
3:L:156:SER:HG	2:I:55:HIS:HE2	1.56	0.52
3:M:182:SER:HB3	3:M:185:ASP:H	1.74	0.52
3:L:142:ARG:HG2	3:L:142:ARG:NH1	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:61:ARG:HG2	3:M:77:ARG:NH1	2.23	0.52
3:M:155:GLN:HB3	3:M:158:ASN:OD1	2.09	0.52
3:M:182:SER:HB2	3:M:185:ASP:CB	2.40	0.52
3:M:60:ASP:N	3:M:60:ASP:OD1	2.43	0.52
2:I:144:ASP:HB3	2:I:175:LEU:HD13	1.91	0.51
2:H:210:ARG:HG2	2:H:211:VAL:N	2.25	0.51
3:L:31:SER:HB3	3:L:51:ALA:HB2	1.92	0.51
3:M:131:SER:HA	3:M:179:LEU:O	2.11	0.51
1:D:10:VAL:HG23	1:D:113:GLN:HB3	1.93	0.50
2:H:193:THR:HB	2:H:210:ARG:HH12	1.74	0.50
2:H:210:ARG:HG3	2:H:211:VAL:H	1.77	0.50
2:I:6:GLU:H	2:I:105:GLN:NE2	2.09	0.50
1:D:104:TYR:HB3	3:M:94:SER:HB3	1.94	0.49
2:I:165:THR:HG23	2:I:180:SER:HB2	1.94	0.49
2:I:35:HIS:HD1	2:I:47:TRP:HE1	1.59	0.49
2:I:72:ASP:OD2	2:I:75:LYS:HG3	2.13	0.49
3:M:140:TYR:CG	3:M:141:PRO:HA	2.47	0.49
3:L:164:THR:CG2	3:L:174:SER:H	2.19	0.49
3:M:138:ASN:HD22	3:M:138:ASN:H	1.60	0.49
3:M:132:VAL:CG2	3:M:179:LEU:HB3	2.38	0.49
3:M:89:GLN:HB2	3:M:98:PHE:CD1	2.48	0.49
2:H:124:LEU:HB3	3:L:118:PHE:CD2	2.48	0.49
2:H:95:THR:HG22	2:H:96:GLY:O	2.12	0.48
3:M:151:ASP:HA	3:M:191:VAL:CG2	2.40	0.48
1:C:98:LEU:HD12	1:C:105:TYR:HB2	1.95	0.48
3:L:78:LEU:HD13	3:L:83:PHE:CZ	2.49	0.48
3:L:12:SER:OG	3:L:105:GLU:OE2	2.30	0.47
3:L:156:SER:OG	2:I:55:HIS:NE2	2.44	0.47
3:M:143:GLU:O	3:M:198:HIS:HD2	1.97	0.47
1:D:67:ILE:O	1:D:82:GLN:HG2	2.15	0.47
3:M:151:ASP:OD2	3:M:189:HIS:HA	2.15	0.47
1:D:59:GLU:OE2	1:D:71:THR:HA	2.15	0.47
1:D:63:LEU:C	1:D:65:ASP:H	2.19	0.46
2:H:165:THR:HG23	2:H:180:SER:HB2	1.98	0.46
3:M:148:TRP:CE2	3:M:179:LEU:HB2	2.51	0.46
3:L:183:LYS:O	3:L:187:GLU:HG3	2.16	0.46
3:L:180:THR:O	3:L:181:LEU:HD23	2.16	0.46
1:C:4:HIS:HE2	4:C:202:NAG:H3	1.80	0.45
2:H:6:GLU:OE2	2:H:104:GLY:HA3	2.16	0.45
2:I:143:LYS:HG2	2:I:144:ASP:OD2	2.16	0.45
3:M:187:GLU:C	3:M:211:ARG:HH21	2.18	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:170:LEU:HD13	2:H:176:TYR:CE1	2.52	0.45
3:L:31:SER:HB3	3:L:51:ALA:CB	2.46	0.45
1:C:4:HIS:CE1	4:C:202:NAG:HN2	2.34	0.45
2:I:87:THR:HG23	2:I:110:THR:HA	1.98	0.45
2:I:168:ALA:HB2	2:I:178:LEU:HD23	1.97	0.45
1:C:117:ILE:HG23	1:C:118:ASP:N	2.32	0.45
2:H:138:LEU:HB2	2:H:211:VAL:HG11	1.99	0.44
2:I:88:ALA:HB3	2:I:90:TYR:CE1	2.52	0.44
2:I:199:ASN:OD1	2:I:201:LYS:HG3	2.16	0.44
2:H:124:LEU:HD12	2:H:140:CYS:N	2.32	0.44
