



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:26 PM UTC

PDB ID : 7Q9H / pdb_00007q9h
Title : Peptide LLKAVAEKQ in complex with human cathepsin V C25A mutant
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Kosec, G.; Impens, F.; Demol, H.; Turk, B.; Gevaert, K.; Turk, D.
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

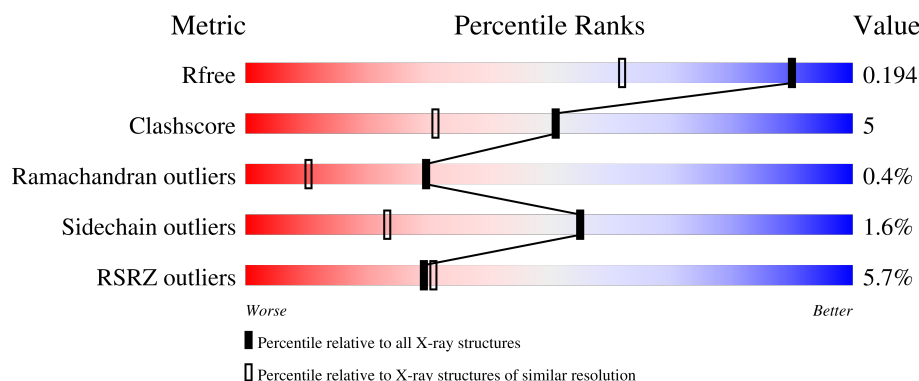
1 Overall quality at a glance

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	3% 86% 13% .
1	BA	221	5% 88% 11% .
2	PAA	11	27% 27% 9% 64%
2	PAC	11	45% 9% 18% 18% 55%
2	PB	11	9% 36% 64%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8708 atoms, of which 4516 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	221	Total	C	H	N	O	S	1715	10	0
			3476	1113	1713	302	338	10			
1	BA	221	Total	C	H	N	O	S	1673	6	0
			3410	1095	1671	299	335	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	25	ALA	CYS	engineered mutation	UNP O60911
AA	108	GLN	ASN	engineered mutation	UNP O60911
AA	179	GLN	ASN	engineered mutation	UNP O60911
BA	246	ALA	CYS	engineered mutation	UNP O60911
BA	329	GLN	ASN	engineered mutation	UNP O60911
BA	400	GLN	ASN	engineered mutation	UNP O60911

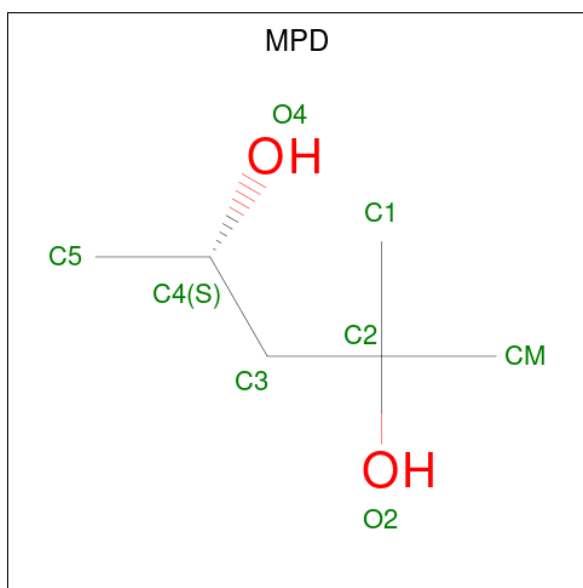
- Molecule 2 is a protein called LLKAVAEKQ Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	PAA	4	Total	C	H	N	O	38	4	0
			66	20	38	4	4			
2	PAC	5	Total	C	H	N	O	38	5	0
			73	22	38	6	7			
2	PB	4	Total	C	H	N	O	38	0	0
			66	20	38	4	4			

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

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

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



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

- 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	1
			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		
5	BA	1	Total	C	O	0	0
			6	3	3		

