



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:28 PM UTC

PDB ID : 7S13 / pdb_00007s13
Title : Crystal structure of Fab in complex with mouse CD96 dimer
Authors : Lee, P.S.; Barman, I.; Strop, P.
Deposited on : 2021-08-31
Resolution : 2.12 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

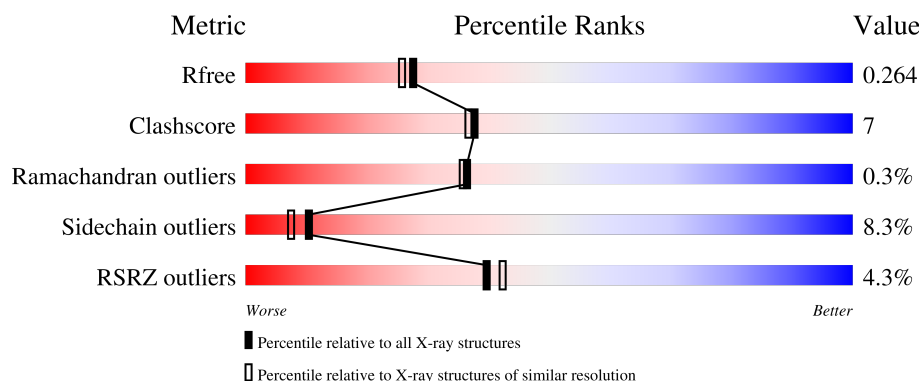
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	H	226	2% 77% 15% 8%
1	I	226	8% 73% 15% • 8%
2	L	213	• 77% 18% • •
2	M	213	71% 23% • •
3	C	125	5% 79% 14% • 6%

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Mol	Chain	Length	Quality of chain
3	D	125	11% 70% 17% 5% 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8274 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 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	209	Total	C	N	O	S	0	0	0
			1569	997	256	308	8			
1	I	208	Total	C	N	O	S	0	0	0
			1565	995	255	307	8			

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	209	Total	C	N	O	S	0	0	0
			1609	1003	266	334	6			
2	M	208	Total	C	N	O	S	0	0	0
			1604	1000	265	333	6			

- Molecule 3 is a protein called T-cell surface protein tactile.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	117	Total	C	N	O	S	0	0	0
			931	595	147	183	6			
3	D	114	Total	C	N	O	S	0	0	0
			906	577	143	180	6			

There are 14 discrepancies between the modelled and reference sequences:

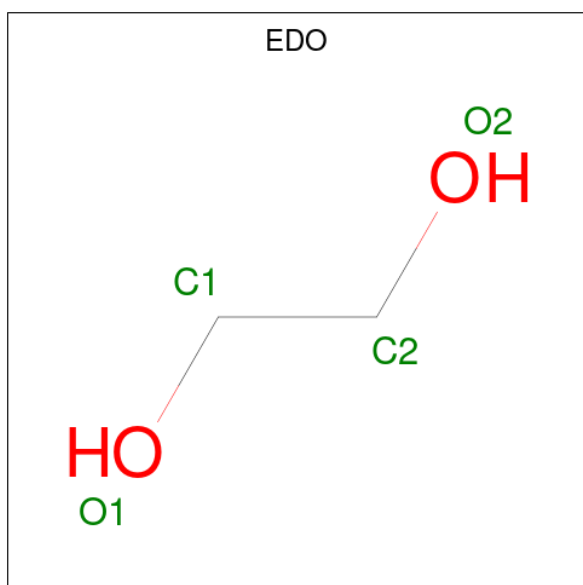
Chain	Residue	Modelled	Actual	Comment	Reference
C	139	GLY	-	expression tag	UNP Q3U0X8
C	140	HIS	-	expression tag	UNP Q3U0X8
C	141	HIS	-	expression tag	UNP Q3U0X8
C	142	HIS	-	expression tag	UNP Q3U0X8
C	143	HIS	-	expression tag	UNP Q3U0X8
C	144	HIS	-	expression tag	UNP Q3U0X8
C	145	HIS	-	expression tag	UNP Q3U0X8
D	139	GLY	-	expression tag	UNP Q3U0X8

