



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:49 PM UTC

PDB ID : 7Q9C / pdb_00007q9c
Title : Peptide RLSAKP in complex with human cathepsin V C25A mutant
Authors : Loboda, J.; Sosnowski, P.; Tusar, L.; Vidmar, R.; Vizovisek, M.; Horvat, J.;
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Deposited on : 2021-11-12
Resolution : 1.40 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

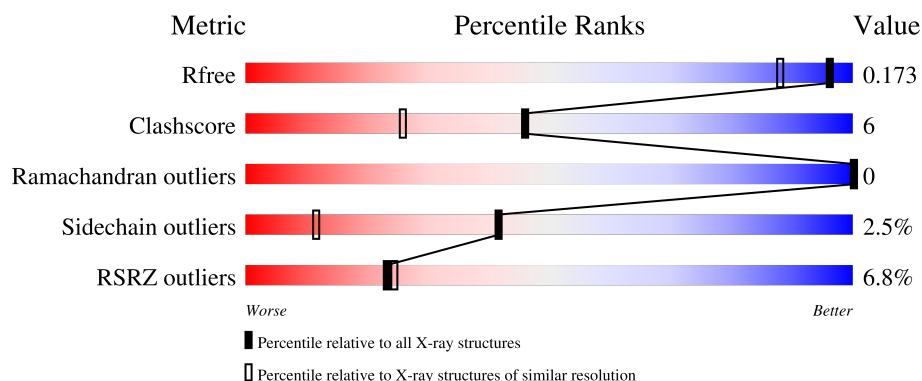
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	AA	221	2% 91% 9%
1	BA	221	7% 89% 9%
2	PAA	8	38% 38% 62%
2	PAC	8	38% 38% 12% 50%
2	PBA	8	50% 25% 50% 25%

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
3	CL	AA	301[B]	-	-	-	X
4	MPD	AA	303[B]	-	-	-	X
4	MPD	BA	508	-	-	X	-
6	TFA	AA	313	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8591 atoms, of which 4420 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 Human cathepsin V.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AA	221	Total	C	H	N	O	S	1660	5	0
			3389	1089	1658	297	335	10			
1	BA	221	Total	C	H	N	O	S	1676	5	0
			3399	1090	1672	297	330	10			

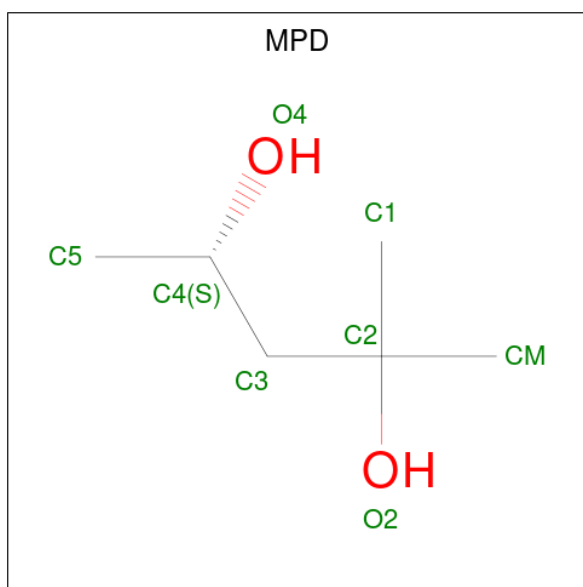
- Molecule 2 is a protein called RLSAKP Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	PAA	3	Total	C	H	N	O	29	3	0
			54	15	29	6	4			
2	PAC	4	Total	C	H	N	O	27	4	1
			49	14	27	5	3			
2	PBA	6	Total	C	H	N	O	54	1	1
			95	27	54	8	6			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AA	4	Total	Cl	0	1
			4	4		
3	BA	1	Total	Cl	0	0
			1	1		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



