



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:04 AM UTC

PDB ID : 7SU0 / pdb_00007su0
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

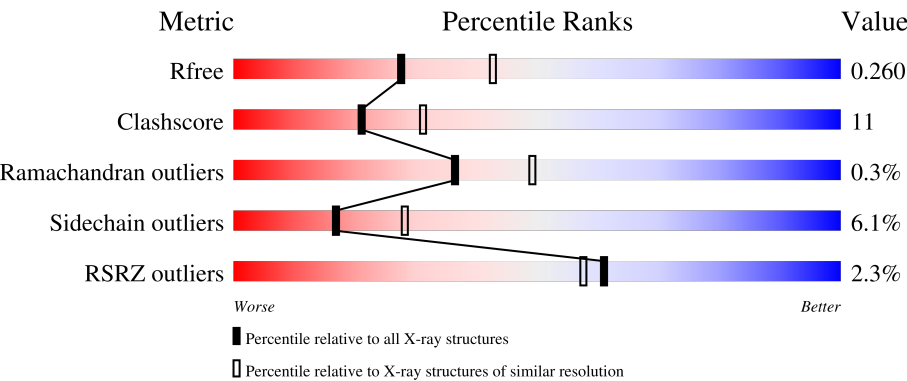
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 _{free}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (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	6% 67%24%6%
1	D	125	4% 66%22%7%
2	H	229	71%21%7%
2	I	229	69%23%8%
3	L	215	77%22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	215	5% 68% 26% • •

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

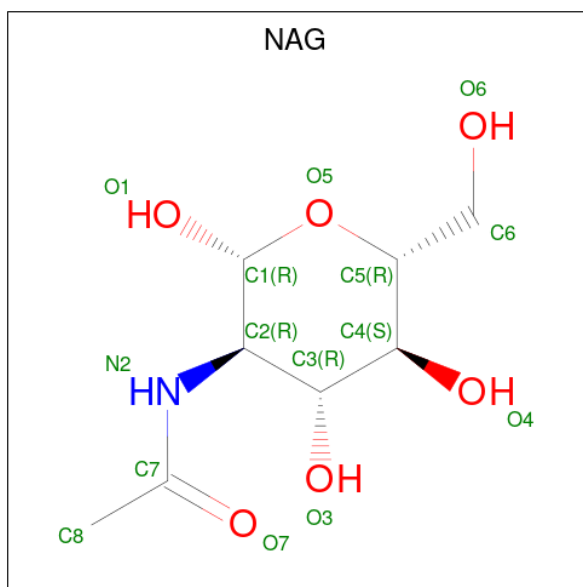
- Molecule 2 is a protein called Fab heavy chain.

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 (CCD ID: 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 (CCD ID: 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 (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

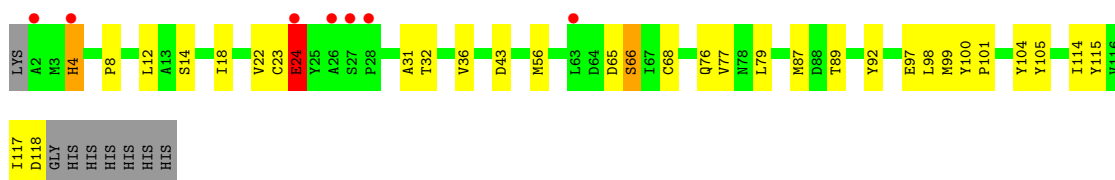
- Molecule 7 is water.

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

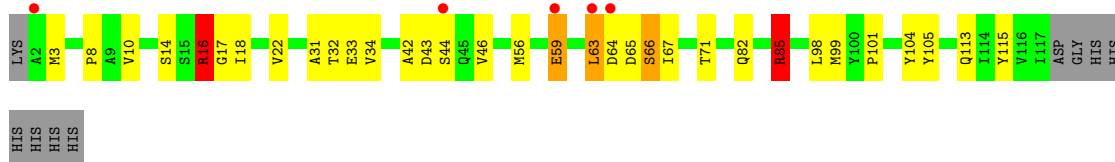
3 Residue-property plots [i](#)

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.