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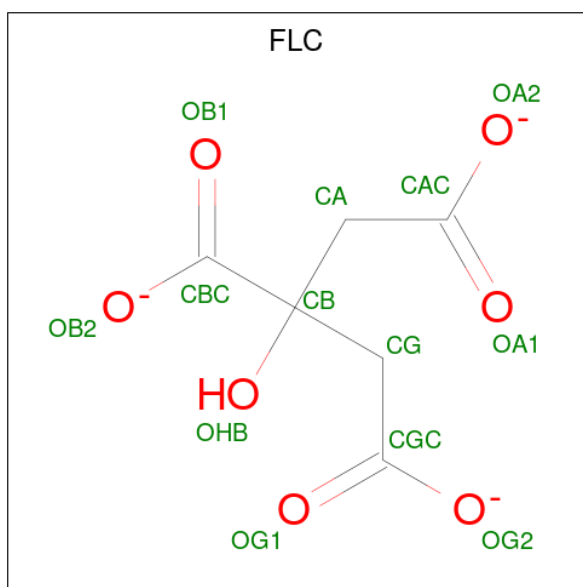
Chain	Residue	Modelled	Actual	Comment	Reference
D	140	HIS	-	expression tag	UNP Q3U0X8
D	141	HIS	-	expression tag	UNP Q3U0X8
D	142	HIS	-	expression tag	UNP Q3U0X8
D	143	HIS	-	expression tag	UNP Q3U0X8
D	144	HIS	-	expression tag	UNP Q3U0X8
D	145	HIS	-	expression tag	UNP Q3U0X8

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



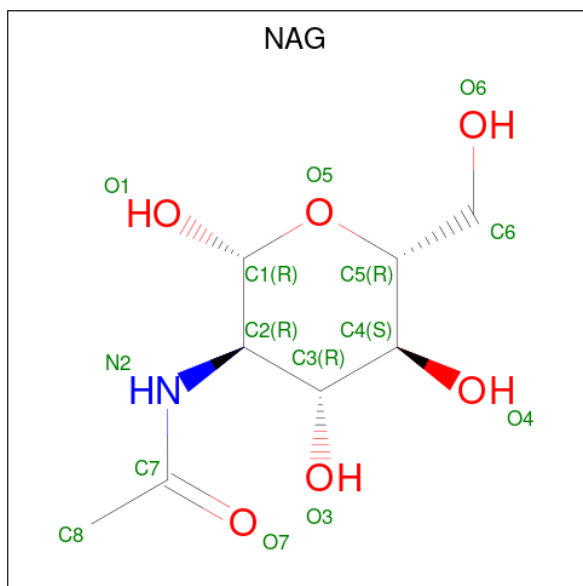
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		

- 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

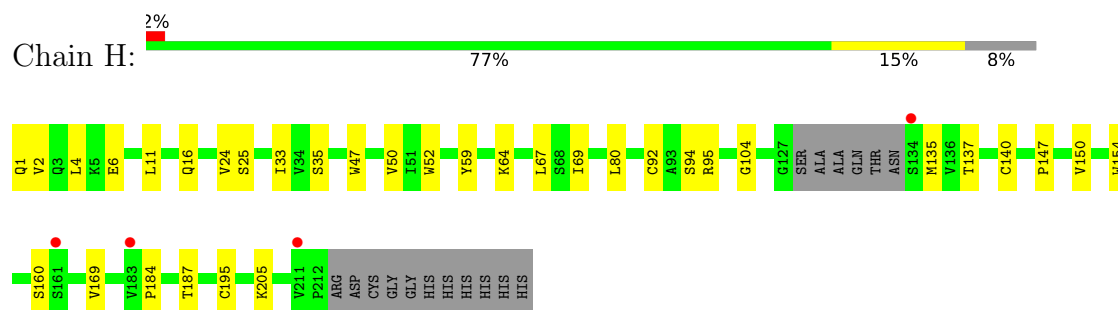
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	15	Total 15	O 15	0	0
7	L	14	Total 14	O 14	0	0
7	I	2	Total 2	O 2	0	0
7	C	5	Total 5	O 5	0	0
7	D	1	Total 1	O 1	0	0

