



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2022 – 12:07 pm GMT

PDB ID : 7OJE
Title : Crystal structure of the covalent complex between *Tribolium castaneum* deubiquitinase ZUP and Ubiquitin-PA
Authors : Pichlo, C.; Hermanns, T.; Hofmann, K.; Baumann, U.
Deposited on : 2021-05-14
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 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 : 2.26
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) : 2.26

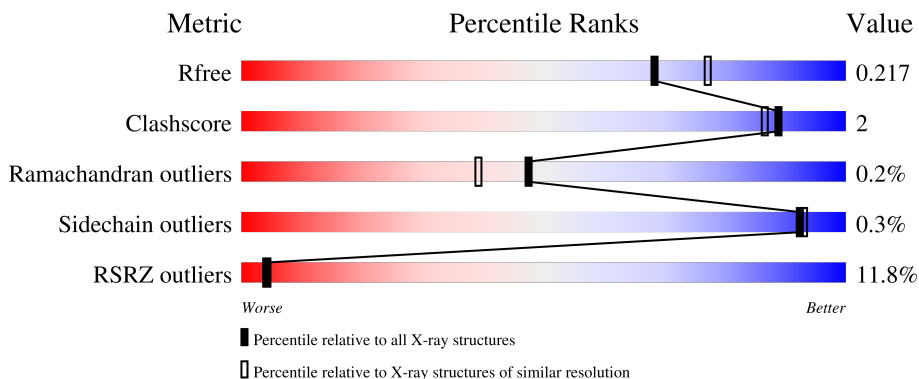
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

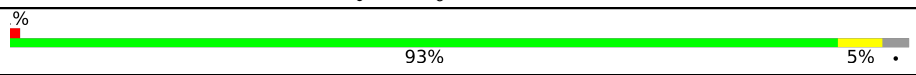
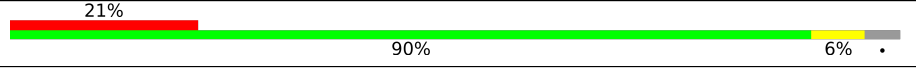
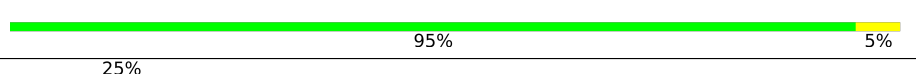
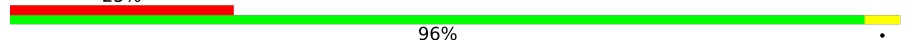
The reported resolution of this entry is 2.05 Å.

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 $\leq 5\%$. 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	375	 93% 5%
1	C	375	 21% 90% 6%
2	B	76	 95% 5%
2	D	76	 25% 96%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7398 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 Lys-63-specific deubiquitinase ZUFSP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	365	2917	1809	542	548	18	0	5	0
1	C	361	2839	1764	523	534	18	0	1	0

- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	76	601	379	105	116	1	0	0	0
2	D	76	601	379	105	116	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	AYE	GLY	engineered mutation	UNP P0CG47
D	76	AYE	GLY	engineered mutation	UNP P0CG47

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	C	1	Total Zn 1 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Na 2 2	0	0
6	C	1	Total Na 1 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	294	Total O 294 294	0	0
7	B	56	Total O 56 56	0	0
7	C	42	Total O 42 42	0	0
7	D	1	Total O 1 1	0	0

3 Residue-property plots [i](#)

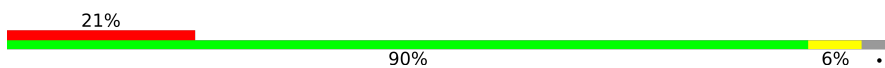
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

