



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2022 – 12:08 pm GMT

PDB ID : 7Q9C
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

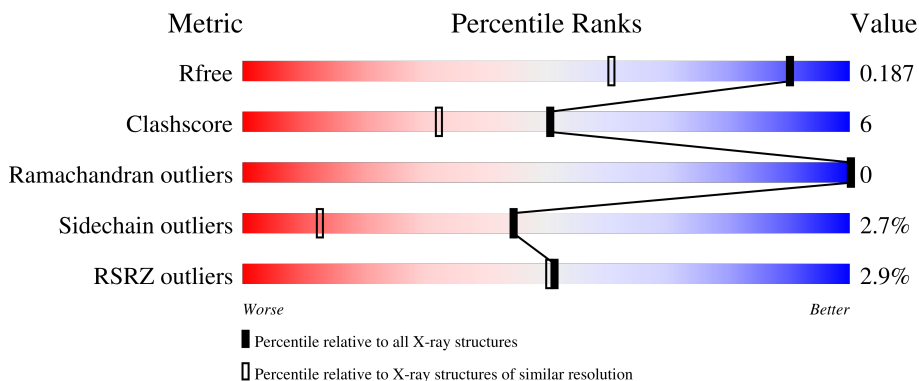
1 Overall quality at a glance

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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (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	
1	BA	221	
2	PAA	8	
2	PAC	8	
2	PBA	8	

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 [i](#)

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	
			Total	C	H	N	O				S
1	AA	221	3389	1089	1658	297	335	10	1660	5	0
1	BA	221	3399	1090	1672	297	330	10	1676	5	0

- Molecule 2 is a protein called RLSAKP Peptide.

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

- Molecule 3 is CHLORIDE ION (three-letter code: 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 (three-letter code: MPD) (formula: C₆H₁₄O₂).



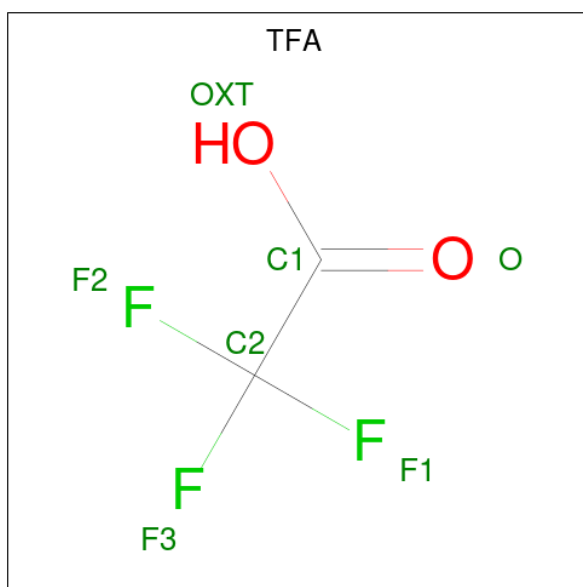
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AA	1	Total C O 8 6 2	0	1
4	AA	1	Total C O 8 6 2	0	1
4	AA	1	Total C O 8 6 2	0	1
4	AA	1	Total C O 8 6 2	0	0
4	BA	1	Total C O 8 6 2	0	0
4	BA	1	Total C O 8 6 2	0	0
4	BA	1	Total C O 8 6 2	0	0
4	BA	1	Total C O 8 6 2	0	0
4	BA	1	Total C O 8 6 2	0	0
4	PBA	1	Total C O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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is trifluoroacetic acid (three-letter code: TFA) (formula: C₂HF₃O₂).



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](#)

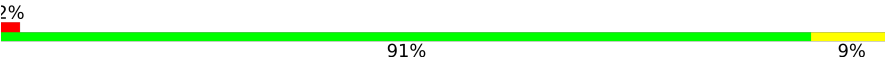
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