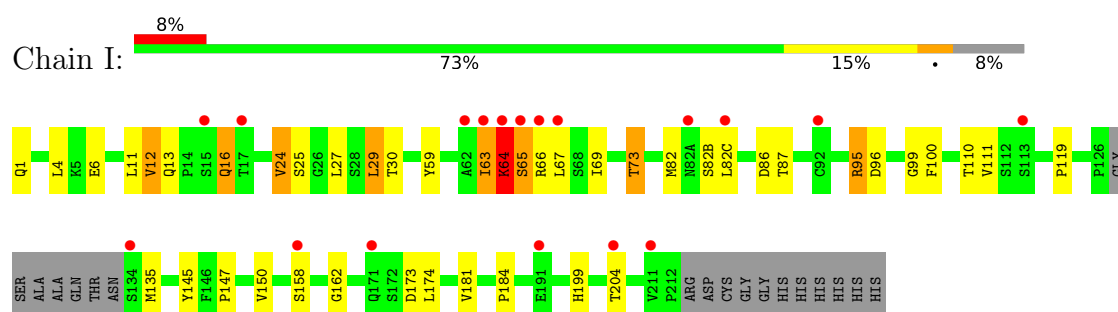
3 Residue-property plots [i](#)

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.

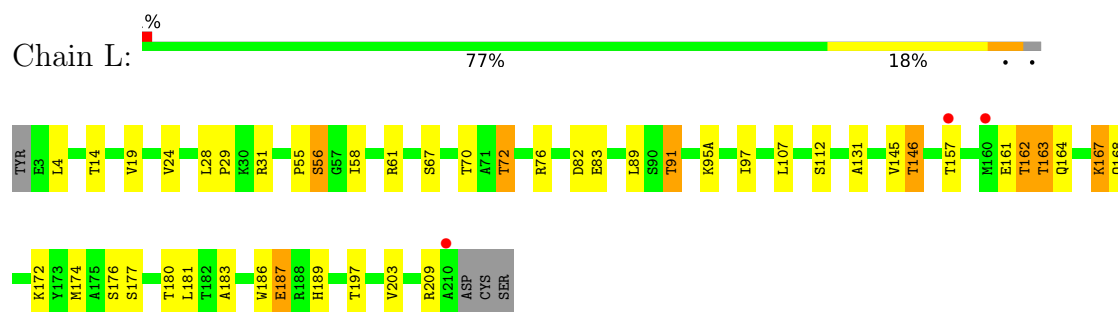
- Molecule 1: Fab heavy chain



- Molecule 1: Fab heavy chain

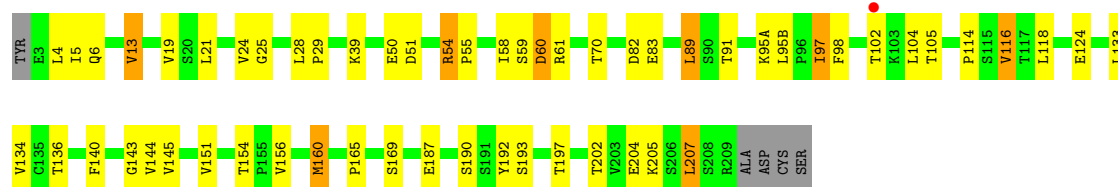


- Molecule 2: Fab light chain

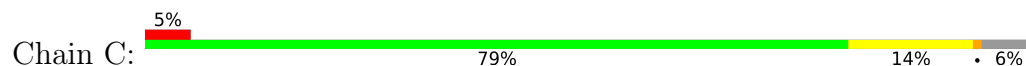


- Molecule 2: Fab light chain





• Molecule 3: T-cell surface protein tactile



• Molecule 3: T-cell surface protein tactile



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.03Å 131.25Å 186.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.77 – 2.12 40.77 – 2.12	Depositor EDS
% Data completeness (in resolution range)	67.5 (40.77-2.12) 67.7 (40.77-2.12)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.217 , 0.265 0.217 , 0.264	Depositor DCC
R_{free} test set	2467 reflections (3.33%)	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.9	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	8274	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: FLC, NAG, PCA, EDO

