



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:03 AM UTC

PDB ID : 5E33 / pdb_00005e33
Title : Structure of human DPP3 in complex with met-enkephalin
Authors : Kumar, P.; Reithofer, V.; Reisinger, M.; Pavkov-Keller, T.; Wallner, S.; Mach-
eroux, P.; Gruber, K.
Deposited on : 2015-10-01
Resolution : 1.84 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
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

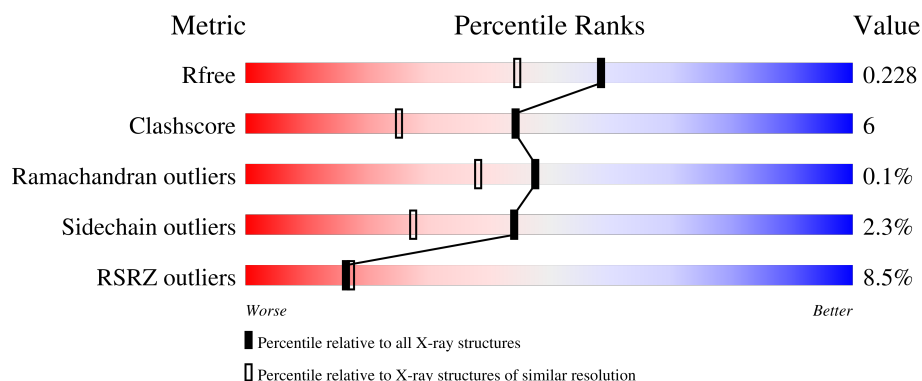
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	A	726	8% 88% 11%
2	B	5	40% 100%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6339 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
1	A	725	Total	C	N	O	S	0	4	0
			5776	3682	977	1105	12			

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 Met-enkephalin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	S	0	0	0
			40	27	5	7	1			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 5 is POTASSIUM ION (CCD ID: K) (formula: K).

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

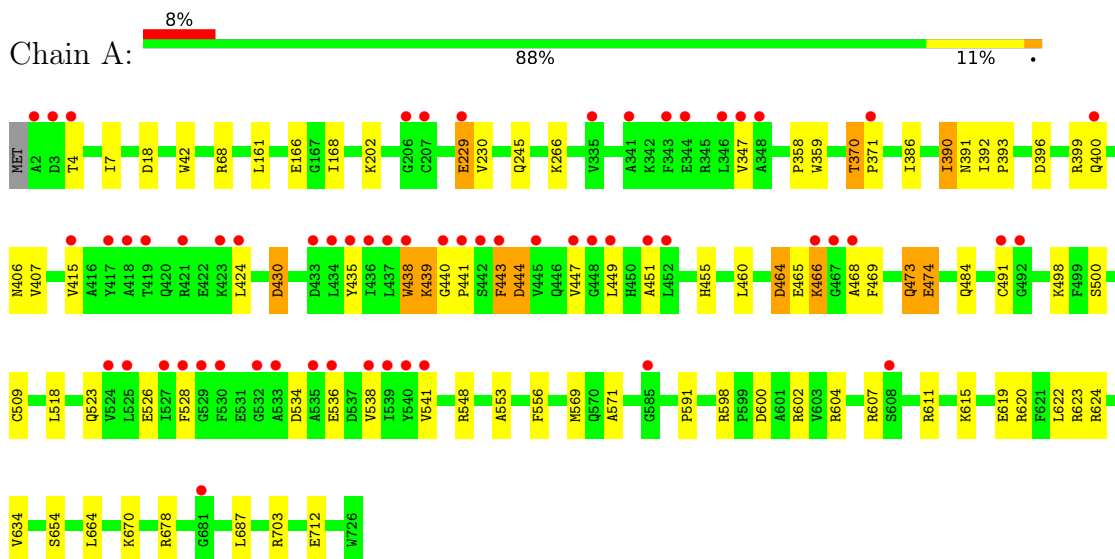
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	517	Total O 517 517	0	0
6	B	2	Total O 2 2	0	0