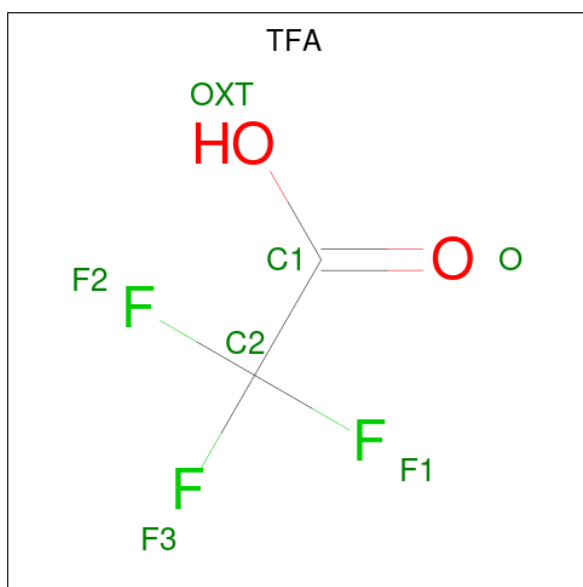
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	AA	1	Total	C	O	0	1
			8	6	2		
4	AA	1	Total	C	O	0	1
			8	6	2		
4	AA	1	Total	C	O	0	1
			8	6	2		
4	AA	1	Total	C	O	0	0
			8	6	2		
4	BA	1	Total	C	O	0	0
			8	6	2		
4	BA	1	Total	C	O	0	0
			8	6	2		
4	BA	1	Total	C	O	0	0
			8	6	2		
4	BA	1	Total	C	O	0	0
			8	6	2		
4	PBA	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is trifluoroacetic acid (CCD ID: TFA) (formula: $C_2HF_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	AA	1	Total	C	F	O	0	0
			7	2	3	2		
6	AA	1	Total	C	F	O	0	0
			7	2	3	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	AA	252	Total	H	O	504	1
			756	504	252		
7	BA	233	Total	H	O	466	0
			699	466	233		
7	PAC	2	Total	H	O	4	0
			6	4	2		
7	PBA	3	Total	H	O	6	0
			9	6	3		

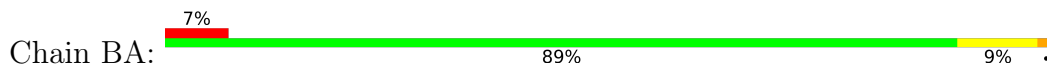
3 Residue-property plots [i](#)

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: Human cathepsin V



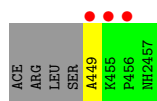
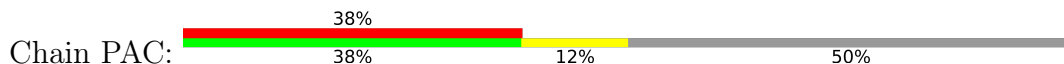
- Molecule 1: Human cathepsin V



- Molecule 2: RLSAKP Peptide



- Molecule 2: RLSAKP Peptide



- Molecule 2: RLSAKP Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.10Å 94.10Å 124.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.05 – 1.40 47.05 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.05-1.40) 100.0 (47.05-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.32Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.184 , 0.210 (Not available) , 0.173	Depositor DCC
R_{free} test set	2100 reflections (1.60%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 56.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8591	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: NH2, MPD, TFA, GOL, CL

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	0.83	0/1773	1.11	6/2396 (0.3%)
1	BA	0.86	1/1772 (0.1%)	1.14	9/2390 (0.4%)
2	PAA	1.64	1/24 (4.2%)	0.99	0/30
2	PAC	1.35	0/21	1.38	0/27
2	PBA	0.49	0/44	1.30	0/58
All	All	0.85	2/3634 (0.1%)	1.13	15/4901 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BA	259	MET	SD-CE	-7.54	1.60	1.79
2	PAA	444[A]	LEU	CA-C	-5.31	1.46	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	109	ASP	CA-CB-CG	7.23	119.83	112.60
1	AA	130	VAL	N-CA-C	6.77	118.11	111.67
1	BA	330	ASP	CA-CB-CG	6.76	119.36	112.60
1	AA	49	SER	N-CA-C	6.49	118.86	108.41
1	BA	351	VAL	N-CA-C	6.47	117.82	111.67
1	AA	52	ASN	CA-CB-CG	6.43	119.03	112.60
1	BA	270	SER	N-CA-C	5.88	118.33	107.99
1	BA	439	TYR	CA-C-N	5.81	125.72	119.85
1	BA	439	TYR	C-N-CA	5.81	125.72	119.85
1	BA	338	PRO	N-CA-C	5.65	119.95	111.14
1	BA	234	VAL	N-CA-C	5.47	115.77	108.11
1	BA	276	ASP	N-CA-C	5.46	118.16	111.82
1	BA	311	PRO	N-CA-C	5.41	119.82	111.21
1	AA	90	PRO	N-CA-C	5.28	119.60	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	55	ASP	N-CA-C	5.07	117.70	111.82