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	H	0.44	0/1602	0.68	2/2195 (0.1%)
1	I	0.39	0/1598	0.61	0/2190
2	L	0.39	0/1645	0.66	0/2242
2	M	0.39	0/1640	0.63	0/2235
3	C	0.47	0/952	0.72	0/1295
3	D	0.43	0/925	0.85	2/1257 (0.2%)
All	All	0.41	0/8362	0.68	4/11414 (0.0%)

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
3	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	85	CYS	CA-CB-SG	-9.57	92.39	114.40
3	D	79	CYS	CA-CB-SG	-7.58	96.96	114.40
1	H	94	SER	CA-C-N	5.23	131.53	121.54
1	H	94	SER	C-N-CA	5.23	131.53	121.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	30	GLY	Peptide

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	H	1569	0	1555	15	0
1	I	1565	0	1552	25	0
2	L	1609	0	1554	24	0
2	M	1604	0	1549	32	0
3	C	931	0	890	10	0
3	D	906	0	868	16	0
4	H	4	0	6	0	0
4	L	8	0	12	0	0
5	I	13	0	5	2	0
6	C	14	0	13	0	0
6	D	14	0	13	0	0
7	C	5	0	0	0	0
7	D	1	0	0	0	0
7	H	15	0	0	1	0
7	I	2	0	0	0	0
7	L	14	0	0	1	0
All	All	8274	0	8017	114	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 7.