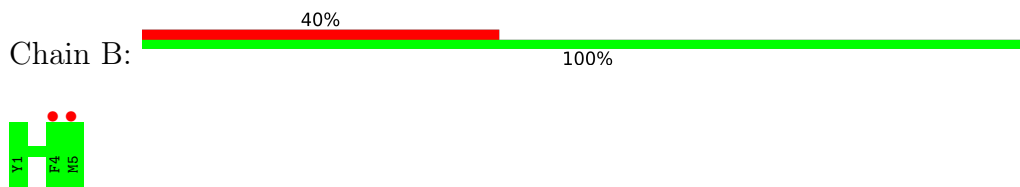
3 Residue-property plots [i](#)

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: Met-enkephalin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.79Å 105.76Å 65.17Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	45.42 – 1.84 45.42 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.42-1.84) 96.8 (45.42-1.84)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.84Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.181 , 0.224 0.188 , 0.228	Depositor DCC
R_{free} test set	3414 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6339	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 4.80% 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: ZN, K, 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	0.67	1/5920 (0.0%)	0.84	9/8019 (0.1%)
2	B	0.38	0/41	1.10	0/51
All	All	0.67	1/5961 (0.0%)	0.84	9/8070 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455	HIS	C-O	-5.32	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	438	TRP	N-CA-C	10.04	125.72	113.38
1	A	466	LYS	N-CA-C	-9.84	94.12	109.76
1	A	370	THR	CA-C-N	6.20	126.17	119.78
1	A	370	THR	C-N-CA	6.20	126.17	119.78
1	A	615	LYS	CA-C-N	-5.74	113.10	119.19
1	A	615	LYS	C-N-CA	-5.74	113.10	119.19
1	A	474	GLU	N-CA-C	5.72	117.59	111.36
1	A	444	ASP	N-CA-C	-5.25	105.64	111.36
1	A	469	PHE	N-CA-C	5.14	117.49	110.55

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	A	5776	0	5657	69	0
2	B	40	0	35	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	517	0	0	12	1
6	B	2	0	0	0	0
All	All	6339	0	5692	69	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 6.