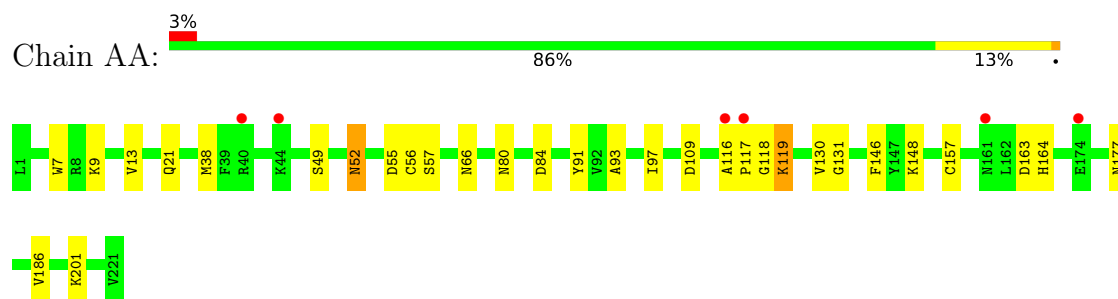
- Molecule 6 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AA	262	Total	H	O	524	2
			786	524	262		
6	BA	238	Total	H	O	476	0
			714	476	238		
6	PAA	3	Total	H	O	6	0
			9	6	3		
6	PAC	2	Total	H	O	4	0
			6	4	2		
6	PB	4	Total	H	O	8	0
			12	8	4		

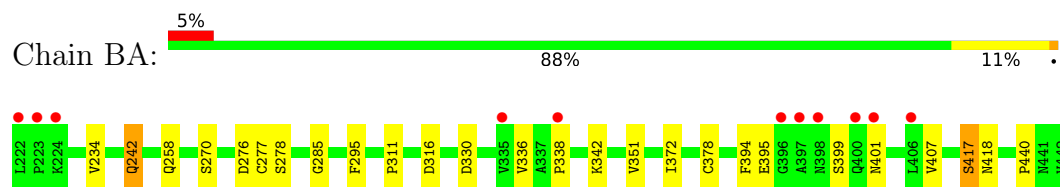
3 Residue-property plots

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.

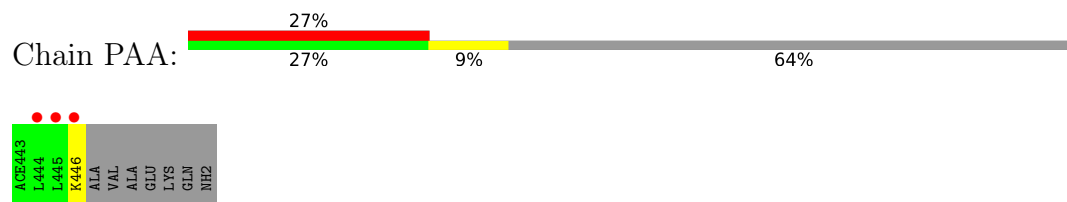
- Molecule 1: Cathepsin L2



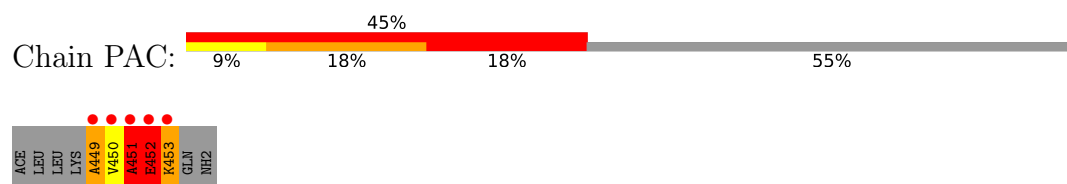
- Molecule 1: Cathepsin L2



- Molecule 2: LLKAVAEKQ Peptide



- Molecule 2: LLKAVAEKQ Peptide



- Molecule 2: LLKAVAEKQ Peptide



ACE457	ALA
L488	VAL
L459	ALA
F460	GLU
	LYS
	GLN
	NH2

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	94.51Å 94.51Å 124.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.26 – 1.40 47.26 – 1.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.26-1.40) 99.9 (47.26-1.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 1.29Å)	Xtriage
Refinement program	MAIN	Depositor
R, R_{free}	0.182 , 0.209 0.188 , 0.194	Depositor DCC
R_{free} test set	2100 reflections (1.48%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.3	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	0.96	EDS
Total number of atoms	8708	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: MPD, CL, ACE, GOL