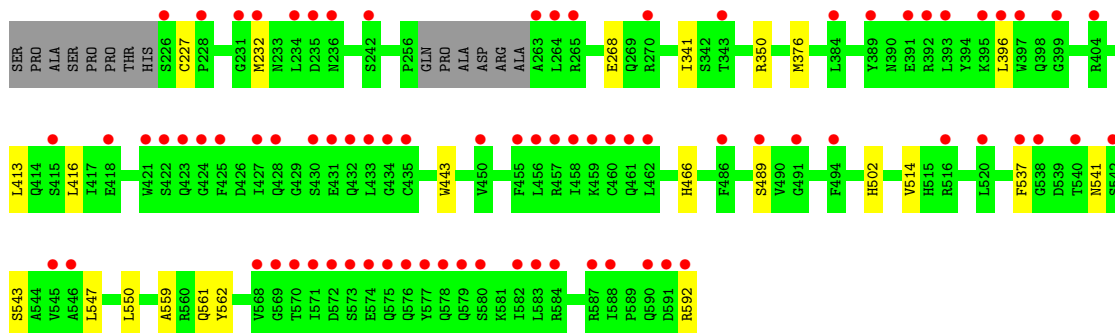
- Molecule 1: Lys-63-specific deubiquitinase ZUFSP

Chain A: 



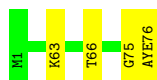
- Molecule 1: Lys-63-specific deubiquitinase ZUFSP

Chain C: 



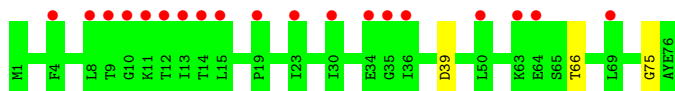
- Molecule 2: Polyubiquitin-B

Chain B: 



- Molecule 2: Polyubiquitin-B

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	151.61Å 151.61Å 83.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.67 – 2.05 75.80 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.9 (51.67-2.05) 88.8 (75.80-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.05Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.185 , 0.219 0.184 , 0.217	Depositor DCC
R_{free} test set	1929 reflections (2.86%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7398	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: EDO, ZN, NA, AYE, CIT

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	0.42	0/2976	0.62	0/4025
1	C	0.28	0/2896	0.54	0/3919
2	B	0.37	0/603	0.60	0/811
2	D	0.26	0/603	0.54	0/811
All	All	0.35	0/7078	0.58	0/9566

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	A	2917	0	2858	12	0
1	C	2839	0	2771	13	0
2	B	601	0	630	4	0
2	D	601	0	630	3	0
3	A	13	0	4	0	0
3	C	13	0	4	0	0
4	A	8	0	12	2	0
4	B	4	0	6	0	0
4	D	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
7	A	294	0	0	1	1
7	B	56	0	0	1	0
7	C	42	0	0	0	0
7	D	1	0	0	0	0
All	All	7398	0	6921	26	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 2.

All (26) 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:C:341:ILE:HG22	1:C:547:LEU:HD22	1.72	0.70
1:C:227:CYS:HB3	1:C:232:MET:H	1.72	0.54
1:C:376:MET:HE3	1:C:413:LEU:HD13	1.89	0.54
1:C:341:ILE:HG12	1:C:543:SER:HB3	1.90	0.54
1:A:421:TRP:CG	1:A:430:SER:HB3	2.44	0.52
1:A:268:GLU:HG3	2:B:66:THR:HB	1.91	0.52
1:A:397:TRP:O	1:A:400:GLN:HG2	2.12	0.48
1:C:592:ARG:HH22	2:D:39:ASP:CG	2.17	0.48
1:C:396:LEU:HD13	1:C:416:LEU:HD11	1.94	0.48
1:C:537:PHE:HZ	1:C:550:LEU:HG	1.79	0.47
1:C:268:GLU:HG3	2:D:66:THR:HB	1.96	0.47
1:A:477:GLU:HG2	7:A:961:HOH:O	2.14	0.46
1:C:466:HIS:HA	1:C:561:GLN:HG3	1.98	0.46
1:A:341:ILE:HG12	1:A:543:SER:HB2	1.98	0.45
1:C:443:TRP:CE3	2:D:75:GLY:HA2	2.51	0.45
1:C:559:ALA:HB3	1:C:562:TYR:CZ	2.52	0.44
1:A:376:MET:HE3	1:A:413:LEU:HD13	1.99	0.44
1:A:559:ALA:HB2	4:A:602:EDO:H11	1.99	0.43
1:A:371:CYS:HB3	2:B:76:AYE:H3A	1.81	0.42
1:A:363:SER:HA	4:A:603:EDO:H12	2.01	0.42
1:A:373:TYR:HA	1:A:376:MET:HE2	2.01	0.42
1:A:443:TRP:CE3	2:B:75:GLY:HA2	2.54	0.42
1:C:350:ARG:HB2	1:C:514:VAL:HB	2.00	0.42
1:C:502:HIS:HB3	1:C:562:TYR:CD1	2.55	0.42
2:B:63:LYS:NZ	7:B:204:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:TYR:HA	1:A:376:MET:CE	2.51	0.41