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	1731	1658	1652	12	0
1	BA	1727	1672	1664	11	0
2	PAA	25	29	28	2	0
2	PAC	22	27	24	2	0
2	PBA	41	54	49	3	0
3	AA	4	0	0	0	0
3	BA	1	0	0	1	0
4	AA	32	0	34	5	0
4	BA	40	0	70	11	0
4	PBA	8	0	14	4	0
5	AA	24	0	32	3	0
5	BA	12	0	16	1	0
6	AA	14	0	0	2	0
7	AA	252	504	0	3	2
7	BA	233	466	0	3	2
7	PAC	2	4	0	0	0
7	PBA	3	6	0	0	0
All	All	4171	4420	3583	42	2

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 6.

All (42) 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:PAA:445[A]:SER:O	2:PAC:449[A]:ALA:N	1.80	1.14
2:PBA:455:LEU:HD21	4:PBA:501:MPD:HM1	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:BA:508:MPD:H53	4:BA:508:MPD:H12	1.46	0.97
4:BA:503:MPD:H52	7:BA:824:HOH:O	1.79	0.83
4:BA:508:MPD:H4	7:BA:762:HOH:O	1.82	0.80
2:PBA:455:LEU:HD21	4:PBA:501:MPD:CM	2.14	0.77
1:AA:145[B]:GLN:NE2	6:AA:313:TFA:OXT	2.18	0.76
4:PBA:501:MPD:HM1	4:PBA:501:MPD:O4	2.02	0.60
1:BA:318:ILE:HD13	4:BA:508:MPD:C5	2.31	0.60
4:AA:303[B]:MPD:H11	4:AA:303[B]:MPD:C5	2.31	0.60
1:AA:18:ASN:HB3	5:AA:309:GOL:H11	1.84	0.59
4:BA:506:MPD:O4	4:BA:506:MPD:CM	2.51	0.59
4:AA:303[B]:MPD:H12	7:AA:422:HOH:O	2.02	0.59
1:AA:199:TYR:HB2	5:AA:306:GOL:H31	1.85	0.58
4:AA:312:MPD:HM1	4:AA:312:MPD:O4	2.04	0.58
1:BA:318:ILE:HD13	4:BA:508:MPD:H51	1.87	0.57
1:BA:320:LYS:O	5:BA:505:GOL:H31	2.06	0.56
1:AA:209:HIS:O	1:AA:212[A]:ILE:HG13	2.08	0.54
1:AA:141:HIS:HD2	7:AA:420:HOH:O	1.90	0.54
1:BA:287[A]:ASN:ND2	7:BA:606:HOH:O	2.41	0.54
2:PAA:445[A]:SER:C	2:PAC:449[A]:ALA:N	2.65	0.51
3:BA:504:CL:CL	4:PBA:501:MPD:HM2	2.49	0.49
1:BA:242:GLN:N	1:BA:242:GLN:CD	2.71	0.48
1:BA:279:ARG:HD2	4:BA:508:MPD:H11	1.95	0.48
1:AA:7:TRP:CE2	1:AA:131:GLY:HA2	2.49	0.47
4:BA:508:MPD:H53	4:BA:508:MPD:C1	2.23	0.46
1:BA:259:MET:SD	1:BA:442[B]:VAL:HG21	2.57	0.45
1:BA:299:LYS:HE2	1:BA:331:THR:O	2.16	0.45
1:BA:336:VAL:O	1:BA:338:PRO:HD3	2.18	0.44
2:PBA:457:ALA:C	2:PBA:458[B]:LYS:HD3	2.42	0.44
1:BA:398:ASN:HB3	1:BA:401:ASN:OD1	2.17	0.43
1:AA:8:ARG:HD3	1:AA:199:TYR:CE2	2.54	0.43
1:AA:40:ARG:NE	7:AA:408:HOH:O	2.50	0.43
4:BA:508:MPD:O2	4:BA:508:MPD:H52	2.18	0.43
4:BA:508:MPD:C5	4:BA:508:MPD:O2	2.67	0.43
1:AA:145[B]:GLN:HE22	6:AA:313:TFA:C1	2.32	0.42
1:AA:163:ASP:OD2	4:AA:303[B]:MPD:O2	2.37	0.42
1:AA:91:TYR:CD2	5:AA:309:GOL:H31	2.54	0.42
4:BA:503:MPD:O4	4:BA:503:MPD:HM1	2.18	0.42
4:AA:302[B]:MPD:O2	4:AA:302[B]:MPD:C5	2.68	0.41
1:BA:368:TYR:CZ	1:BA:421:VAL:HG23	2.56	0.41
1:AA:212[A]:ILE:HG13	1:AA:212[A]:ILE:H	1.63	0.41