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	1.25	3/1817 (0.2%)	1.34	18/2451 (0.7%)
1	BA	1.25	1/1781 (0.1%)	1.33	11/2407 (0.5%)
2	PAA	1.19	0/25	0.85	0/32
2	PAC	1.75	1/34 (2.9%)	2.14	3/44 (6.8%)
2	PB	0.92	0/25	1.18	0/32
All	All	1.25	5/3682 (0.1%)	1.34	32/4966 (0.6%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	97	ILE	CA-CB	8.25	1.62	1.54
2	PAC	449[A]	ALA	N-CA	-7.09	1.32	1.46
1	BA	417	SER	N-CA	5.40	1.53	1.46
1	AA	38	MET	SD-CE	-5.19	1.66	1.79
1	AA	119	LYS	CA-CB	5.14	1.59	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	130	VAL	N-CA-C	8.33	118.73	111.56
1	AA	177	ASN	OD1-CG-ND2	-7.97	114.63	122.60
1	BA	351	VAL	N-CA-C	7.32	118.11	111.81
1	AA	109	ASP	CA-CB-CG	7.12	119.72	112.60
1	BA	270	SER	N-CA-C	6.94	120.17	108.23
1	AA	118	GLY	CA-C-N	-6.73	113.49	122.85
1	AA	118	GLY	C-N-CA	-6.73	113.49	122.85
1	AA	49	SER	N-CA-C	6.67	119.70	108.23
1	AA	52	ASN	CA-CB-CG	6.60	119.20	112.60
2	PAC	451[A]	ALA	CA-C-N	6.52	133.99	121.54
2	PAC	451[A]	ALA	C-N-CA	6.52	133.99	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BA	407	VAL	N-CA-C	6.36	117.02	108.11
1	AA	130	VAL	N-CA-CB	-6.30	104.47	111.41
1	BA	330	ASP	CA-CB-CG	6.22	118.82	112.60
1	AA	55	ASP	CA-CB-CG	6.13	118.73	112.60
1	BA	311	PRO	N-CA-C	5.76	120.54	111.38
1	BA	278	SER	N-CA-C	5.69	119.21	112.72
1	BA	277	CYS	N-CA-C	5.64	121.05	113.72
2	PAC	452[A]	GLU	N-CA-C	5.62	122.77	110.80
1	AA	56	CYS	N-CA-C	5.55	120.93	113.72
1	AA	80	ASN	CB-CG-ND2	5.52	124.68	116.40
1	AA	146	PHE	N-CA-C	5.43	118.91	112.72
1	BA	234	VAL	N-CA-C	5.39	115.66	108.11
1	AA	57	SER	N-CA-C	5.35	118.81	112.72
1	AA	117	PRO	N-CA-C	5.35	119.48	111.14
1	AA	84	ASP	N-CA-C	5.28	117.67	110.55
1	AA	13	VAL	N-CA-CB	-5.25	104.17	111.41
1	AA	186	VAL	N-CA-C	5.22	115.42	108.11
1	BA	401	ASN	CA-CB-CG	5.19	117.79	112.60
1	BA	276	ASP	N-CA-C	5.18	117.83	111.82
1	AA	13	VAL	N-CA-C	5.10	115.25	108.11
1	BA	258	GLN	OE1-CD-NE2	-5.10	117.50	122.60

