wwPDB X-ray Structure Validation Summary Report (i)

Oct 10, 2023 – 12:53 AM EDT

PDB ID	:	7S13
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)

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

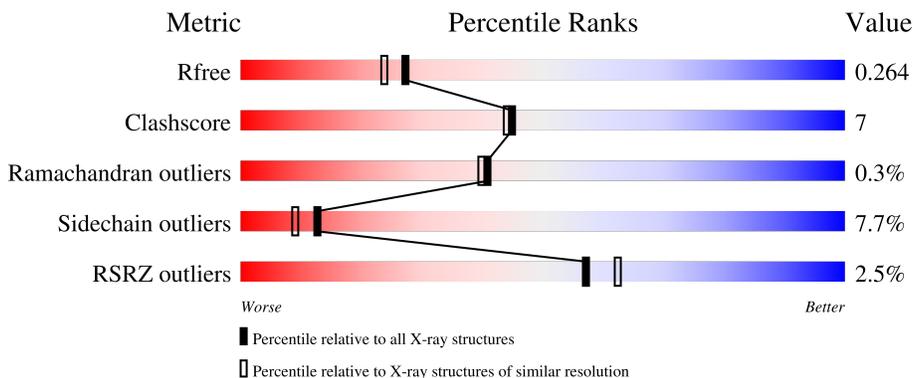|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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	Percentile Ranks	Value
Rfree		0.264
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		7.7%
RSRZ outliers		2.5%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (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 <=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	80% 12% 8%
1	I	226	6% / 72% 16% · 8%
2	L	213	77% 18% · ·
2	M	213	71% 23% · ·
3	C	125	3% / 82% 11% · 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	125	

2 Entry composition (i)

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

Continued on next page...

Continued from previous page...

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 (three-letter code: EDO) (formula: $C_2H_6O_2$).
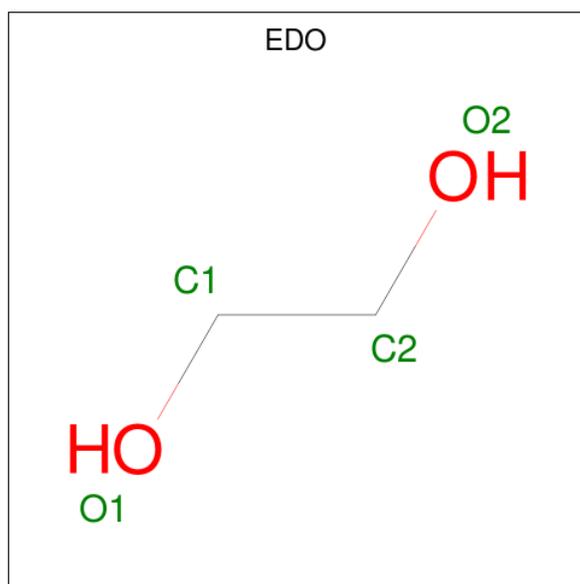
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total 4	C 2	O 2	0	0
4	L	1	Total 4	C 2	O 2	0	0
4	L	1	Total 4	C 2	O 2	0	0

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

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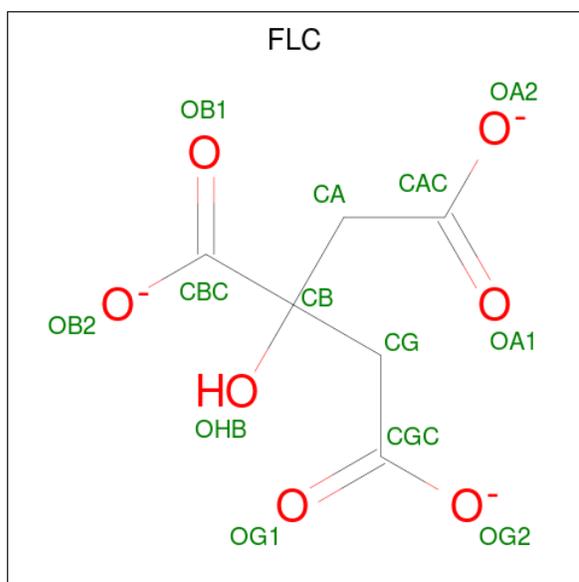
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	I	1	Total C O			0	0
			13	6	7		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

