



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:00 PM UTC

PDB ID : 7Q8J / pdb_00007q8j
Title : Peptide IILKEK in complex with human cathepsin V C25S mutant
Authors : Loboda, J.; Sosnowski, P.; Tusar, L.; Vidmar, R.; Vizovisek, M.; Horvat, J.;
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Deposited on : 2021-11-11
Resolution : 1.64 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

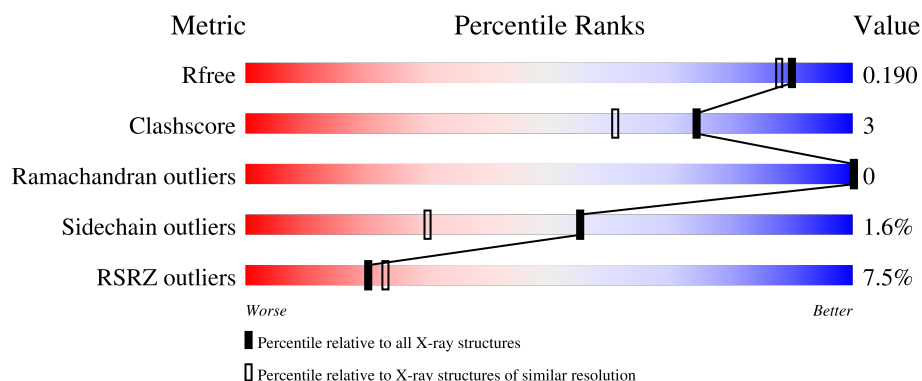
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.64 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	1141 (1.64-1.64)
Clashscore	190562	1171 (1.64-1.64)
Ramachandran outliers	187476	1151 (1.64-1.64)
Sidechain outliers	187428	1150 (1.64-1.64)
RSRZ outliers	180081	1141 (1.64-1.64)

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	AA	222	6% 86% 12% .
1	BA	222	6% 86% 13%
2	A	6	33% 33% 17% 50%
2	PA	6	50% 50% 50%
3	PB	3	67% 67% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	AA	301	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3834 atoms, of which 11 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 Cathepsin L2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AA	222	Total	C	H	N	O	S	9	0	0
			1701	1069	3	291	328	10			
1	BA	221	Total	C	H	N	O	S	15	0	0
			1698	1065	8	290	325	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	26	SER	CYS	engineered mutation	UNP O60911
AA	109	GLN	ASN	engineered mutation	UNP O60911
AA	180	GLN	ASN	engineered mutation	UNP O60911
BA	247	SER	CYS	engineered mutation	UNP O60911
BA	330	GLN	ASN	engineered mutation	UNP O60911
BA	401	GLN	ASN	engineered mutation	UNP O60911

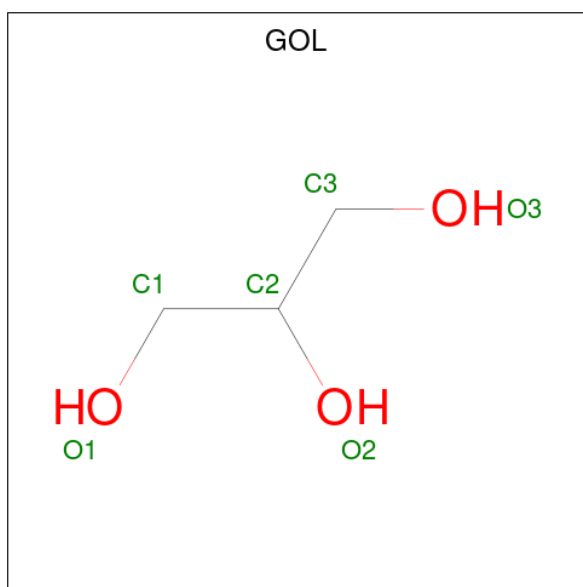
- Molecule 2 is a protein called IILKEK Peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	PA	6	Total	C	N	O	3	0	0
			52	35	8	9			
2	A	3	Total	C	N	O	0	0	0
			24	18	3	3			

- Molecule 3 is a protein called EYS Peptide.