All (69) 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:438:TRP:O	1:A:441:PRO:HD2	1.43	1.18
1:A:438:TRP:C	1:A:441:PRO:HD2	1.75	1.10
1:A:68[B]:ARG:NH2	1:A:712:GLU:OE2	2.05	0.90
1:A:439:LYS:NZ	1:A:443:PHE:HE1	1.71	0.87
1:A:473:GLN:O	1:A:473:GLN:NE2	2.06	0.87
1:A:439:LYS:HZ3	1:A:443:PHE:HE1	0.85	0.81
1:A:68[A]:ARG:NH2	1:A:712:GLU:OE2	2.15	0.80
1:A:464:ASP:OD1	1:A:466:LYS:N	2.15	0.79
1:A:473:GLN:HE21	1:A:473:GLN:C	1.92	0.78
1:A:623:ARG:NH1	6:A:902:HOH:O	2.25	0.69
1:A:358:PRO:HB3	1:A:619:GLU:HG3	1.75	0.67
1:A:438:TRP:O	1:A:441:PRO:CD	2.34	0.66
1:A:391:ASN:HD22	1:A:451:ALA:HB1	1.62	0.64
1:A:435:TYR:CZ	1:A:439:LYS:HD2	2.33	0.63
1:A:604:ARG:NH2	6:A:904:HOH:O	2.30	0.62
1:A:390:ILE:HG12	1:A:407:VAL:HB	1.83	0.61
1:A:430:ASP:OD1	1:A:430:ASP:N	2.27	0.59
1:A:440:GLY:N	1:A:441:PRO:CD	2.66	0.58
1:A:391:ASN:ND2	1:A:406:ASN:OD1	2.36	0.58
1:A:393:PRO:O	1:A:399:ARG:HD3	2.04	0.57
1:A:245:GLN:NE2	6:A:908:HOH:O	2.37	0.57
1:A:68[A]:ARG:HH22	1:A:712:GLU:CD	2.12	0.57
1:A:678:ARG:HG3	1:A:687:LEU:HD11	1.87	0.56
1:A:465:GLU:HG2	1:A:491:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLN:NE2	6:A:911:HOH:O	2.40	0.54
1:A:438:TRP:HA	1:A:441:PRO:HG2	1.89	0.54
1:A:415:VAL:CG1	1:A:670:LYS:HD2	2.38	0.53
1:A:620:ARG:O	1:A:624:ARG:HG3	2.08	0.53
1:A:607:ARG:NH2	6:A:903:HOH:O	2.28	0.52
1:A:435:TYR:CE1	1:A:439:LYS:HD2	2.45	0.52
1:A:553:ALA:HA	1:A:569:MET:HE3	1.92	0.52
1:A:444:ASP:HB3	1:A:528:PHE:CE2	2.46	0.51
1:A:536:GLU:HG2	6:A:903:HOH:O	2.10	0.51
1:A:447:VAL:HG11	6:A:1151:HOH:O	2.10	0.51
1:A:600:ASP:OD2	1:A:602:ARG:NH1	2.45	0.50
1:A:359:TRP:HZ3	1:A:622:LEU:HG	1.77	0.50
1:A:534:ASP:O	1:A:538:VAL:HG23	2.12	0.50
1:A:556:PHE:CD2	1:A:569:MET:HG3	2.47	0.49
1:A:611:ARG:NH1	6:A:918:HOH:O	2.45	0.49
1:A:444:ASP:HB3	1:A:528:PHE:HE2	1.78	0.49
1:A:466:LYS:O	1:A:468:ALA:N	2.36	0.49
1:A:424:LEU:HA	1:A:424:LEU:HD23	1.68	0.49
1:A:438:TRP:C	1:A:441:PRO:CD	2.67	0.48
1:A:474:GLU:O	1:A:484:GLN:NE2	2.47	0.48
1:A:591:PRO:HD3	6:A:1059:HOH:O	2.14	0.47
1:A:347:VAL:HG22	1:A:371:PRO:HB2	1.96	0.47
1:A:598:ARG:NH1	1:A:664:LEU:HG	2.31	0.46
1:A:415:VAL:HG13	1:A:670:LYS:HD2	1.96	0.46
1:A:634:VAL:HG12	6:A:1307:HOH:O	2.16	0.46
1:A:229:GLU:HG3	1:A:230:VAL:N	2.30	0.46
1:A:466:LYS:C	1:A:468:ALA:H	2.22	0.46
1:A:370:THR:HA	1:A:371:PRO:HD3	1.73	0.45
1:A:509:CYS:HA	1:A:571:ALA:HB1	1.98	0.45
1:A:42:TRP:CD2	1:A:703:ARG:HD3	2.51	0.45
1:A:391:ASN:OD1	1:A:399:ARG:NH2	2.41	0.45
1:A:202:LYS:NZ	6:A:920:HOH:O	2.46	0.44
1:A:548:ARG:HD3	6:A:1265:HOH:O	2.18	0.43
1:A:347:VAL:HG13	1:A:371:PRO:HD2	2.00	0.43
1:A:449:LEU:HD13	1:A:518:LEU:HB2	2.00	0.43
1:A:464:ASP:OD1	1:A:465:GLU:N	2.52	0.42
1:A:161:LEU:HA	1:A:168:ILE:O	2.20	0.42
1:A:386:ILE:HD13	1:A:386:ILE:HG21	1.87	0.42
1:A:4:THR:HB	1:A:7:ILE:HG12	2.01	0.42
1:A:390:ILE:CG1	1:A:407:VAL:HB	2.48	0.42
1:A:438:TRP:HA	1:A:441:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HB3	1:A:266:LYS:HE2	1.80	0.41
1:A:523:GLN:O	1:A:526:GLU:HB2	2.20	0.41
1:A:396:ASP:HA	1:A:399:ARG:HG3	2.03	0.41
1:A:466:LYS:C	1:A:468:ALA:N	2.78	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:A:1273:HOH:O	6:A:1339:HOH:O[2_757]	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	A	727/726 (100%)	713 (98%)	13 (2%)	1 (0%)	48	38
2	B	3/5 (60%)	3 (100%)	0	0	100	100
All	All	730/731 (100%)	716 (98%)	13 (2%)	1 (0%)	48	38