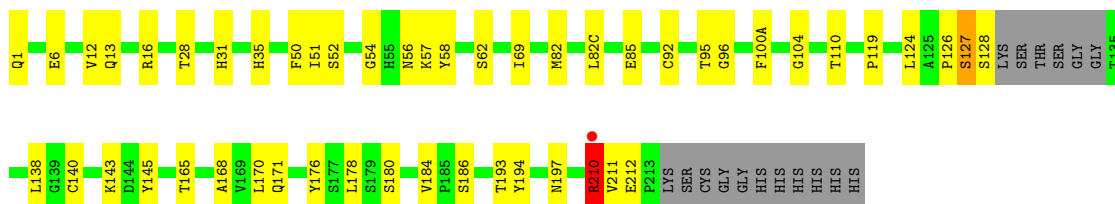
- Molecule 1: Cytotoxic T-lymphocyte protein 4



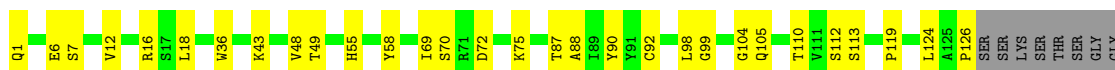
- Molecule 1: Cytotoxic T-lymphocyte protein 4



- Molecule 2: Fab heavy chain

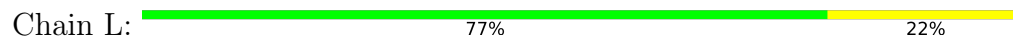


- Molecule 2: Fab heavy chain

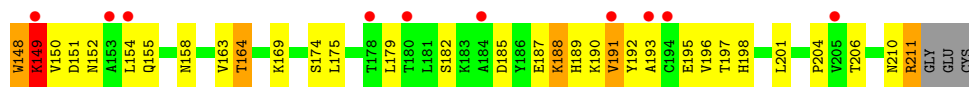




• Molecule 3: Fab light chain



• 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) 70.2 (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 0.205 , 0.260	Depositor DCC
R_{free} test set	1909 reflections (3.48%)	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 , 34.9	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: PCA, FLC, NAG, PEG

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	0.52	0/887	0.80	2/1208 (0.2%)
1	D	0.45	0/879	0.81	2/1197 (0.2%)
2	H	0.46	1/1656 (0.1%)	0.78	4/2260 (0.2%)
2	I	0.38	0/1644	0.60	0/2244
3	L	0.43	0/1686	0.65	0/2289
3	M	0.46	0/1673	0.81	4/2272 (0.2%)
All	All	0.45	1/8425 (0.0%)	0.74	12/11470 (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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	210	ARG	CG-CD	-7.51	1.29	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	210	ARG	CA-CB-CG	-15.86	82.38	114.10
2	H	210	ARG	CG-CD-NE	9.66	133.25	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	16	ARG	CG-CD-NE	-9.23	91.69	112.00
2	H	210	ARG	N-CA-C	7.88	121.65	110.23
3	M	149	LYS	CA-CB-CG	7.68	129.46	114.10
2	H	210	ARG	CB-CG-CD	7.24	127.96	111.30
1	D	16	ARG	CB-CG-CD	7.06	127.54	111.30
1	C	4	HIS	N-CA-CB	6.01	121.29	110.83
1	C	4	HIS	CB-CA-C	-5.92	98.06	109.37
3	M	149	LYS	CG-CD-CE	5.26	123.40	111.30
3	M	149	LYS	N-CA-CB	-5.13	103.79	111.64
3	M	149	LYS	CD-CE-NZ	-5.04	95.78	111.90

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 [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	C	873	0	860	23	0
1	D	865	0	857	21	0
2	H	1619	0	1570	37	0
2	I	1607	0	1560	33	0
3	L	1649	0	1593	25	0
3	M	1636	0	1584	50	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	180	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 11.