All (114) 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:D:25:GLU:HG3	3:D:29:VAL:HG11	1.61	0.80
2:L:189:HIS:O	2:L:209:ARG:NH1	2.15	0.79
1:H:47:TRP:HZ2	1:H:50:VAL:HG23	1.49	0.77
2:L:168:GLN:HG2	2:L:174:MET:HE3	1.71	0.73
1:I:66:ARG:NH2	1:I:86:ASP:OD2	2.22	0.71
2:M:13:VAL:HG13	2:M:19:VAL:HB	1.73	0.69
1:H:47:TRP:CZ2	1:H:50:VAL:HG23	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:56:SER:HB2	3:D:82:GLU:HB3	1.79	0.63
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.80	0.63
5:I:301:FLC:OG1	5:I:301:FLC:OHB	2.14	0.62
2:L:61:ARG:NH2	2:L:82:ASP:OD2	2.33	0.61
2:M:197:THR:OG1	2:M:202:THR:HG22	2.01	0.61
1:H:35:SER:OG	1:H:50:VAL:HG22	2.02	0.59
2:M:21:LEU:HD22	2:M:102:THR:HG21	1.85	0.58
2:M:61:ARG:NH2	2:M:82:ASP:OD2	2.37	0.58
1:I:73:THR:HG22	5:I:301:FLC:OB1	2.04	0.58
2:M:13:VAL:HG22	2:M:104:LEU:HD11	1.87	0.57
2:M:116:VAL:HG22	2:M:205:LYS:HG2	1.86	0.56
1:H:11:LEU:HB2	1:H:147:PRO:HG3	1.87	0.56
1:H:4:LEU:HD22	1:H:24:VAL:HG22	1.88	0.56
3:D:56:MET:HE3	3:D:101:TRP:CE3	2.41	0.56
2:L:146:THR:HG23	2:L:197:THR:HB	1.88	0.56
1:I:66:ARG:HH22	1:I:86:ASP:CG	2.15	0.55
3:D:85:CYS:SG	3:D:86:GLU:N	2.79	0.55
1:I:95:ARG:HH11	1:I:96:ASP:CG	2.14	0.54
2:M:60:ASP:N	2:M:60:ASP:OD1	2.40	0.54
3:C:46:GLN:HE21	3:C:98:VAL:HG11	1.72	0.54
1:I:63:ILE:HB	1:I:67:LEU:HD23	1.89	0.54
2:M:51:ASP:OD2	3:D:50:LYS:NZ	2.29	0.54
1:I:87:THR:HG23	1:I:110:THR:HA	1.88	0.54
2:M:4:LEU:HD23	2:M:25:GLY:HA3	1.91	0.53
1:H:67:LEU:HD11	1:H:80:LEU:HD11	1.91	0.53
2:L:112:SER:OG	2:L:172:LYS:NZ	2.42	0.53
2:L:24:VAL:HG22	2:L:70:THR:HG22	1.91	0.53
3:C:56:MET:HE3	3:C:101:TRP:CE3	2.44	0.52
1:I:59:TYR:HE1	1:I:69:ILE:HG13	1.75	0.52
2:M:192:TYR:HB2	2:M:207:LEU:HD22	1.89	0.52
2:L:131:ALA:N	2:L:181:LEU:O	2.42	0.52
3:C:127:ILE:HG13	3:D:119:ILE:HG21	1.91	0.51
1:I:66:ARG:O	1:I:82:MET:HA	2.10	0.51
1:H:135:MET:HE1	1:H:184:PRO:HG3	1.93	0.51
1:I:13:GLN:O	1:I:16:GLN:HB2	2.11	0.51
1:I:82(B):SER:O	1:I:82(B):SER:OG	2.22	0.50
1:I:66:ARG:HH21	1:I:82(C):LEU:HA	1.75	0.50
2:M:28:LEU:N	2:M:29:PRO:HD2	2.27	0.49
1:H:33:ILE:HG13	7:H:402:HOH:O	2.12	0.49
2:M:124:GLU:OE1	2:M:124:GLU:N	2.35	0.49
1:I:16:GLN:O	1:I:82(C):LEU:HD11	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:163:THR:HB	2:L:176:SER:O	2.12	0.49
1:I:199:HIS:HB3	1:I:204:THR:HB	1.95	0.49
3:C:119:ILE:HG21	3:D:127:ILE:HG13	1.95	0.49
1:H:59:TYR:HD1	1:H:67:LEU:HD23	1.79	0.48
2:L:168:GLN:HG2	2:L:174:MET:CE	2.41	0.48
2:M:114:PRO:HB3	2:M:140:PHE:HB3	1.96	0.48
3:C:46:GLN:NE2	3:C:98:VAL:HG11	2.29	0.48
2:L:55:PRO:HG2	2:L:58:ILE:HG13	1.95	0.47
3:D:44:THR:OG1	3:D:102:THR:HB	2.14	0.47
1:H:59:TYR:HE1	1:H:69:ILE:HG13	1.79	0.47
1:H:6:GLU:OE2	1:H:104:GLY:HA3	2.15	0.47
2:M:116:VAL:HA	2:M:136:THR:O	2.15	0.47
2:L:4:LEU:HG	2:L:97:ILE:HD12	1.96	0.46