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.99	0.44
2:H:28:THR:HB	2:H:31:HIS:HD2	1.82	0.44
3:L:11:LEU:HD22	3:L:13:LEU:HD11	1.99	0.44
3:M:146:VAL:HG23	3:M:196:VAL:HG12	1.99	0.44
3:M:190:LYS:HD2	3:M:210:ASN:OD1	2.18	0.44
1:D:32:THR:O	1:D:56:MET:N	2.44	0.44
2:H:85:GLU:CD	2:H:85:GLU:H	2.17	0.43
2:I:98:LEU:N	5:I:301:FLC:OG2	2.34	0.43
3:M:136:LEU:HD13	3:M:175:LEU:HD22	2.00	0.43
2:H:28:THR:HB	2:H:31:HIS:CD2	2.53	0.43
1:D:85:ARG:HH21	1:D:85:ARG:CB	2.29	0.43
2:I:18:LEU:HD12	2:I:18:LEU:HA	1.90	0.43
1:D:34:VAL:HG22	1:D:98:LEU:HD23	2.01	0.43
2:I:199:ASN:ND2	2:I:206:LYS:CE	2.80	0.43
2:I:99:GLY:HA3	3:M:91:TYR:CE1	2.54	0.43
3:M:150:VAL:HG22	3:M:192:TYR:CD2	2.54	0.43
3:L:158:ASN:OD1	3:L:158:ASN:N	2.51	0.42
2:I:12:VAL:CG1	2:I:16:ARG:HB3	2.49	0.42
2:I:170:LEU:HD13	2:I:176:TYR:CE1	2.53	0.42
3:M:185:ASP:HA	3:M:188:LYS:CE	2.49	0.42
2:H:51:ILE:HD11	2:H:54:GLY:HA2	1.99	0.42
2:H:100(A):PHE:N	2:H:100(A):PHE:CD1	2.88	0.42
2:H:126:PRO:HG3	2:H:138:LEU:HB3	2.00	0.42
3:L:90:GLN:HE21	3:L:90:GLN:HB3	1.70	0.42
3:L:95:PRO:O	3:L:97:THR:HG23	2.19	0.42
2:H:170:LEU:HD13	2:H:176:TYR:CZ	2.55	0.42
3:M:112:ALA:HB1	3:M:201:LEU:CD1	2.50	0.42
3:M:140:TYR:CD1	3:M:141:PRO:HA	2.54	0.42
2:H:165:THR:HA	2:H:180:SER:HA	2.02	0.42
2:I:124:LEU:HD22	3:M:118:PHE:HB3	2.02	0.42
2:I:147:PRO:HD2	2:I:202:PRO:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:187:GLU:HA	3:M:211:ARG:HH21	1.84	0.42
2:I:6:GLU:OE1	2:I:104:GLY:HA3	2.19	0.42
2:I:112:SER:HB3	2:I:146:PHE:CZ	2.56	0.41
1:D:17:GLY:C	1:D:18:ILE:HD13	2.40	0.41
3:M:182:SER:CB	3:M:185:ASP:H	2.33	0.41
1:D:113:GLN:HG2	1:D:115:TYR:CE2	2.55	0.41
1:C:8:PRO:HD3	1:C:22:VAL:O	2.20	0.41
3:M:197:THR:HG22	3:M:204:PRO:HB3	2.01	0.41
1:C:97:GLU:HG2	1:C:104:TYR:OH	2.21	0.41
1:D:42:ALA:O	1:D:44:SER:N	2.53	0.41
2:H:184:VAL:HG11	2:H:194:TYR:CE1	2.56	0.41
1:D:82:GLN:HG2	1:D:82:GLN:H	1.81	0.41
2:I:210:ARG:NH1	2:I:212:GLU:OE2	2.47	0.41
3:L:1:GLU:HA	7:L:312:HOH:O	2.21	0.41
3:L:188:LYS:HB2	3:L:188:LYS:HE3	1.94	0.41
3:M:11:LEU:HD23	3:M:11:LEU:HA	1.95	0.40
3:M:149:LYS:HD2	3:M:195:GLU:HB2	2.02	0.40
3:M:151:ASP:O	3:M:152:ASN:HB2	2.20	0.40
3:L:135:LEU:HD12	3:L:136:LEU:N	2.36	0.40
3:M:142:ARG:O	3:M:142:ARG:HG2	2.22	0.40
3:M:190:LYS:O	3:M:210:ASN:OD1	2.39	0.40
1:C:36:VAL:HG21	1:C:77:VAL:HG21	2.04	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	16	ARG
1	C	23	CYS
1	C	24	GLU
1	C	66	SER
1	C	73	SER