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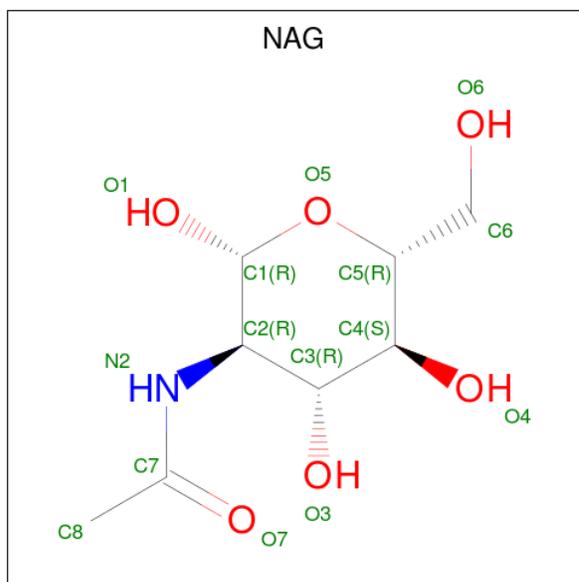
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

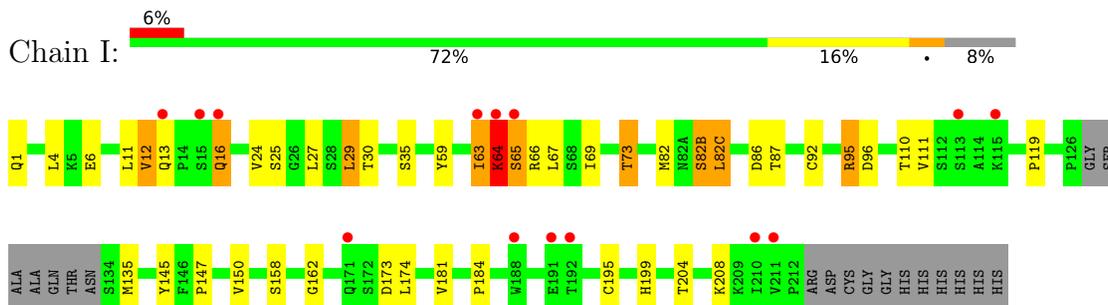| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	15	Total 15	O 15	0	0
7	L	14	Total 14	O 14	0	0
7	I	2	Total 2	O 2	0	0
7	C	5	Total 5	O 5	0	0
7	D	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

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.
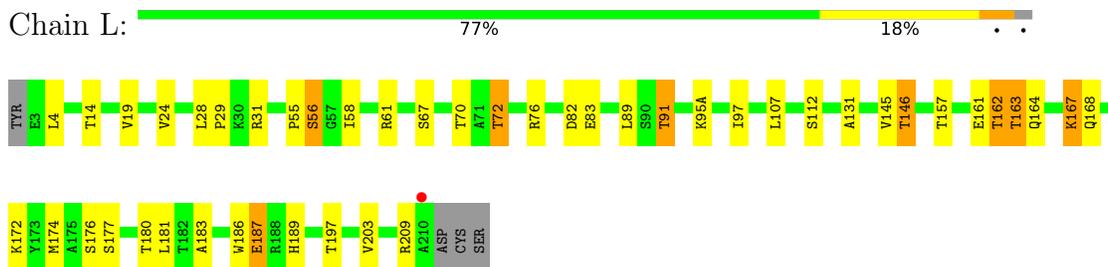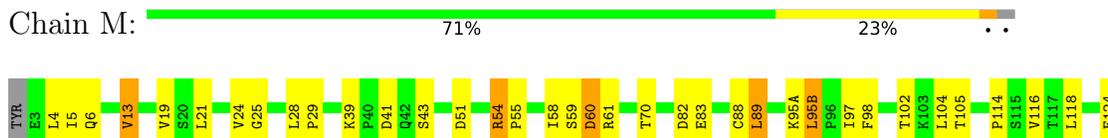
- Molecule 1: Fab heavy chain
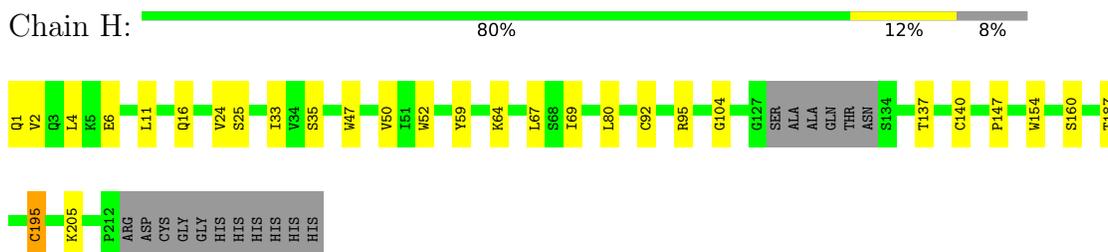
- Molecule 1: Fab heavy chain
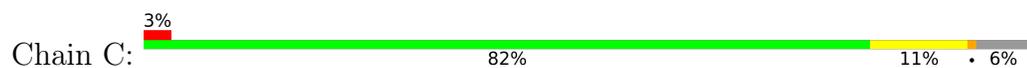