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:AA:614:HOH:O	7:BA:773:HOH:O[6_555]	2.13	0.07
7:AA:579:HOH:O	7:BA:646:HOH:O[4_445]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AA	224/221 (101%)	218 (97%)	6 (3%)	0	100	100
1	BA	223/221 (101%)	216 (97%)	7 (3%)	0	100	100
2	PAA	1/8 (12%)	1 (100%)	0	0	100	100
2	PAC	2/8 (25%)	2 (100%)	0	0	100	100
2	PBA	5/8 (62%)	5 (100%)	0	0	100	100
All	All	455/466 (98%)	442 (97%)	13 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	183/178 (103%)	179 (98%)	4 (2%)	45	14
1	BA	183/178 (103%)	179 (98%)	4 (2%)	45	14
2	PAA	3/5 (60%)	2 (67%)	1 (33%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	PAC	2/5 (40%)	2 (100%)	0	100	100
2	PBA	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	376/371 (101%)	366 (97%)	10 (3%)	42	10

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	157	CYS
1	AA	196	SER
1	AA	212[A]	ILE
1	AA	212[B]	ILE
1	BA	242	GLN
1	BA	299	LYS
1	BA	366	GLN
1	BA	378	CYS
2	PAA	443[A]	ARG
2	PBA	456	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	141	HIS
1	AA	179	GLN
1	AA	220	ASN
1	BA	240	GLN
1	BA	366	GLN
1	BA	382	ASN
1	BA	441	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 23 ligands modelled in this entry, 5 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	AA	310	-	5,5,5	0.90	0	5,5,5	1.31	1 (20%)
4	MPD	AA	303[B]	-	7,7,7	1.70	2 (28%)	9,10,10	0.97	0
5	GOL	AA	306	-	5,5,5	0.40	0	5,5,5	0.66	0
5	GOL	BA	505	-	5,5,5	0.90	0	5,5,5	1.55	1 (20%)
4	MPD	AA	312	-	7,7,7	0.80	0	9,10,10	0.63	0
5	GOL	AA	309	-	5,5,5	0.59	0	5,5,5	1.21	1 (20%)
6	TFA	AA	313	-	6,6,6	2.62	2 (33%)	9,9,9	1.65	1 (11%)