2:L:91:THR:HG23	2:L:95(A):LYS:HA	1.97	0.46
2:M:83:GLU:HG3	2:M:105:THR:HA	1.98	0.46
2:L:61:ARG:HB3	2:L:76:ARG:O	2.16	0.46
2:M:54:ARG:NH2	2:M:60:ASP:HB3	2.31	0.46
3:C:57:GLN:NE2	3:C:67:MET:HG3	2.31	0.46
1:I:135:MET:HE1	1:I:184:PRO:HG3	1.98	0.46
2:M:118:LEU:HG	2:M:207:LEU:HD13	1.98	0.45
2:M:97:ILE:HD12	2:M:97:ILE:O	2.15	0.45
2:L:4:LEU:HD23	2:L:4:LEU:HA	1.77	0.45
1:I:162:GLY:O	1:I:181:VAL:HA	2.16	0.45
2:M:55:PRO:HD2	2:M:58:ILE:HG13	1.99	0.45
1:I:29:LEU:HD23	1:I:29:LEU:HA	1.82	0.45
2:M:89:LEU:HD23	2:M:98:PHE:CZ	2.52	0.44
1:H:35:SER:O	1:H:92:CYS:HA	2.18	0.44
2:L:28:LEU:N	2:L:29:PRO:HD2	2.33	0.44
2:M:95(B):LEU:HD12	2:M:95(B):LEU:HA	1.80	0.44
3:D:28:ASN:CG	3:D:29:VAL:H	2.25	0.44
1:I:135:MET:HE2	1:I:184:PRO:HA	1.99	0.44
3:D:56:MET:HE2	3:D:71:TYR:CD2	2.54	0.43
2:M:95(A):LYS:HD3	3:D:52:PHE:CD1	2.53	0.43
3:D:28:ASN:O	3:D:30:GLY:N	2.42	0.43
2:M:156:VAL:HB	2:M:160:MET:HE3	2.00	0.43
2:L:83:GLU:OE2	2:L:167:LYS:HE2	2.19	0.43
1:I:27:LEU:HD23	3:C:86:GLU:HB2	2.00	0.43
1:I:64:LYS:HD2	1:I:65:SER:N	2.34	0.43
2:M:89:LEU:HD23	2:M:98:PHE:CE1	2.54	0.42
2:L:183:ALA:O	2:L:187:GLU:HG2	2.20	0.42
2:L:72:THR:HG23	7:L:412:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:24:VAL:HG22	2:M:70:THR:HG22	2.01	0.42
2:L:163:THR:HG23	2:L:164:GLN:O	2.19	0.42
2:M:143:GLY:O	2:M:165:PRO:HG2	2.20	0.42
2:L:56:SER:CB	3:D:82:GLU:HB3	2.48	0.42
3:C:56:MET:HE2	3:C:71:TYR:CD2	2.55	0.42
1:I:12:VAL:O	1:I:111:VAL:HA	2.20	0.42
2:M:133:LEU:HD12	2:M:133:LEU:N	2.35	0.42
2:M:59:SER:OG	2:M:61:ARG:HG3	2.20	0.41
1:H:33:ILE:HG22	1:H:52:TRP:HA	2.03	0.41
1:I:11:LEU:HB2	1:I:147:PRO:HG3	2.01	0.41
1:I:99:GLY:O	1:I:100:PHE:C	2.63	0.41
2:M:95(A):LYS:HD3	3:D:52:PHE:CE1	2.55	0.41
3:C:117:GLU:HG3	3:C:131:VAL:HG22	2.02	0.41
1:I:173:ASP:O	1:I:174:LEU:HD23	2.21	0.41
3:D:37:PRO:HA	3:D:108:ILE:O	2.20	0.41
1:H:154:TRP:CZ3	1:H:195:CYS:HB3	2.56	0.41
2:L:162:THR:HB	2:L:177:SER:OG	2.20	0.41
2:M:204:GLU:HG2	2:M:205:LYS:N	2.34	0.41
2:M:28:LEU:HA	2:M:28:LEU:HD23	1.88	0.41
1:I:4:LEU:HD22	1:I:24:VAL:HG12	2.03	0.40
3:D:51:ASN:OD1	3:D:125:GLU:HG3	2.21	0.40
2:L:14:THR:HG22	2:L:107:LEU:HB2	2.02	0.40
2:L:186:TRP:CE2	2:L:209:ARG:HD2	2.57	0.40
2:M:50:GLU:OE2	3:C:78:TYR:OH	2.32	0.40
1:H:67:LEU:HD12	1:H:67:LEU:HA	1.87	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	H	205/226 (91%)	196 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	204/226 (90%)	193 (95%)	10 (5%)	1 (0%)	24	22
2	L	207/213 (97%)	201 (97%)	6 (3%)	0	100	100
2	M	206/213 (97%)	198 (96%)	8 (4%)	0	100	100
3	C	115/125 (92%)	107 (93%)	8 (7%)	0	100	100
3	D	112/125 (90%)	104 (93%)	6 (5%)	2 (2%)	6	3
All	All	1049/1128 (93%)	999 (95%)	47 (4%)	3 (0%)	36	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	64	LYS
3	D	28	ASN
3	D	29	VAL