- Molecule 2: Fab light chain

- Molecule 2: Fab light chain

E125 L126 L133 V134 C135 T136 F140 G143 V144 V145 T154 M160 P165 S169 S190 S191 Y192 S193 C194 T197 T202 V203 E204 K205 S206 L207 S208 R209 ALA ASP CYS SER

• Molecule 3: T-cell surface protein tactile

Chain C:

3%

82%   11%   • 6%

G21 V29 G30 C45 Q46 Q57 V61 T62 D63 K64 M67 L70 E86 E95 K96 G97 V98 E117 C118 I119 I127 V131 E137 PRO GLY HIS HIS HIS HIS HIS HIS

• Molecule 3: T-cell surface protein tactile

Chain D:

6%

73%   14%   5%   9%

GLY VAL TRP E24 E25 L26 F27 N28 V29 G30 Y34 P37 T44 K50 N51 F52 L70 C79 G80 Q81 E82 C85 E86 K96 G97 V98 T102 I108 S109 C118 I119 F120 T121 E125 G126 I127 E137 PRO GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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) 67.5 (40.77-2.12)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.217 , 0.265 0.216 , 0.264	Depositor DCC
R_{free} test set	2465 reflections (4.94%)	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)	0.32 , 32.5	EDS
L-test for twinning [2]	$< |L| > = 0.50, < L^2 > = 0.34$	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.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: NAG, FLC, 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	0.52	0/1602	0.68	0/2195
1	I	0.50	1/1598 (0.1%)	0.67	0/2190
2	L	0.46	0/1645	0.70	1/2242 (0.0%)
2	M	0.49	2/1640 (0.1%)	0.71	2/2235 (0.1%)
3	C	0.55	1/952 (0.1%)	0.74	1/1295 (0.1%)
3	D	0.51	0/925	0.87	3/1257 (0.2%)
All	All	0.50	4/8362 (0.0%)	0.72	7/11414 (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
3	C	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	92	CYS	CB-SG	-8.66	1.67	1.82
2	M	88	CYS	CB-SG	-7.48	1.69	1.82
3	C	45	CYS	CB-SG	-7.25	1.70	1.82
2	M	194	CYS	CB-SG	-5.14	1.73	1.81

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	85	CYS	CA-CB-SG	-12.00	92.39	114.00
3	D	79	CYS	CA-CB-SG	-9.47	96.96	114.00
2	M	207	LEU	CA-CB-CG	6.93	131.24	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	89	LEU	CA-CB-CG	5.86	128.77	115.30
2	M	89	LEU	CA-CB-CG	5.66	128.33	115.30

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	14	0
1	I	1565	0	1552	24	0
2	L	1609	0	1554	24	0
2	M	1604	0	1549	31	0
3	C	931	0	890	7	0
3	D	906	0	868	13	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	106	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.