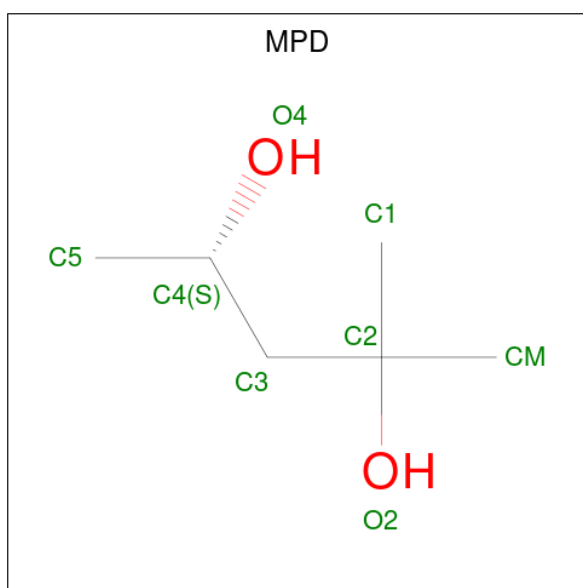
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	PB	3	Total	C	N	O	0	0	0
			28	17	3	8			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	BA	1	Total	C	O	0	0
			8	6	2		
5	BA	1	Total	C	O	0	0
			8	6	2		

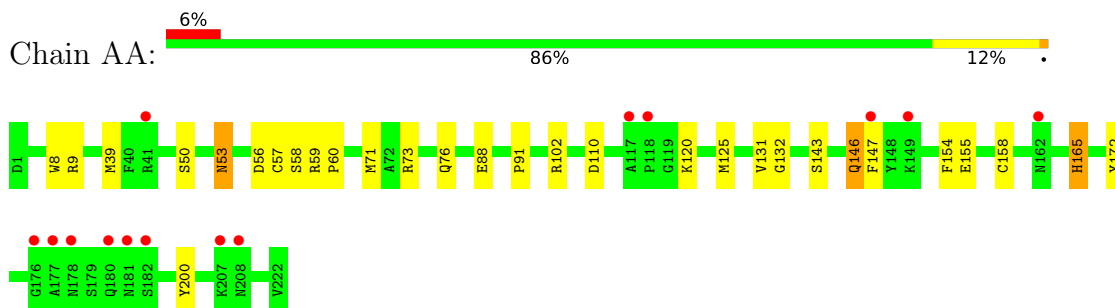
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	AA	155	Total 155	O 155	0	0
6	BA	146	Total 146	O 146	0	0
6	PA	1	Total 1	O 1	0	0
6	PB	1	Total 1	O 1	0	0

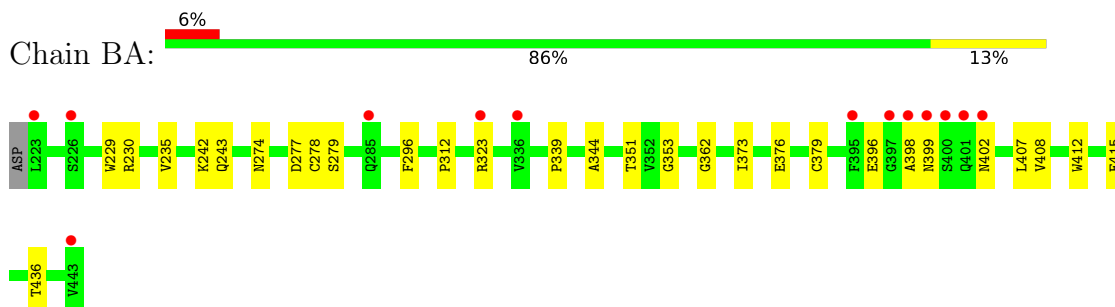
3 Residue-property plots [i](#)

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: Cathepsin L2



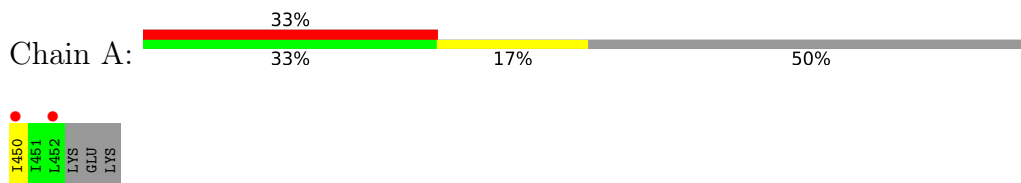
- Molecule 1: Cathepsin L2



- Molecule 2: IILKEK Peptide



- Molecule 2: IILKEK Peptide



- Molecule 3: EYS Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.82Å 93.82Å 125.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.91 – 1.64 46.91 – 1.64	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.91-1.64) 99.8 (46.91-1.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 1.64Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.193 , 0.217 0.191 , 0.190	Depositor DCC
R_{free} test set	2100 reflections (3.05%)	wwPDB-VP
Wilson B-factor (Å ²)	22.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3834	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MPD