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)
7:A:835:HOH:O	7:A:874:HOH:O[3_454]	2.02	0.18

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	366/375 (98%)	357 (98%)	8 (2%)	1 (0%)	41	31
1	C	358/375 (96%)	346 (97%)	10 (3%)	2 (1%)	25	15
2	B	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
2	D	73/76 (96%)	72 (99%)	1 (1%)	0	100	100
All	All	870/902 (96%)	847 (97%)	20 (2%)	3 (0%)	47	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	542	SER
1	C	489[A]	SER
1	C	489[B]	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	319/322 (99%)	318 (100%)	1 (0%)	92	93
1	C	307/322 (95%)	306 (100%)	1 (0%)	92	93
2	B	68/68 (100%)	68 (100%)	0	100	100
2	D	68/68 (100%)	68 (100%)	0	100	100
All	All	762/780 (98%)	760 (100%)	2 (0%)	92	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	541	ASN
1	C	541	ASN

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

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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.50	0
4	EDO	D	101	-	3,3,3	0.45	0	2,2,2	0.52	0
4	EDO	B	101	-	3,3,3	0.47	0	2,2,2	0.48	0
3	CIT	A	601	6	3,12,12	1.19	0	3,17,17	1.01	0
3	CIT	C	601	6	3,12,12	1.29	0	3,17,17	0.40	0
4	EDO	A	603	-	3,3,3	0.44	0	2,2,2	0.35	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
4	EDO	A	602	-	-	1/1/1/1	-
4	EDO	D	101	-	-	1/1/1/1	-
4	EDO	B	101	-	-	0/1/1/1	-
3	CIT	A	601	6	-	0/6/16/16	-
3	CIT	C	601	6	-	0/6/16/16	-
4	EDO	A	603	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	EDO	O1-C1-C2-O2
4	D	101	EDO	O1-C1-C2-O2
4	A	602	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	EDO	1	0
4	A	603	EDO	1	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	A	365/375 (97%)	0.21	4 (1%) 80 82	19, 35, 75, 121	0
1	C	361/375 (96%)	1.11	80 (22%) 0 0	38, 81, 128, 154	0
2	B	75/76 (98%)	-0.13	0 100 100	26, 36, 48, 52	0
2	D	75/76 (98%)	1.46	19 (25%) 0 0	64, 93, 112, 116	0
All	All	876/902 (97%)	0.66	103 (11%) 4 4	19, 60, 116, 154	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	571	ILE	10.4
1	C	577	TYR	7.6
1	C	264	LEU	6.4
2	D	13	ILE	6.3
1	C	457	ARG	5.8
1	C	450	VAL	5.7
1	C	583	LEU	5.6
1	C	592	ARG	5.4
1	C	570	THR	5.2
1	C	462	LEU	5.1
1	C	435	CYS	5.0
1	C	491	GLY	4.8