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	H	183/196 (93%)	171 (93%)	12 (7%)	15	12
1	I	183/196 (93%)	169 (92%)	14 (8%)	12	9
2	L	186/190 (98%)	169 (91%)	17 (9%)	9	6
2	M	186/190 (98%)	165 (89%)	21 (11%)	5	3
3	C	102/109 (94%)	97 (95%)	5 (5%)	22	21
3	D	100/109 (92%)	91 (91%)	9 (9%)	9	6
All	All	940/990 (95%)	862 (92%)	78 (8%)	10	7

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	VAL
1	H	16	GLN
1	H	25	SER

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Mol	Chain	Res	Type
1	H	64	LYS
1	H	95	ARG
1	H	137	THR
1	H	140	CYS
1	H	150	VAL
1	H	160	SER
1	H	169	VAL
1	H	187	THR
1	H	205	LYS
2	L	19	VAL
2	L	31	ARG
2	L	56	SER
2	L	67	SER
2	L	72	THR
2	L	89	LEU
2	L	91	THR
2	L	145	VAL
2	L	146	THR
2	L	157	THR
2	L	161	GLU
2	L	162	THR
2	L	163	THR
2	L	167	LYS
2	L	180	THR
2	L	187	GLU
2	L	203	VAL
1	I	6	GLU
1	I	12	VAL
1	I	16	GLN
1	I	24	VAL
1	I	25	SER
1	I	29	LEU
1	I	30	THR
1	I	63	ILE
1	I	64	LYS
1	I	65	SER
1	I	73	THR
1	I	95	ARG
1	I	150	VAL
1	I	158	SER
2	M	5	ILE
2	M	6	GLN

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Mol	Chain	Res	Type
2	M	13	VAL
2	M	39	LYS
2	M	54	ARG
2	M	60	ASP
2	M	89	LEU
2	M	91	THR
2	M	97	ILE
2	M	116	VAL
2	M	134	VAL
2	M	144	VAL
2	M	145	VAL
2	M	151	VAL
2	M	154	THR
2	M	160	MET
2	M	169	SER
2	M	187	GLU
2	M	190	SER
2	M	193	SER
2	M	207	LEU
3	C	29	VAL
3	C	61	VAL
3	C	98	VAL
3	C	106	ARG
3	C	137	GLU
3	D	47	THR
3	D	60	LYS
3	D	82	GLU
3	D	86	GLU
3	D	98	VAL
3	D	102	THR
3	D	109	SER
3	D	118	CYS
3	D	121	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	77	GLN
2	L	38	GLN
2	L	42	GLN
1	I	39	GLN

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Mol	Chain	Res	Type
2	M	38	GLN
2	M	171	ASN
3	C	46	GLN
3	C	88	GLN
3	D	100	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
1	PCA	H	1	1	7,8,9	2.01	1 (14%)	9,10,12	2.22	4 (44%)
1	PCA	I	1	1	7,8,9	2.03	1 (14%)	9,10,12	2.30	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
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1
1	PCA	I	1	1	-	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)
1	H	1	PCA	CD-N	5.14	1.47	1.34
1	I	1	PCA	CD-N	5.14	1.47	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	1	PCA	CA-N-CD	-3.55	101.42	113.58
1	I	1	PCA	CB-CA-C	-3.47	107.90	112.66
1	H	1	PCA	CB-CA-N	3.27	112.23	103.24
1	I	1	PCA	CA-N-CD	-3.15	102.80	113.58
1	I	1	PCA	CB-CA-N	2.74	110.77	103.24
1	H	1	PCA	CG-CD-N	2.59	114.72	108.39
1	H	1	PCA	OE-CD-CG	-2.44	122.36	126.72
1	I	1	PCA	CG-CD-N	2.39	114.25	108.39
1	I	1	PCA	OE-CD-CG	-2.18	122.83	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 [i](#)