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	1763	1713	1699	14	0
1	BA	1739	1671	1661	10	0
2	PAA	28	38	38	2	0
2	PAC	35	38	37	7	0
2	PB	28	38	38	0	0
3	AA	3	0	0	0	0
3	BA	1	0	0	1	0
4	AA	24	0	41	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BA	32	0	56	5	0
5	AA	12	0	11	2	0
5	BA	18	0	24	1	0
6	AA	262	524	0	6	1
6	BA	238	476	0	2	1
6	PAA	3	6	0	0	0
6	PAC	2	4	0	0	0
6	PB	4	8	0	0	0
All	All	4192	4516	3605	38	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 5.

All (38) 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:446[A]:LYS:O	2:PAC:449[A]:ALA:N	1.71	1.23
4:AA:308:MPD:H12	6:AA:409:HOH:O	1.50	1.09
4:AA:308:MPD:C1	6:AA:409:HOH:O	2.07	1.00
4:BA:505:MPD:HM2	4:BA:505:MPD:H52	1.45	0.95
2:PAA:446[A]:LYS:C	2:PAC:449[A]:ALA:N	2.41	0.79
4:BA:505:MPD:HM2	4:BA:505:MPD:C5	2.15	0.75
1:AA:148[B]:LYS:HD2	1:BA:418[B]:ASN:HD21	1.52	0.73
1:AA:163:ASP:OD2	4:AA:302[B]:MPD:H32	1.90	0.71
3:BA:504:CL:CL	4:BA:505:MPD:HM3	2.30	0.68
1:BA:417:SER:O	1:BA:418[B]:ASN:ND2	2.31	0.63
1:AA:66[B]:ASN:ND2	6:AA:401:HOH:O	2.33	0.61
2:PAC:453[A]:LYS:HG2	2:PAC:453[A]:LYS:O	2.02	0.58
4:BA:505:MPD:C5	4:BA:505:MPD:CM	2.82	0.57
4:AA:307:MPD:H12	6:AA:640:HOH:O	2.05	0.56
1:AA:9:LYS:HE2	6:BA:653:HOH:O	2.05	0.56
1:AA:116:ALA:HB3	1:AA:119:LYS:HD2	1.88	0.55
1:BA:285:GLY:HA3	1:BA:316:ASP:OD1	2.06	0.55
1:AA:164:HIS:HD1	2:PAC:449[A]:ALA:N	2.05	0.54
1:BA:336:VAL:O	1:BA:338:PRO:HD3	2.10	0.51
1:AA:148[B]:LYS:CD	1:BA:418[B]:ASN:HD21	2.21	0.50
4:AA:307:MPD:H13	6:AA:514:HOH:O	2.13	0.49
1:AA:201[A]:LYS:HG3	5:AA:306:GOL:H31	1.95	0.48
1:AA:116:ALA:CB	1:AA:119:LYS:HD2	2.43	0.48
5:BA:507:GOL:H11	5:BA:508:GOL:O3	2.13	0.48
1:BA:372:ILE:HD11	1:BA:395[B]:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:242:GLN:N	1:BA:242:GLN:CD	2.72	0.47
1:AA:21:GLN:OE1	2:PAC:452[A]:GLU:HG2	2.16	0.45
2:PAC:450[A]:VAL:O	2:PAC:451[A]:ALA:HB2	2.18	0.44
4:BA:503:MPD:O2	6:BA:601:HOH:O	2.13	0.43
1:AA:148[A]:LYS:CE	6:AA:412:HOH:O	2.66	0.43
1:BA:394:PHE:CG	1:BA:399:SER:HA	2.54	0.43
1:AA:201[B]:LYS:HG3	5:AA:306:GOL:H31	2.01	0.42
4:AA:308:MPD:H12	4:AA:308:MPD:O4	2.20	0.41
1:BA:295:PHE:CZ	1:BA:440:PRO:HD3	2.55	0.41
1:AA:91:TYR:CE2	1:AA:93:ALA:HB2	2.55	0.41
1:BA:342:LYS:HD3	1:BA:342:LYS:HA	1.99	0.40
1:AA:7:TRP:CE2	1:AA:131: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)
6:AA:552:HOH:O	6:BA:612:HOH:O[3_554]	1.94	0.26

