Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 12:29 pm GMT

PDB ID	:	5E3A
Title	:	Structure of human DPP3 in complex with opioid peptide leu-enkephalin
Authors	:	Kumar, P.; Reithofer, V.; Reisinger, M.; Pavkov-Keller, T.; Wallner, S.; Macheroux, P.; Gruber, K.
Deposited on	:	2015-10-02
Resolution	:	2.05 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:

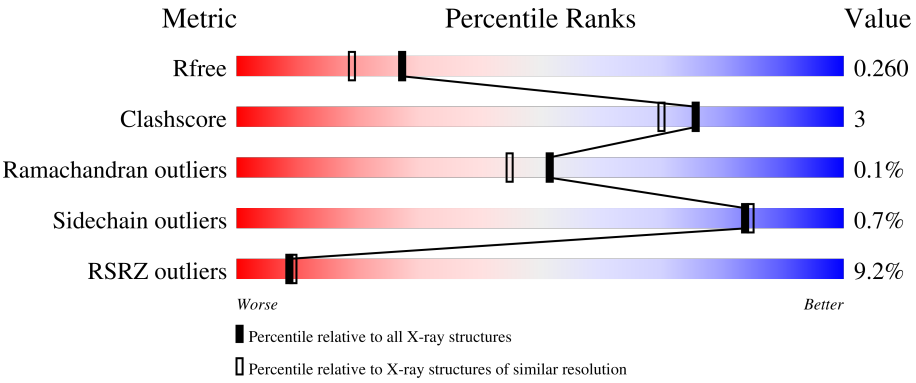
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	A	726	9% 91% 8%
2	B	5	20% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6165 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 Dipeptidyl peptidase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5758	3670	975	1101	12	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	SER	CYS	engineered mutation	UNP Q9NY33
A	207	CYS	GLU	engineered mutation	UNP Q9NY33
A	451	ALA	GLU	engineered mutation	UNP Q9NY33
A	491	CYS	SER	engineered mutation	UNP Q9NY33
A	519	SER	CYS	engineered mutation	UNP Q9NY33
A	654	SER	CYS	engineered mutation	UNP Q9NY33

- Molecule 2 is a protein called Leu-enkephalin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	5	40	28	5	7	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	2	2	2	0	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total K 1 1	0	0

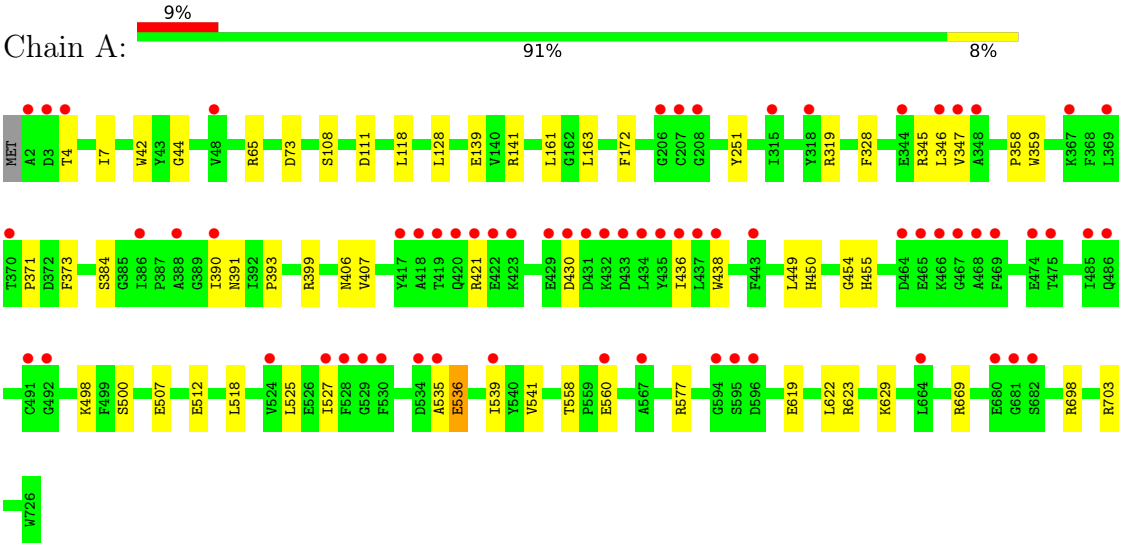
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	363	Total O 363 363	0	0