4	MPD	AA	302[B]	-	7,7,7	0.34	0	9,10,10	0.26	0
4	MPD	BA	506	-	7,7,7	0.70	0	9,10,10	0.73	0
4	MPD	BA	508	-	7,7,7	1.00	1 (14%)	9,10,10	0.43	0
4	MPD	BA	501	-	7,7,7	0.37	0	9,10,10	0.58	0
4	MPD	BA	502	-	7,7,7	0.45	0	9,10,10	0.35	0
4	MPD	PBA	501	-	7,7,7	0.70	0	9,10,10	0.39	0
5	GOL	AA	314	-	5,5,5	0.33	0	5,5,5	0.50	0
6	TFA	AA	311	-	6,6,6	1.74	2 (33%)	9,9,9	1.10	1 (11%)
4	MPD	BA	503	-	7,7,7	0.41	0	9,10,10	0.35	0
5	GOL	BA	507	-	5,5,5	0.57	0	5,5,5	0.44	0
4	MPD	AA	304[B]	-	7,7,7	0.29	0	9,10,10	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	AA	310	-	-	1/4/4/4	-
4	MPD	AA	303[B]	-	-	2/5/5/5	-
5	GOL	AA	306	-	-	1/4/4/4	-
5	GOL	BA	505	-	-	2/4/4/4	-
4	MPD	AA	312	-	-	0/5/5/5	-
5	GOL	AA	309	-	-	0/4/4/4	-
6	TFA	AA	313	-	-	0/6/6/6	-
4	MPD	AA	302[B]	-	-	0/5/5/5	-
4	MPD	BA	506	-	-	2/5/5/5	-
4	MPD	BA	508	-	-	1/5/5/5	-
4	MPD	BA	501	-	-	0/5/5/5	-
4	MPD	BA	502	-	-	2/5/5/5	-
4	MPD	PBA	501	-	-	0/5/5/5	-
5	GOL	AA	314	-	-	0/4/4/4	-
6	TFA	AA	311	-	-	1/6/6/6	-
4	MPD	BA	503	-	-	1/5/5/5	-
5	GOL	BA	507	-	-	2/4/4/4	-
4	MPD	AA	304[B]	-	-	3/5/5/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AA	313	TFA	OXT-C1	-5.23	1.11	1.30
4	AA	303[B]	MPD	O2-C2	-3.60	1.36	1.44
6	AA	313	TFA	F3-C2	-3.14	1.19	1.32
6	AA	311	TFA	F1-C2	-2.69	1.21	1.32
4	BA	508	MPD	C5-C4	-2.50	1.41	1.51
4	AA	303[B]	MPD	C3-C2	-2.35	1.47	1.54
6	AA	311	TFA	OXT-C1	-2.27	1.22	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AA	313	TFA	F1-C2-C1	-3.82	98.28	111.90
5	BA	505	GOL	C3-C2-C1	2.64	121.50	111.80
5	AA	310	GOL	O1-C1-C2	-2.22	100.36	110.38
5	AA	309	GOL	C3-C2-C1	2.15	119.67	111.80
6	AA	311	TFA	OXT-C1-C2	2.08	120.71	112.58