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	229/221 (104%)	220 (96%)	9 (4%)	0	100	100
1	BA	225/221 (102%)	217 (96%)	8 (4%)	0	100	100
2	PAA	2/11 (18%)	2 (100%)	0	0	100	100
2	PAC	3/11 (27%)	1 (33%)	0	2 (67%)	0	0
2	PB	2/11 (18%)	2 (100%)	0	0	100	100
All	All	461/475 (97%)	442 (96%)	17 (4%)	2 (0%)	30	10

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	PAC	451[A]	ALA
2	PAC	452[A]	GLU

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	188/178 (106%)	186 (99%)	2 (1%)	65	37
1	BA	184/178 (103%)	182 (99%)	2 (1%)	65	37
2	PAA	3/7 (43%)	3 (100%)	0	100	100
2	PAC	3/7 (43%)	1 (33%)	2 (67%)	0	0
2	PB	3/7 (43%)	3 (100%)	0	100	100
All	All	381/377 (101%)	375 (98%)	6 (2%)	55	23

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

Mol	Chain	Res	Type
1	AA	52	ASN
1	AA	157	CYS
1	BA	242	GLN
1	BA	378	CYS
2	PAC	452[A]	GLU
2	PAC	453[A]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	80	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	BA	507	-	5,5,5	0.64	0	5,5,5	0.89	0
4	MPD	AA	308	-	7,7,7	0.56	0	9,10,10	0.57	0
4	MPD	BA	502	-	7,7,7	0.80	0	9,10,10	0.62	0
4	MPD	AA	302[B]	-	7,7,7	0.30	0	9,10,10	0.34	0
4	MPD	BA	506	-	7,7,7	0.23	0	9,10,10	0.32	0
5	GOL	BA	508	-	5,5,5	0.32	0	5,5,5	1.06	1 (20%)
5	GOL	AA	306	-	5,5,5	0.85	0	5,5,5	1.06	0
5	GOL	BA	501	-	5,5,5	0.47	0	5,5,5	0.78	0
4	MPD	BA	503	-	7,7,7	1.09	1 (14%)	9,10,10	1.60	2 (22%)
5	GOL	AA	303[B]	-	5,5,5	0.13	0	5,5,5	0.35	0
4	MPD	AA	307	-	7,7,7	0.39	0	9,10,10	1.53	1 (11%)
4	MPD	BA	505	-	7,7,7	0.46	0	9,10,10	0.57	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	BA	507	-	-	2/4/4/4	-
4	MPD	AA	308	-	-	1/5/5/5	-
4	MPD	BA	502	-	-	0/5/5/5	-
4	MPD	AA	302[B]	-	-	4/5/5/5	-
4	MPD	BA	506	-	-	1/5/5/5	-
5	GOL	BA	508	-	-	0/4/4/4	-
5	GOL	AA	306	-	-	0/4/4/4	-
5	GOL	BA	501	-	-	0/4/4/4	-
4	MPD	BA	503	-	-	0/5/5/5	-
5	GOL	AA	303[B]	-	-	0/4/4/4	-
4	MPD	AA	307	-	-	0/5/5/5	-
4	MPD	BA	505	-	-	3/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	BA	503	MPD	CM-C2	-2.28	1.45	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	AA	307	MPD	CM-C2-C1	-4.19	101.25	110.63
4	BA	503	MPD	CM-C2-C1	3.67	118.84	110.63
4	BA	503	MPD	O4-C4-C5	-2.43	99.01	109.45
5	BA	508	GOL	C3-C2-C1	-2.14	103.95	111.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AA	302[B]	MPD	C2-C3-C4-O4
4	AA	302[B]	MPD	C2-C3-C4-C5
4	BA	505	MPD	C2-C3-C4-O4
4	BA	505	MPD	O2-C2-C3-C4
5	BA	507	GOL	O2-C2-C3-O3
4	BA	505	MPD	C2-C3-C4-C5
5	BA	507	GOL	C1-C2-C3-O3
4	AA	302[B]	MPD	O2-C2-C3-C4
4	AA	308	MPD	C2-C3-C4-O4
4	BA	506	MPD	C2-C3-C4-O4
4	AA	302[B]	MPD	CM-C2-C3-C4