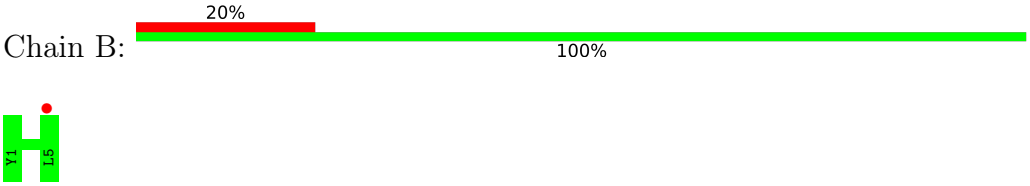
3 Residue-property plots (i)

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: Dipeptidyl peptidase 3



• Molecule 2: Leu-enkephalin



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.56Å 105.76Å 64.99Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	39.58 – 2.05 39.58 – 2.05	Depositor EDS
% Data completeness (in resolution range)	94.8 (39.58-2.05) 95.1 (39.58-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.41 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.209 , 0.260 0.211 , 0.260	Depositor DCC
R_{free} test set	2414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 40.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6165	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: K, ZN, MG

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	A	0.22	0/5893	0.37	0/7983
2	B	0.27	0/41	0.38	0/52
All	All	0.22	0/5934	0.37	0/8035

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

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	A	5758	0	5635	36	0
2	B	40	0	37	0	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
5	A	1	0	0	0	0
6	A	363	0	0	6	0
All	All	6165	0	5672	36	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 3.

All (36) 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:A:421:ARG:HB3	1:A:436:ILE:HD11	1.75	0.67
1:A:346:LEU:HA	1:A:527:ILE:HD13	1.77	0.66
1:A:319:ARG:NH1	6:A:902:HOH:O	2.29	0.65
1:A:391:ASN:ND2	1:A:406:ASN:OD1	2.32	0.62
1:A:358:PRO:HB3	1:A:619:GLU:HG3	1.83	0.60
1:A:438:TRP:HB2	1:A:541:VAL:HG21	1.83	0.59
1:A:345:ARG:HG3	1:A:527:ILE:HG23	1.87	0.55
1:A:391:ASN:OD1	1:A:399:ARG:NH1	2.33	0.55
1:A:141:ARG:NH1	6:A:911:HOH:O	2.39	0.54
1:A:345:ARG:NH1	1:A:527:ILE:O	2.38	0.53
1:A:430:ASP:N	1:A:430:ASP:OD1	2.44	0.50
1:A:669:ARG:NH1	6:A:924:HOH:O	2.44	0.49
1:A:347:VAL:HG22	1:A:371:PRO:HG2	1.94	0.49
1:A:623:ARG:NH1	6:A:905:HOH:O	2.34	0.49
1:A:128:LEU:HD22	1:A:141:ARG:HG2	1.96	0.47
1:A:73:ASP:OD2	1:A:698:ARG:NH2	2.38	0.47
1:A:42:TRP:CD2	1:A:703:ARG:HD3	2.50	0.47
1:A:498:LYS:NZ	6:A:930:HOH:O	2.47	0.47
1:A:65:ARG:NH1	1:A:139:GLU:HG2	2.29	0.47
1:A:108:SER:HB3	1:A:384:SER:HB2	1.96	0.47
1:A:577:ARG:NH2	6:A:928:HOH:O	2.47	0.46
1:A:393:PRO:O	1:A:399:ARG:HD3	2.16	0.46
1:A:450:HIS:ND1	1:A:512:GLU:OE1	2.47	0.46
1:A:525:LEU:HD13	1:A:535:ALA:HB1	1.98	0.45
1:A:536:GLU:O	1:A:539:ILE:HB	2.17	0.44
1:A:44:GLY:HA3	1:A:328:PHE:CE1	2.53	0.44
1:A:4:THR:HB	1:A:7:ILE:HG12	1.99	0.43
1:A:449:LEU:HD13	1:A:518:LEU:HB2	2.01	0.43
1:A:359:TRP:HZ3	1:A:622:LEU:HG	1.83	0.43
1:A:558:THR:HG22	1:A:560:GLU:HG2	2.00	0.42
1:A:507:GLU:OE1	1:A:629:LYS:NZ	2.44	0.42
1:A:449:LEU:O	1:A:454:GLY:N	2.53	0.41
1:A:390:ILE:HG13	1:A:407:VAL:HB	2.02	0.41
1:A:399:ARG:HH22	1:A:455:HIS:HB3	1.86	0.41
1:A:163:LEU:HD21	1:A:172:PHE:CG	2.56	0.40
1:A:111:ASP:HB3	1:A:161:LEU:HB2	2.03	0.40