The worst 5 of 106 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
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

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
1	I	204/226 (90%)	193 (95%)	10 (5%)	1 (0%)	29	25
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%)	8	3
All	All	1049/1128 (93%)	999 (95%)	47 (4%)	3 (0%)	41	40

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%)	172 (94%)	11 (6%)	19	16
1	I	183/196 (93%)	165 (90%)	18 (10%)	8	4
2	L	186/190 (98%)	170 (91%)	16 (9%)	10	6
2	M	186/190 (98%)	170 (91%)	16 (9%)	10	6
3	C	102/109 (94%)	98 (96%)	4 (4%)	32	32
3	D	100/109 (92%)	93 (93%)	7 (7%)	15	11
All	All	940/990 (95%)	868 (92%)	72 (8%)	13	9

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	M	169	SER
3	D	121	THR
2	M	193	SER
3	D	82	GLU
2	L	180	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	46	GLN

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	I	1	1	7,8,9	1.91	1 (14%)	9,10,12	2.27	5 (55%)
1	PCA	H	1	1	7,8,9	1.89	1 (14%)	9,10,12	2.17	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
1	PCA	I	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	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	4.81	1.47	1.34
1	I	1	PCA	CD-N	4.81	1.47	1.34

The worst 5 of 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	-3.49	107.90	112.70
1	I	1	PCA	CA-N-CD	-3.15	102.80	113.58
1	H	1	PCA	CB-CA-N	3.11	112.23	103.30
1	I	1	PCA	CB-CA-N	2.60	110.77	103.30

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 ⓘ

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	#$|Z| > 2$
4	EDO	L	301	-	3,3,3	0.54	0	2,2,2	0.26	0
6	NAG	C	201	3	14,14,15	0.34	0	17,19,21	0.43	0
4	EDO	H	301	-	3,3,3	0.64	0	2,2,2	0.21	0
5	FLC	I	301	-	12,12,12	1.15	1 (8%)	17,17,17	1.64	2 (11%)
4	EDO	L	302	-	3,3,3	0.54	0	2,2,2	0.54	0
6	NAG	D	201	3	14,14,15	0.60	0	17,19,21	0.59	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	EDO	L	301	-	-	0/1/1/1	-
6	NAG	C	201	3	-	2/6/23/26	0/1/1/1
4	EDO	H	301	-	-	0/1/1/1	-
5	FLC	I	301	-	-	4/16/16/16	-
4	EDO	L	302	-	-	1/1/1/1	-
6	NAG	D	201	3	-	0/6/23/26	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	-2.21	1.51	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
5	I	301	FLC	OB2-CBC-CB	4.32	120.55	113.05
5	I	301	FLC	OB1-CBC-CB	-4.05	116.52	122.25

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	I	301	FLC	CA-CB-CG-CGC
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	CBC-CB-CG-CGC

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	H	208/226 (92%)	-0.09	0	100	100	32, 41, 57, 70	0
1	I	207/226 (91%)	0.30	14 (6%)	17	21	35, 55, 82, 122	0
2	L	209/213 (98%)	-0.16	1 (0%)	91	92	31, 46, 62, 101	0
2	M	208/213 (97%)	0.01	1 (0%)	91	92	39, 54, 68, 87	0
3	C	117/125 (93%)	0.18	4 (3%)	45	51	30, 41, 76, 116	0
3	D	114/125 (91%)	0.52	7 (6%)	21	25	30, 48, 87, 110	0
All	All	1063/1128 (94%)	0.09	27 (2%)	57	62	30, 48, 74, 122	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	29	VAL	6.5
1	I	65	SER	4.5
3	D	27	PHE	4.3
1	I	64	LYS	3.5
3	D	28	ASN	3.2

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

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(Å²)	Q<0.9
1	PCA	H	1	8/9	0.86	0.22	49,59,70,77	0
1	PCA	I	1	8/9	0.86	0.17	57,61,75,78	0

6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4   Ligands ⓘ

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	EDO	H	301	4/4	0.74	0.12	49,51,58,61	0
6	NAG	C	201	14/15	0.82	0.23	66,71,74,75	0
6	NAG	D	201	14/15	0.87	0.20	82,87,91,92	0
5	FLC	I	301	13/13	0.89	0.24	62,72,85,89	0
4	EDO	L	302	4/4	0.93	0.09	40,44,45,48	0
4	EDO	L	301	4/4	0.96	0.11	35,35,36,37	0

6.5   Other polymers ⓘ

There are no such residues in this entry.