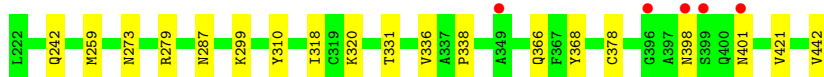
- Molecule 1: Human cathepsin V

Chain AA:  93% 7%



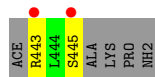
- Molecule 1: Human cathepsin V

Chain BA:  2% 91% 9%



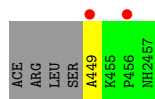
- Molecule 2: RLSAKP Peptide

Chain PAA:  12% 25% 62%




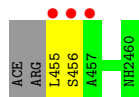
- Molecule 2: RLSAKP Peptide

Chain PAC:  25% 38% 12% 50%



- Molecule 2: RLSAKP Peptide

Chain PBA:  38% 50% 25% 25%



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 – 1.32	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.05-1.40) 99.8 (47.05-1.32)	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 0.190 , 0.187	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)	(Not available) , (Not available)	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, TFA, MPD, 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	0.58	0/1773	0.74	0/2396
1	BA	0.58	0/1772	0.75	0/2390
2	PAA	1.07	0/24	0.78	0/30
2	PAC	1.23	0/21	1.30	0/27
2	PBA	0.48	0/44	0.82	0/58
All	All	0.59	0/3634	0.75	0/4901

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	2	0
3	AA	4	0	0	0	0
3	BA	1	0	0	1	0
4	AA	32	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3581	41	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 (41) 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
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
3:BA:504:CL:CL	4:PBA:501:MPD:HM2	2.49	0.49
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
2:PAA:445[A]:SER:C	2:PAC:449[A]:ALA:N	2.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:BA:242:GLN:N	1:BA:242:GLN:CD	2.71	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 symmetry 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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	52	19
1	BA	183/178 (103%)	179 (98%)	4 (2%)	52	19
2	PAA	3/5 (60%)	2 (67%)	1 (33%)	0	0
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%)	44	13

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

Mol	Chain	Res	Type
1	AA	52	ASN
1	AA	89	TYR
1	AA	157	CYS
1	AA	196	SER
1	BA	273	ASN
1	BA	310	TYR
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 (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	AA	141	HIS
1	AA	179	GLN
1	BA	382	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 monosaccharides 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
4	MPD	AA	312	-	7,7,7	0.77	0	9,10,10	0.63	0
6	TFA	AA	313	-	6,6,6	2.48	2 (33%)	9,9,9	1.58	1 (11%)
4	MPD	BA	502	-	7,7,7	0.42	0	9,10,10	0.35	0
5	GOL	AA	306	-	5,5,5	0.38	0	5,5,5	0.59	0
4	MPD	BA	503	-	7,7,7	0.37	0	9,10,10	0.33	0
5	GOL	BA	505	-	5,5,5	0.83	0	5,5,5	1.45	1 (20%)
4	MPD	AA	304[B]	-	7,7,7	0.26	0	9,10,10	0.30	0
4	MPD	BA	506	-	7,7,7	0.65	0	9,10,10	0.75	0
4	MPD	AA	302[B]	-	7,7,7	0.32	0	9,10,10	0.26	0
4	MPD	PBA	501	-	7,7,7	0.66	0	9,10,10	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	TFA	AA	311	-	6,6,6	1.64	2 (33%)	9,9,9	1.05	0
4	MPD	AA	303[B]	-	7,7,7	1.66	2 (28%)	9,10,10	1.00	1 (11%)
5	GOL	AA	309	-	5,5,5	0.57	0	5,5,5	1.14	1 (20%)
5	GOL	AA	314	-	5,5,5	0.32	0	5,5,5	0.44	0
4	MPD	BA	508	-	7,7,7	0.94	1 (14%)	9,10,10	0.38	0
4	MPD	BA	501	-	7,7,7	0.35	0	9,10,10	0.56	0
5	GOL	BA	507	-	5,5,5	0.54	0	5,5,5	0.40	0
5	GOL	AA	310	-	5,5,5	0.84	0	5,5,5	1.23	1 (20%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AA	313	TFA	OXT-C1	-4.99	1.11	1.30
4	AA	303[B]	MPD	O2-C2	-3.45	1.36	1.44
6	AA	313	TFA	F3-C2	-2.95	1.19	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	AA	311	TFA	F1-C2	-2.52	1.21	1.32
4	BA	508	MPD	C5-C4	-2.37	1.41	1.51
4	AA	303[B]	MPD	C3-C2	-2.35	1.47	1.53
6	AA	311	TFA	OXT-C1	-2.15	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	-3.65	98.28	111.85
5	BA	505	GOL	C3-C2-C1	2.52	121.50	111.70
4	AA	303[B]	MPD	O2-C2-C3	-2.09	101.94	109.80
5	AA	310	GOL	O1-C1-C2	-2.05	100.36	110.20
5	AA	309	GOL	C3-C2-C1	2.05	119.67	111.70

There are no chirality outliers.