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	AA	1.33	6/1740 (0.3%)	1.27	11/2351 (0.5%)
1	BA	1.24	4/1732 (0.2%)	1.35	14/2340 (0.6%)
2	A	0.26	0/23	0.76	0/30
2	PA	1.32	0/51	1.50	1/64 (1.6%)
3	PB	0.83	0/28	1.09	0/35
All	All	1.28	10/3574 (0.3%)	1.31	26/4820 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	39	MET	SD-CE	-12.93	1.47	1.79
1	AA	155	GLU	C-O	-7.90	1.18	1.25
1	BA	376	GLU	C-O	-7.25	1.19	1.25
1	AA	76	GLN	C-O	-6.63	1.16	1.24
1	AA	102	ARG	C-O	-5.85	1.19	1.25
1	BA	242	LYS	C-O	-5.75	1.18	1.24
1	BA	243	GLN	C-N	-5.32	1.25	1.33
1	AA	50	SER	C-N	5.22	1.41	1.34
1	BA	408	VAL	C-O	-5.22	1.18	1.24
1	AA	154	PHE	C-N	-5.09	1.28	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	279	SER	N-CA-C	10.71	124.32	112.97
1	AA	57	CYS	N-CA-C	10.07	125.77	113.38
1	BA	278	CYS	N-CA-C	9.63	125.34	113.50
1	BA	398	ALA	N-CA-C	9.33	123.16	111.69
1	AA	58	SER	N-CA-C	8.41	121.89	112.97
1	BA	408	VAL	N-CA-C	7.73	118.94	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	56	ASP	N-CA-C	7.05	120.00	111.82
1	BA	296	PHE	CA-CB-CG	6.83	120.63	113.80
1	BA	436	THR	N-CA-C	6.77	119.68	111.82
1	AA	53	ASN	N-CA-C	-6.44	104.26	111.28
1	BA	277	ASP	N-CA-C	6.32	119.15	111.82
1	AA	76	GLN	N-CA-C	-6.20	104.45	111.14
1	BA	344	ALA	N-CA-C	-6.04	104.78	111.36
1	AA	50	SER	N-CA-C	5.94	118.44	108.23
1	BA	339	PRO	N-CA-C	5.76	119.91	111.03
1	AA	131	VAL	N-CA-CB	-5.76	105.07	111.41
1	BA	243	GLN	N-CA-C	5.73	118.64	110.68
2	PA	448	GLU	N-CA-C	5.73	120.27	113.28
1	AA	71	MET	N-CA-C	5.60	117.38	111.28
1	BA	312	PRO	N-CA-C	5.58	119.77	111.41
1	BA	351	THR	N-CA-C	5.54	120.17	113.41
1	AA	110	ASP	CA-CB-CG	5.49	118.09	112.60
1	BA	235	VAL	N-CA-CB	-5.44	103.90	111.41
1	BA	274	ASN	N-CA-C	-5.44	105.25	111.07
1	AA	91	PRO	N-CA-C	5.19	119.19	111.41
1	AA	165	HIS	N-CA-CB	-5.05	102.33	110.71

There are no chirality outliers.

There are no planarity outliers.

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	AA	1698	3	1626	9	1
1	BA	1690	8	1619	7	1
2	A	24	0	32	1	0
2	PA	52	0	64	3	0
3	PB	28	0	19	0	0
4	AA	12	0	16	0	0
5	BA	16	0	28	6	0
6	AA	155	0	0	1	0
6	BA	146	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	PA	1	0	0	0	0
6	PB	1	0	0	0	0
All	All	3823	11	3404	21	1

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 3.

All (21) 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)
1:AA:73:ARG:HH21	2:PA:444:ILE:N	1.61	0.98
5:BA:502:MPD:H53	5:BA:502:MPD:H11	1.45	0.95
5:BA:502:MPD:H11	5:BA:502:MPD:C5	2.09	0.82
1:AA:73:ARG:NH2	2:PA:444:ILE:N	2.37	0.69
1:BA:230:ARG:NH1	1:BA:407:LEU:HD21	2.13	0.64
1:AA:165:HIS:HD1	2:A:450:ILE:N	1.96	0.64
1:BA:373:ILE:HD11	1:BA:396:GLU:HG3	1.79	0.64
1:BA:399:ASN:OD1	1:BA:402:ASN:HB2	2.00	0.61
1:BA:229:TRP:CE2	1:BA:353:GLY:HA2	2.37	0.59
1:AA:120:LYS:NZ	6:AA:401:HOH:O	2.26	0.54
5:BA:502:MPD:C5	5:BA:502:MPD:C1	2.81	0.52
5:BA:502:MPD:H4	6:BA:665:HOH:O	2.10	0.52
1:AA:146:GLN:HG2	1:AA:147:PHE:CD2	2.45	0.52
1:BA:415:GLU:HG3	6:BA:688:HOH:O	2.16	0.46
1:AA:9:ARG:HD3	1:AA:200:TYR:CE2	2.52	0.45
1:AA:125:MET:HE3	1:AA:172:TYR:CE1	2.53	0.44
1:AA:59:ARG:N	1:AA:60:PRO:CD	2.80	0.44
1:BA:362:GLY:HA2	5:BA:502:MPD:H52	1.99	0.44
1:BA:412:TRP:CD1	5:BA:501:MPD:H52	2.53	0.43
2:PA:445:ILE:HD12	2:PA:445:ILE:C	2.43	0.42
1:AA:8:TRP:CE2	1:AA:132:GLY:HA2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:88:GLU:OE2	1:BA:323:ARG:NH1[3_554]	2.09	0.11