All (180) 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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:D:56:MET:HE3	1:D:56:MET:HA	1.84	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
2:H:127:SER:OG	2:H:128:SER:N	2.32	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:182:SER:HB2	3:M:185:ASP:CB	2.40	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
1:D:63:LEU:C	1:D:65:ASP:H	2.19	0.51
3:M:60:ASP:N	3:M:60:ASP:OD1	2.43	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
3:M:187:GLU:C	3:M:211:ARG:HH21	2.18	0.50
2:H:85:GLU:H	2:H:85:GLU:CD	2.17	0.49
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
1:C:99:MET:HE3	1:C:104:TYR:CE2	2.48	0.49
2:I:72:ASP:OD2	2:I:75:LYS:HG3	2.13	0.49
1:C:99:MET:HE3	1:C:104:TYR:CD2	2.48	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: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
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:105:GLU:OE2	3:L:140:TYR:OH	2.34	0.46
3:L:180:THR:O	3:L:181:LEU:HD23	2.16	0.46
1:D:17:GLY:C	1:D:18:ILE:HD13	2.40	0.45
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:143:LYS:HG2	2:I:144:ASP:OD2	2.16	0.45
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: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:145:LYS:NZ	1:D:33:GLU:OE1	2.51	0.42
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
2:I:146:PHE:CD1	2:I:146:PHE:C	2.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:M:187:GLU:HA	3:M:211:ARG:HH21	1.84	0.42
1:D:3:MET:HE2	1:D:98:LEU:HG	2.01	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
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
1:C:87:MET:HE2	1:C:87:MET:HB3	1.88	0.41
3:M:197:THR:HG22	3:M:204:PRO:HB3	2.01	0.41
2:H:143:LYS:NZ	2:H:171:GLN:OE1	2.53	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
3:L:125:LEU:C	3:L:127:SER:H	2.28	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
2:H:178:LEU:HD12	2:H:178:LEU:C	2.45	0.40
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
3:M:125:LEU:C	3:M:127:SER:H	2.29	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	C	115/125 (92%)	108 (94%)	5 (4%)	2 (2%)	7	9
1	D	114/125 (91%)	108 (95%)	5 (4%)	1 (1%)	14	20
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%)	36	49

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%)	92 (96%)	4 (4%)	26	43
1	D	95/103 (92%)	88 (93%)	7 (7%)	13	20
2	H	179/192 (93%)	173 (97%)	6 (3%)	32	52
2	I	177/192 (92%)	168 (95%)	9 (5%)	21	35
3	L	184/185 (100%)	169 (92%)	15 (8%)	10	17
3	M	183/185 (99%)	168 (92%)	15 (8%)	10	17
All	All	914/960 (95%)	858 (94%)	56 (6%)	17	28

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	12	LEU
1	C	23	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	24	GLU
1	C	66	SER
2	H	62	SER
2	H	92	CYS
2	H	110	THR
2	H	127	SER
2	H	186	SER
2	H	197	ASN
3	L	22	SER
3	L	27	GLN
3	L	27(A)	GLU
3	L	30	GLU
3	L	33	LEU
3	L	72	THR
3	L	94	SER
3	L	105	GLU
3	L	106	ILE
3	L	114	SER
3	L	131	SER
3	L	154	LEU
3	L	171	SER
3	L	197	THR
3	L	203	SER
1	D	14	SER
1	D	16	ARG
1	D	46	VAL
1	D	59	GLU
1	D	63	LEU
1	D	66	SER
1	D	85	ARG
2	I	7	SER
2	I	43	LYS
2	I	70	SER
2	I	92	CYS
2	I	113	SER
2	I	150	VAL
2	I	161	SER
2	I	173	SER
2	I	192	GLN
3	M	31	SER
3	M	61	ARG
3	M	72	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	105	GLU
3	M	122	ASP
3	M	123	GLU
3	M	133	VAL
3	M	149	LYS
3	M	154	LEU
3	M	163	VAL
3	M	164	THR
3	M	169	LYS
3	M	188	LYS
3	M	191	VAL
3	M	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	31	HIS
3	L	124	GLN
1	D	4	HIS
1	D	58	ASN
1	D	75	ASN
2	I	56	ASN
2	I	76	ASN
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	H	1	2	7,8,9	2.02	1 (14%)	9,10,12	2.15	4 (44%)
2	PCA	I	1	2	7,8,9	1.90	1 (14%)	9,10,12	2.33	5 (55%)

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	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	I	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	5.06	1.47	1.34
2	I	1	PCA	CD-N	4.79	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	101.56	113.58
2	I	1	PCA	CA-N-CD	-3.44	101.80	113.58
2	H	1	PCA	CB-CA-N	3.26	112.21	103.24
2	I	1	PCA	CB-CA-N	2.98	111.44	103.24
2	I	1	PCA	CB-CA-C	-2.80	108.81	112.66
2	I	1	PCA	CG-CD-N	2.72	115.06	108.39
2	H	1	PCA	CG-CD-N	2.55	114.63	108.39
2	I	1	PCA	OE-CD-CG	-2.33	122.57	126.72
2	H	1	PCA	OE-CD-CG	-2.12	122.94	126.72

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 oligosaccharides in this entry.