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AA	303[B]	MPD	C2-C3-C4-C5
4	AA	304[B]	MPD	C1-C2-C3-C4
4	AA	304[B]	MPD	O2-C2-C3-C4
4	BA	506	MPD	C2-C3-C4-C5
4	BA	508	MPD	C2-C3-C4-C5
5	BA	505	GOL	O1-C1-C2-O2
5	BA	505	GOL	O1-C1-C2-C3
5	BA	507	GOL	O2-C2-C3-O3
5	BA	507	GOL	C1-C2-C3-O3
5	AA	310	GOL	O1-C1-C2-O2
4	BA	503	MPD	C2-C3-C4-O4
4	AA	304[B]	MPD	CM-C2-C3-C4
4	AA	303[B]	MPD	O2-C2-C3-C4
4	BA	502	MPD	O2-C2-C3-C4
4	BA	502	MPD	CM-C2-C3-C4
4	BA	506	MPD	C1-C2-C3-C4
6	AA	311	TFA	OXT-C1-C2-F1
5	AA	306	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AA	303[B]	MPD	3	0
5	AA	306	GOL	1	0
5	BA	505	GOL	1	0
4	AA	312	MPD	1	0
5	AA	309	GOL	2	0
6	AA	313	TFA	2	0
4	AA	302[B]	MPD	1	0
4	BA	506	MPD	1	0
4	BA	508	MPD	8	0
4	PBA	501	MPD	4	0
4	BA	503	MPD	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	AA	221/221 (100%)	-0.04	5 (2%) 61 63	4, 8, 14, 28	6 (2%)
1	BA	221/221 (100%)	0.61	16 (7%) 21 22	5, 11, 20, 39	7 (3%)
2	PAA	3/8 (37%)	3.53	3 (100%) 0 0	10, 10, 14, 20	3 (100%)
2	PAC	3/8 (37%)	4.45	3 (100%) 0 0	12, 12, 15, 17	3 (100%)
2	PBA	5/8 (62%)	4.61	4 (80%) 0 0	9, 12, 39, 44	1 (20%)
All	All	453/466 (97%)	0.38	31 (6%) 23 24	4, 9, 18, 44	20 (4%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PBA	455	LEU	8.0
2	PBA	456	SER	5.8
2	PAC	449[A]	ALA	4.9
1	AA	116	ALA	4.8
2	PAC	455[A]	LYS	4.6
1	BA	442[A]	VAL	4.3
2	PAA	445[A]	SER	4.3
2	PBA	457	ALA	4.1
1	BA	222	LEU	3.9
2	PAC	456[A]	PRO	3.8
2	PAA	443[A]	ARG	3.7
1	BA	400	GLN	3.6
1	BA	401	ASN	3.5
2	PBA	458[A]	LYS	3.2
1	BA	381[A]	LYS	3.0
1	BA	397	ALA	2.8
1	AA	66[A]	ASN	2.8
2	PAA	444[A]	LEU	2.6
1	BA	335	VAL	2.6
1	BA	338	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	BA	337	ALA	2.5
1	AA	117	PRO	2.5
1	BA	428	ASN	2.4
1	BA	398	ASN	2.4
1	BA	433[A]	ILE	2.3
1	BA	343	ALA	2.2
1	BA	344	LEU	2.2
1	AA	87	GLU	2.2
1	BA	399	SER	2.1
1	AA	212[A]	ILE	2.0
1	BA	351	VAL	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	MPD	AA	304[B]	8/8	0.58	0.23	38,43,52,53	8
4	MPD	BA	508	8/8	0.58	0.30	69,85,95,96	0
3	CL	AA	301[B]	1/1	0.59	0.58	53,53,53,53	1
6	TFA	AA	313	7/7	0.66	0.17	96,97,102,104	0
5	GOL	AA	314	6/6	0.67	0.18	30,30,30,30	0
4	MPD	AA	303[B]	8/8	0.67	0.59	46,51,52,53	8
4	MPD	PBA	501	8/8	0.71	0.26	82,87,93,94	0
5	GOL	AA	310	6/6	0.75	0.20	35,63,77,84	0
5	GOL	AA	309	6/6	0.80	0.24	47,57,63,67	0
4	MPD	BA	506	8/8	0.83	0.34	71,80,86,87	0
4	MPD	AA	302[B]	8/8	0.86	0.30	50,55,58,58	8
5	GOL	AA	306	6/6	0.87	0.16	21,26,36,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MPD	AA	312	8/8	0.88	0.31	75,86,96,97	0
4	MPD	BA	502	8/8	0.88	0.16	27,33,41,42	0
4	MPD	BA	501	8/8	0.89	0.12	22,25,27,28	0
4	MPD	BA	503	8/8	0.89	0.28	67,76,81,83	0
6	TFA	AA	311	7/7	0.91	0.10	21,32,35,36	0
5	GOL	BA	505	6/6	0.91	0.13	30,35,39,40	0
5	GOL	BA	507	6/6	0.92	0.13	22,35,52,53	0
3	CL	AA	307	1/1	0.95	0.09	23,23,23,23	0
3	CL	BA	504	1/1	0.97	0.12	25,25,25,25	0
3	CL	AA	308	1/1	0.99	0.10	22,22,22,22	0
3	CL	AA	305	1/1	0.99	0.14	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.