All (15) 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	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
4	BA	502	MPD	O2-C2-C3-C4
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	BA	506	MPD	O2-C2-C3-C4
4	AA	302[B]	MPD	C2-C3-C4-C5
6	AA	311	TFA	OXT-C1-C2-F1

There are no ring outliers.

11 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AA	312	MPD	1	0
6	AA	313	TFA	2	0
5	AA	306	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	BA	503	MPD	2	0
5	BA	505	GOL	1	0
4	BA	506	MPD	1	0
4	AA	302[B]	MPD	1	0
4	PBA	501	MPD	4	0
4	AA	303[B]	MPD	3	0
5	AA	309	GOL	2	0
4	BA	508	MPD	8	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.15	1 (0%) 91 89	10, 15, 27, 46	1 (0%)
1	BA	221/221 (100%)	0.27	5 (2%) 60 60	12, 20, 42, 73	2 (0%)
2	PAA	3/8 (37%)	2.91	2 (66%) 0 0	33, 33, 36, 63	3 (100%)
2	PAC	3/8 (37%)	2.73	2 (66%) 0 0	33, 33, 48, 53	3 (100%)
2	PBA	5/8 (62%)	4.20	3 (60%) 0 0	23, 37, 81, 92	0
All	All	453/466 (97%)	0.14	13 (2%) 51 50	10, 17, 39, 92	9 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PBA	455	LEU	12.1
2	PAA	443[A]	ARG	4.5
1	BA	396	GLY	4.1
2	PBA	456	SER	3.9
2	PAC	449[A]	ALA	3.5
1	BA	398	ASN	3.4
1	AA	116	ALA	3.2
1	BA	401	ASN	3.0
2	PBA	457	ALA	2.9
2	PAA	445[A]	SER	2.8
2	PAC	456[A]	PRO	2.7
1	BA	399	SER	2.2
1	BA	349	ALA	2.2

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 monosaccharides 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
3	CL	AA	301[B]	1/1	0.34	0.63	53,53,53,53	1
4	MPD	BA	503	8/8	0.41	0.34	67,76,81,83	0
4	MPD	AA	303[B]	8/8	0.48	0.45	46,51,52,53	8
6	TFA	AA	313	7/7	0.57	0.39	96,97,102,104	0
5	GOL	AA	314	6/6	0.59	0.36	30,30,30,30	0
4	MPD	PBA	501	8/8	0.62	0.28	82,87,93,94	0
4	MPD	AA	304[B]	8/8	0.65	0.26	38,43,52,53	8
5	GOL	AA	309	6/6	0.68	0.20	47,57,63,67	0
6	TFA	AA	311	7/7	0.75	0.13	21,32,35,36	0
4	MPD	BA	508	8/8	0.75	0.21	69,85,95,96	0
4	MPD	BA	501	8/8	0.76	0.13	22,25,27,28	0
4	MPD	BA	506	8/8	0.78	0.28	71,80,86,87	0
4	MPD	AA	312	8/8	0.83	0.34	75,86,96,97	0
5	GOL	BA	505	6/6	0.83	0.12	30,35,39,40	0
4	MPD	AA	302[B]	8/8	0.86	0.16	50,55,58,58	8
5	GOL	AA	306	6/6	0.88	0.12	21,26,36,42	0
4	MPD	BA	502	8/8	0.90	0.10	27,33,41,42	0
5	GOL	AA	310	6/6	0.91	0.17	35,63,77,84	0
3	CL	AA	307	1/1	0.94	0.07	23,23,23,23	0
5	GOL	BA	507	6/6	0.95	0.13	22,35,52,53	0
3	CL	AA	305	1/1	0.98	0.04	23,23,23,23	0
3	CL	AA	308	1/1	0.98	0.04	22,22,22,22	0
3	CL	BA	504	1/1	0.98	0.04	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.