6 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	$\# Z > 2$
6	NAG	D	201	3	14,14,15	0.60	0	17,19,21	0.59	0
4	EDO	L	301	-	3,3,3	0.50	0	2,2,2	0.25	0
5	FLC	I	301	-	12,12,12	1.19	1 (8%)	17,17,17	1.42	2 (11%)
4	EDO	H	301	-	3,3,3	0.61	0	2,2,2	0.26	0
4	EDO	L	302	-	3,3,3	0.51	0	2,2,2	0.57	0
6	NAG	C	201	3	14,14,15	0.35	0	17,19,21	0.44	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
6	NAG	D	201	3	-	0/6/23/26	0/1/1/1
4	EDO	L	301	-	-	0/1/1/1	-
5	FLC	I	301	-	-	4/16/16/16	-
4	EDO	H	301	-	-	0/1/1/1	-
4	EDO	L	302	-	-	1/1/1/1	-
6	NAG	C	201	3	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	301	FLC	CB-CBC	-2.27	1.51	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	301	FLC	OB2-CBC-CB	3.86	120.55	113.14
5	I	301	FLC	OB1-CBC-CB	-2.88	116.52	122.09

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	301	FLC	OHB-CB-CG-CGC
6	C	201	NAG	O5-C5-C6-O6
6	C	201	NAG	C4-C5-C6-O6
5	I	301	FLC	CA-CB-CG-CGC
5	I	301	FLC	CBC-CB-CG-CGC
4	L	302	EDO	O1-C1-C2-O2
5	I	301	FLC	CAC-CA-CB-OHB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
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	H	208/226 (92%)	0.13	4 (1%) 66 69	32, 41, 57, 70	0
1	I	207/226 (91%)	0.75	18 (8%) 16 17	35, 55, 82, 122	0
2	L	209/213 (98%)	0.21	3 (1%) 73 76	31, 46, 62, 101	0
2	M	208/213 (97%)	0.64	1 (0%) 87 89	39, 54, 68, 87	0
3	C	117/125 (93%)	0.29	6 (5%) 33 36	30, 41, 76, 116	0
3	D	114/125 (91%)	0.69	14 (12%) 8 9	30, 48, 87, 110	0
All	All	1063/1128 (94%)	0.44	46 (4%) 40 42	30, 48, 74, 122	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	29	VAL	4.9
3	D	27	PHE	4.2
1	I	65	SER	3.6
2	L	157	THR	3.6
1	I	64	LYS	3.3
3	C	96	LYS	3.3
1	H	134	SER	3.2
3	D	26	LEU	3.1
3	D	82	GLU	3.1
3	D	97	GLY	3.1
2	L	210	ALA	3.0
1	I	171	GLN	2.8
1	I	82(C)	LEU	2.8
3	D	45	CYS	2.7
3	D	81	GLN	2.7
1	I	191	GLU	2.6
1	H	211	VAL	2.6
1	I	211	VAL	2.6
1	I	63	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
3	D	34	TYR	2.5
3	D	28	ASN	2.5
3	D	83	HIS	2.5
3	D	30	GLY	2.5
3	C	45	CYS	2.4
1	I	15	SER	2.4
3	C	94	THR	2.4
1	I	158	SER	2.4
3	D	85	CYS	2.4
1	I	67	LEU	2.3
2	L	160	MET	2.3
1	I	204	THR	2.3
3	C	21	GLY	2.2
1	I	17	THR	2.2
1	I	113	SER	2.2
3	C	23	TRP	2.2
3	D	137	GLU	2.1
1	I	134	SER	2.1
1	I	82(A)	ASN	2.1
1	I	62	ALA	2.1
1	I	92	CYS	2.1
1	I	66	ARG	2.1
3	D	80	GLY	2.1
1	H	183	VAL	2.0
1	H	161	SER	2.0
3	C	64	LYS	2.0
2	M	102	THR	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
1	PCA	H	1	8/9	0.79	0.15	49,59,70,77	0
1	PCA	I	1	8/9	0.79	0.13	57,61,75,78	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($\text{\AA}^2$)	Q<0.9
4	EDO	H	301	4/4	0.54	0.23	49,51,58,61	0
6	NAG	D	201	14/15	0.60	0.19	82,87,91,92	0
6	NAG	C	201	14/15	0.73	0.13	66,71,74,75	0
5	FLC	I	301	13/13	0.79	0.10	62,72,85,89	0
4	EDO	L	302	4/4	0.86	0.11	40,44,45,48	0
4	EDO	L	301	4/4	0.95	0.09	35,35,36,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.