5.6 Ligand geometry

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
4	NAG	C	202	1	14,14,15	0.83	2 (14%)	17,19,21	0.51	0
4	NAG	C	201	1	14,14,15	0.94	1 (7%)	17,19,21	0.91	1 (5%)
6	PEG	M	301	-	6,6,6	0.66	0	5,5,5	0.48	0
4	NAG	D	201	1	14,14,15	0.50	0	17,19,21	0.73	0
5	FLC	I	301	-	12,12,12	1.14	1 (8%)	17,17,17	1.16	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	C	202	1	-	0/6/23/26	0/1/1/1
4	NAG	C	201	1	-	2/6/23/26	0/1/1/1
6	PEG	M	301	-	-	2/4/4/4	-
4	NAG	D	201	1	-	2/6/23/26	0/1/1/1
5	FLC	I	301	-	-	7/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	201	NAG	O5-C1	3.30	1.49	1.43
4	C	202	NAG	O5-C1	2.18	1.47	1.43
4	C	202	NAG	C1-C2	2.05	1.55	1.52
5	I	301	FLC	CB-CBC	-2.00	1.51	1.53

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	201	NAG	C1-O5-C5	2.65	115.74	112.19

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	301	FLC	CA-CB-CBC-OB1
5	I	301	FLC	CA-CB-CBC-OB2
5	I	301	FLC	OHB-CB-CBC-OB1
5	I	301	FLC	OHB-CB-CBC-OB2
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
5	I	301	FLC	CBC-CB-CG-CGC
6	M	301	PEG	O2-C3-C4-O4
5	I	301	FLC	CA-CB-CG-CGC
6	M	301	PEG	C4-C3-O2-C2
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
4	C	202	NAG	2	0
5	I	301	FLC	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, 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%)	0.40	7 (5%) 27 24	35, 50, 89, 110	0
1	D	116/125 (92%)	0.29	5 (4%) 40 35	30, 49, 80, 115	0
2	H	211/229 (92%)	-0.28	1 (0%) 87 86	27, 38, 56, 88	0
2	I	209/229 (91%)	0.10	1 (0%) 87 86	26, 45, 71, 88	0
3	L	214/215 (99%)	-0.42	0 100 100	24, 35, 47, 59	0
3	M	212/215 (98%)	0.24	11 (5%) 33 29	23, 47, 88, 108	0
All	All	1079/1138 (94%)	0.00	25 (2%) 61 57	23, 41, 80, 115	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	63	LEU	4.3
1	D	63	LEU	4.2
2	H	210	ARG	4.1
3	M	154	LEU	3.8
1	C	4	HIS	3.6
3	M	149	LYS	3.5
1	C	24	GLU	3.4
1	C	27	SER	3.4
1	D	64	ASP	3.2
1	D	2	ALA	3.2
1	C	2	ALA	3.0
3	M	184	ALA	2.9
1	C	28	PRO	2.6
3	M	194	CYS	2.6
3	M	193	ALA	2.4
3	M	153	ALA	2.3
1	D	59	GLU	2.3
3	M	117	ILE	2.3
3	M	191	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	180	THR	2.3
3	M	178	THR	2.1
1	C	26	ALA	2.1
3	M	205	VAL	2.1
1	D	44	SER	2.1
2	I	196	CYS	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, 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	0.73	0.15	45,51,61,66	0
2	PCA	I	1	8/9	0.77	0.13	48,52,55,58	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
4	NAG	C	201	14/15	0.81	0.10	54,60,67,73	0
5	FLC	I	301	13/13	0.81	0.14	58,68,75,76	0
4	NAG	C	202	14/15	0.84	0.12	52,62,67,73	0
4	NAG	D	201	14/15	0.86	0.08	48,50,54,58	0
6	PEG	M	301	7/7	0.89	0.10	33,36,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.