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	AA	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
1	BA	219/222 (99%)	213 (97%)	6 (3%)	0	100	100
2	A	1/6 (17%)	1 (100%)	0	0	100	100
2	PA	4/6 (67%)	4 (100%)	0	0	100	100
3	PB	1/3 (33%)	1 (100%)	0	0	100	100
All	All	445/459 (97%)	432 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	AA	180/180 (100%)	176 (98%)	4 (2%)	45	18
1	BA	179/180 (99%)	178 (99%)	1 (1%)	78	66
2	A	3/6 (50%)	3 (100%)	0	100	100
2	PA	6/6 (100%)	6 (100%)	0	100	100
3	PB	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	371/375 (99%)	365 (98%)	6 (2%)	55	30

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	53	ASN
1	AA	143	SER
1	AA	146	GLN
1	AA	158	CYS
1	BA	379	CYS
3	PB	453	GLU

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

Mol	Chain	Res	Type
1	AA	109	GLN
1	AA	146	GLN
1	AA	181	ASN
1	AA	198	ASN
1	AA	221	ASN
1	BA	241	GLN
1	BA	259	GLN
1	BA	383	ASN
1	BA	442	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	GOL	AA	301	-	5,5,5	0.16	0	5,5,5	0.18	0
5	MPD	BA	501	-	7,7,7	0.31	0	9,10,10	0.39	0
4	GOL	AA	302	-	5,5,5	0.14	0	5,5,5	0.49	0
5	MPD	BA	502	-	7,7,7	0.33	0	9,10,10	0.28	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	GOL	AA	301	-	-	0/4/4/4	-
5	MPD	BA	501	-	-	0/5/5/5	-
4	GOL	AA	302	-	-	0/4/4/4	-
5	MPD	BA	502	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	BA	502	MPD	O2-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BA	501	MPD	1	0
5	BA	502	MPD	5	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(Å ²)	Q < 0.9
1	AA	222/222 (100%)	0.21	14 (6%)	26 29	10, 18, 43, 73	3 (1%)
1	BA	221/222 (99%)	0.21	13 (5%)	28 31	11, 19, 44, 105	3 (1%)
2	A	3/6 (50%)	2.53	2 (66%)	0 0	29, 29, 38, 46	0
2	PA	6/6 (100%)	3.10	3 (50%)	0 0	24, 30, 68, 69	1 (16%)
3	PB	3/3 (100%)	1.74	2 (66%)	0 0	24, 24, 29, 65	0
All	All	455/459 (99%)	0.27	34 (7%)	20 23	10, 19, 47, 105	7 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PA	444	ILE	7.8
1	AA	177	ALA	5.9
1	BA	402	ASN	5.4
2	PA	449	LYS	4.4
1	AA	180	GLN	4.3
1	AA	117	ALA	4.2
1	AA	181	ASN	4.1
1	BA	397	GLY	4.0
1	BA	398	ALA	4.0
2	PA	445	ILE	3.6
1	BA	223	LEU	3.6
2	A	452	LEU	3.5
1	AA	118	PRO	3.4
1	AA	178	ASN	3.4
1	BA	400	SER	3.2
1	AA	176	GLY	3.2
1	BA	443	VAL	3.0
1	BA	399	ASN	2.7
1	BA	226	SER	2.6
1	AA	162	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
3	PB	453	GLU	2.6
1	BA	395	PHE	2.5
1	BA	323	ARG	2.4
1	AA	149	LYS	2.4
1	AA	41	ARG	2.3
1	AA	182	SER	2.3
3	PB	454	TYR	2.3
2	A	450	ILE	2.2
1	BA	401	GLN	2.2
1	AA	208	ASN	2.2
1	BA	336	VAL	2.1
1	AA	147	PHE	2.1
1	BA	285	GLN	2.0
1	AA	207	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

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	GOL	AA	301	6/6	0.72	0.46	124,125,125,126	0
4	GOL	AA	302	6/6	0.78	0.25	57,65,67,67	0
5	MPD	BA	501	8/8	0.85	0.20	52,55,57,57	0
5	MPD	BA	502	8/8	0.90	0.25	49,54,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.