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	BA	507	GOL	1	0
4	AA	308	MPD	3	0
4	AA	302[B]	MPD	1	0
5	BA	508	GOL	1	0
5	AA	306	GOL	2	0
4	BA	503	MPD	1	0
4	AA	307	MPD	2	0
4	BA	505	MPD	4	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%)	0.15	6 (2%) 56 58	3, 7, 13, 18	12 (5%)
1	BA	221/221 (100%)	0.47	11 (4%) 34 36	3, 9, 16, 36	8 (3%)
2	PAA	3/11 (27%)	4.62	3 (100%) 0 0	5, 5, 10, 11	3 (100%)
2	PAC	5/11 (45%)	10.90	5 (100%) 0 0	9, 11, 14, 19	5 (100%)
2	PB	3/11 (27%)	1.66	1 (33%) 1 1	8, 8, 13, 13	0
All	All	453/475 (95%)	0.46	26 (5%) 29 31	3, 8, 15, 36	28 (6%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	PAC	451[A]	ALA	14.8
2	PAC	453[A]	LYS	12.0
2	PAC	452[A]	GLU	9.5
2	PAC	449[A]	ALA	9.4
2	PAC	450[A]	VAL	8.9
1	AA	116	ALA	6.2
2	PAA	444[A]	LEU	5.8
2	PAA	446[A]	LYS	5.7
1	BA	397	ALA	4.8
1	AA	44[A]	LYS	4.4
1	AA	117	PRO	4.3
1	BA	400	GLN	4.2
1	AA	40	ARG	3.8
1	BA	406[A]	LEU	3.2
1	AA	174[A]	GLU	2.9
1	BA	401	ASN	2.6
1	AA	161	ASN	2.6
1	BA	222	LEU	2.6
1	BA	396	GLY	2.4
2	PAA	445[A]	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	BA	338	PRO	2.3
1	BA	224	LYS	2.3
1	BA	223	PRO	2.2
1	BA	398	ASN	2.2
1	BA	335	VAL	2.2
2	PB	458	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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	MPD	AA	308	8/8	0.78	0.31	64,75,76,77	0
5	GOL	BA	507	6/6	0.78	0.24	64,72,83,87	0
4	MPD	AA	307	8/8	0.80	0.26	38,46,77,88	0
4	MPD	BA	505	8/8	0.81	0.27	74,83,94,98	0
4	MPD	BA	503	8/8	0.81	0.16	23,26,29,29	0
5	GOL	BA	508	6/6	0.82	0.20	35,72,81,84	0
4	MPD	AA	302[B]	8/8	0.83	0.54	66,71,76,76	8
4	MPD	BA	506	8/8	0.84	0.31	76,79,86,88	0
5	GOL	AA	306	6/6	0.84	0.16	19,24,34,34	0
5	GOL	AA	303[B]	6/6	0.86	0.24	56,62,63,65	6
4	MPD	BA	502	8/8	0.88	0.14	27,31,37,39	0
3	CL	AA	301[B]	1/1	0.91	0.31	27,27,27,27	1
5	GOL	BA	501	6/6	0.91	0.11	24,25,28,31	0
3	CL	AA	304	1/1	0.96	0.08	20,20,20,20	0
3	CL	BA	504	1/1	0.98	0.07	19,19,19,19	0
3	CL	AA	305	1/1	0.99	0.09	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.