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Mol	Chain	Res	Type
1	C	87	MET
1	C	118	ASP
2	H	82(B)	SER
2	H	92	CYS
2	H	127	SER
2	H	177	SER
2	H	186	SER
2	H	197	ASN
2	H	201	LYS
2	H	209	LYS
3	L	22	SER
3	L	33	LEU
3	L	45	ARG
3	L	72	THR
3	L	90	GLN
3	L	94	SER
3	L	100	GLN
3	L	105	GLU
3	L	114	SER
3	L	131	SER
3	L	171	SER
3	L	203	SER
1	D	14	SER
1	D	16	ARG
1	D	40	ARG
1	D	46	VAL
1	D	59	GLU
1	D	63	LEU
1	D	65	ASP
1	D	66	SER
1	D	73	SER
1	D	76	GLN
1	D	82	GLN
1	D	85	ARG
2	I	43	LYS
2	I	64	LYS
2	I	70	SER
2	I	82(B)	SER
2	I	92	CYS
2	I	113	SER
2	I	150	VAL
2	I	161	SER

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Mol	Chain	Res	Type
2	I	192	GLN
3	M	31	SER
3	M	33	LEU
3	M	60	ASP
3	M	61	ARG
3	M	72	THR
3	M	77	ARG
3	M	105	GLU
3	M	122	ASP
3	M	123	GLU
3	M	138	ASN
3	M	142	ARG
3	M	149	LYS
3	M	154	LEU
3	M	164	THR
3	M	169	LYS
3	M	188	LYS
3	M	191	VAL
3	M	210	ASN

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

All (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
2	I	1	PCA	CG-CD-N	2.57	115.06	108.39
2	H	1	PCA	CG-CD-N	2.41	114.63	108.39
2	I	1	PCA	OE-CD-CG	-2.40	122.57	126.76
2	H	1	PCA	OE-CD-CG	-2.19	122.94	126.76

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
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.

All (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
6	M	301	PEG	C4-C3-O2-C2
5	I	301	FLC	CA-CB-CG-CGC
5	I	301	FLC	CBC-CB-CG-CGC
5	I	301	FLC	OHB-CB-CG-CGC

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

### 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	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

All (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
3	M	153	ALA	3.8
2	I	158	ALA	3.7
2	I	184	VAL	3.3
2	H	210	ARG	3.3
1	C	24	GLU	3.2
1	C	2	ALA	3.1
3	M	184	ALA	3.1
3	M	188	LYS	3.0
3	M	181	LEU	3.0
3	M	191	VAL	2.8
2	I	190	GLY	2.7
1	D	16	ARG	2.6
1	C	4	HIS	2.4
1	D	30	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
3	M	186	TYR	2.3
3	M	150	VAL	2.3
1	C	57	GLY	2.3
3	M	148	TRP	2.2
1	C	56	MET	2.2
1	D	64	ASP	2.2
3	M	147	GLN	2.1
3	M	152	ASN	2.1
2	I	193	THR	2.1
3	M	151	ASP	2.0

## 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
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.