1	C	591	ASP	4.8
1	C	542	SER	4.8
1	C	584	ARG	4.8
1	C	231	GLY	4.6
1	C	236	ASN	4.6
1	C	576	GLN	4.5
1	C	575	GLN	4.4
1	C	579	GLN	4.4
2	D	35	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	234	LEU	4.3
1	C	458	ILE	4.2
2	D	36	ILE	4.2
2	D	4	PHE	4.2
1	C	389	TYR	4.2
1	C	455	PHE	4.1
1	C	431	GLU	4.1
1	C	228	PRO	4.1
2	D	14	THR	4.0
1	A	224	THR	3.9
2	D	15	LEU	3.8
1	C	460	CYS	3.8
2	D	11	LYS	3.8
2	D	30	ILE	3.7
2	D	10	GLY	3.7
1	C	516	ARG	3.6
1	C	421	TRP	3.5
1	C	384	LEU	3.5
2	D	63	LYS	3.5
1	C	270	ARG	3.5
1	C	569	GLY	3.4
1	C	461	GLN	3.4
1	C	415	SER	3.3
1	A	490	VAL	3.2
2	D	9	THR	3.2
1	C	572	ASP	3.2
1	C	235	ASP	3.2
1	C	582	ILE	3.2
1	C	422	SER	3.1
1	C	427	ILE	3.1
1	C	423	GLN	3.0
1	C	432	GLN	3.0
1	C	399	GLY	3.0
1	C	393	LEU	3.0
2	D	23	ILE	2.9
1	C	397	TRP	2.9
1	C	568	VAL	2.9
1	C	494	PHE	2.9
1	C	265	ARG	2.8
2	D	19	PRO	2.8
1	C	433	LEU	2.7
1	C	590	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	424	GLY	2.7
1	C	540	THR	2.6
1	C	537	PHE	2.6
1	C	242	SER	2.6
1	C	489[A]	SER	2.6
1	C	580	SER	2.6
2	D	34	GLU	2.5
1	C	396	LEU	2.5
1	C	573	SER	2.5
1	C	392	ARG	2.5
1	C	428	GLN	2.5
1	C	226	SER	2.5
1	C	391	GLU	2.5
2	D	69	LEU	2.4
1	A	543	SER	2.4
2	D	12	THR	2.4
1	C	434	GLY	2.4
1	C	520	LEU	2.4
2	D	8	LEU	2.3
1	C	232	MET	2.3
1	A	542	SER	2.3
1	C	588	ILE	2.3
1	C	538	GLY	2.3
1	C	456	LEU	2.2
1	C	587	ARG	2.2
1	C	418	GLU	2.2
1	C	343	THR	2.2
1	C	425	PHE	2.2
1	C	395	LYS	2.2
1	C	578	GLN	2.1
1	C	574	GLU	2.1
1	C	486	PHE	2.1
2	D	64	GLU	2.1
1	C	430	SER	2.1
1	C	263	ALA	2.1
1	C	459	LYS	2.1
1	C	546	ALA	2.0
1	C	404	ARG	2.0
2	D	50	LEU	2.0
1	C	545	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 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(\AA^2)	Q<0.9
4	EDO	D	101	4/4	0.78	0.19	70,71,72,78	0
3	CIT	C	601	13/13	0.82	0.18	61,64,75,80	0
6	NA	C	603	1/1	0.82	0.06	63,63,63,63	0
4	EDO	B	101	4/4	0.92	0.14	35,36,37,39	0
5	ZN	C	602	1/1	0.94	0.09	101,101,101,101	0
3	CIT	A	601	13/13	0.96	0.10	32,36,45,46	0
4	EDO	A	602	4/4	0.96	0.12	30,37,42,53	0
4	EDO	A	603	4/4	0.97	0.12	38,39,43,58	0
5	ZN	A	604	1/1	0.97	0.09	54,54,54,54	0
6	NA	A	606	1/1	0.99	0.08	34,34,34,34	0
6	NA	A	605	1/1	0.99	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.