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	612/609 (100%)	598 (98%)	14 (2%)	44	27
2	B	3/3 (100%)	3 (100%)	0	100	100
All	All	615/612 (100%)	601 (98%)	14 (2%)	44	27

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	166	GLU
1	A	229	GLU
1	A	390	ILE
1	A	392	ILE
1	A	430	ASP
1	A	439	LYS
1	A	443	PHE
1	A	460	LEU
1	A	464	ASP
1	A	473	GLN
1	A	498	LYS
1	A	541	VAL
1	A	654	SER

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

Mol	Chain	Res	Type
1	A	77	GLN
1	A	563	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 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 [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	A	725/726 (99%)	0.28	60 (8%) 17 18	16, 32, 70, 94	4 (0%)
2	B	5/5 (100%)	1.66	2 (40%) 1 1	34, 39, 50, 76	0
All	All	730/731 (99%)	0.29	62 (8%) 16 17	16, 32, 71, 94	4 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	ALA	4.7
1	A	527	ILE	4.7
1	A	346	LEU	4.3
1	A	528	PHE	4.2
1	A	417	TYR	4.1
1	A	434	LEU	4.0
1	A	437	LEU	3.9
1	A	447	VAL	3.8
1	A	443	PHE	3.8
1	A	435	TYR	3.8
2	B	5	MET	3.7
1	A	532	GLY	3.6
1	A	421	ARG	3.5
1	A	438	TRP	3.4
1	A	541	VAL	3.3
1	A	419	THR	3.3
1	A	467	GLY	3.3
1	A	343	PHE	3.2
1	A	445	VAL	3.2
1	A	442	SER	3.2
1	A	533	ALA	3.1
1	A	524	VAL	3.1
1	A	436	ILE	3.1
1	A	440	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	525	LEU	3.0
1	A	529	GLY	3.0
1	A	207	CYS	3.0
1	A	538	VAL	2.9
1	A	3	ASP	2.9
1	A	347	VAL	2.9
1	A	585	GLY	2.9
1	A	335	VAL	2.8
1	A	418	ALA	2.8
1	A	448	GLY	2.7
1	A	530	PHE	2.7
1	A	468	ALA	2.6
1	A	539	ILE	2.5
1	A	451	ALA	2.5
1	A	540	TYR	2.5
1	A	206	GLY	2.5
1	A	348	ALA	2.5
1	A	452	LEU	2.4
1	A	371	PRO	2.4
1	A	491	CYS	2.4
1	A	441	PRO	2.4
1	A	424	LEU	2.4
1	A	341	ALA	2.4
1	A	466	LYS	2.3
2	B	4	PHE	2.3
1	A	492	GLY	2.2
1	A	229	GLU	2.2
1	A	608	SER	2.2
1	A	415	VAL	2.1
1	A	400	GLN	2.1
1	A	681	GLY	2.1
1	A	449	LEU	2.1
1	A	2	ALA	2.1
1	A	433	ASP	2.1
1	A	344	GLU	2.0
1	A	536	GLU	2.0
1	A	423	LYS	2.0
1	A	4	THR	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 [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($\text{\AA}^2$)	Q<0.9
3	ZN	A	801	1/1	0.97	0.05	40,40,40,40	1
4	MG	A	802	1/1	0.99	0.06	24,24,24,24	0
4	MG	A	803	1/1	0.99	0.07	21,21,21,21	0
5	K	A	804	1/1	1.00	0.07	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.