There are no symmetry-related clashes.

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	A	724/726 (100%)	701 (97%)	22 (3%)	1 (0%)	51 45
2	B	3/5 (60%)	2 (67%)	1 (33%)	0	100 100
All	All	727/731 (100%)	703 (97%)	23 (3%)	1 (0%)	51 45

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	SER

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	A	609/609 (100%)	605 (99%)	4 (1%)	84 84
2	B	3/3 (100%)	3 (100%)	0	100 100
All	All	612/612 (100%)	608 (99%)	4 (1%)	84 84

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	LEU
1	A	251	TYR
1	A	373	PHE
1	A	536	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95^{th} 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	A	725/726 (99%)	0.50	66 (9%)	9	9	16, 32, 67, 93	0
2	B	5/5 (100%)	2.22	1 (20%)	1	0	37, 38, 49, 67	0
All	All	730/731 (99%)	0.51	67 (9%)	9	9	16, 32, 67, 93	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	467	GLY	8.8
2	B	5	LEU	6.3
1	A	466	LYS	5.9
1	A	2	ALA	5.7
1	A	534	ASP	5.5
1	A	420	GLN	5.4
1	A	465	GLU	5.2
1	A	468	ALA	4.7
1	A	207	CYS	4.6
1	A	436	ILE	4.5
1	A	417	TYR	4.5
1	A	418	ALA	4.5
1	A	469	PHE	4.4
1	A	421	ARG	3.9
1	A	206	GLY	3.8
1	A	530	PHE	3.8
1	A	535	ALA	3.8
1	A	419	THR	3.8
1	A	437	LEU	3.7
1	A	3	ASP	3.6
1	A	681	GLY	3.4
1	A	422	GLU	3.3
1	A	528	PHE	3.2
1	A	464	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	680	GLU	3.1
1	A	315	ILE	3.1
1	A	344	GLU	3.0
1	A	435	TYR	3.0
1	A	594	GLY	2.9
1	A	4	THR	2.9
1	A	369	LEU	2.9
1	A	682	SER	2.8
1	A	474	GLU	2.8
1	A	438	TRP	2.8
1	A	367	LYS	2.7
1	A	423	LYS	2.7
1	A	529	GLY	2.7
1	A	443	PHE	2.7
1	A	524	VAL	2.7
1	A	431	ASP	2.7
1	A	318	TYR	2.7
1	A	346	LEU	2.7
1	A	208	GLY	2.5
1	A	430	ASP	2.5
1	A	595	SER	2.5
1	A	433	ASP	2.5
1	A	491	CYS	2.5
1	A	48	VAL	2.4
1	A	432	LYS	2.4
1	A	390	ILE	2.4
1	A	347	VAL	2.4
1	A	348	ALA	2.4
1	A	560	GLU	2.3
1	A	567	ALA	2.2
1	A	664	LEU	2.2
1	A	475	THR	2.2
1	A	386	ILE	2.2
1	A	539	ILE	2.2
1	A	527	ILE	2.2
1	A	429	GLU	2.1
1	A	492	GLY	2.1
1	A	370	THR	2.1
1	A	434	LEU	2.1
1	A	486	GLN	2.1
1	A	485	ILE	2.0
1	A	388	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	596	ASP	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 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, 95^{th} 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	ZN	A	801	1/1	0.80	0.13	52,52,52,52	1
5	K	A	804	1/1	0.97	0.07	29,29,29,29	0
4	MG	A	803	1/1	0.99	0.11	19,19,19,19	0
4	MG	A	802	1/1	0.99	0.11	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.