Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:53 AM GMT

PDB ID	:	2YPT
Title	:	Crystal structure of the human nuclear membrane zinc metalloprotease ZMPSTE24 mutant (E336A) in complex with a synthetic CSIM tetrapeptide from the C-terminus of prelamin A
Authors	:	Pike, A.C.W.; Dong, Y.Y.; Quigley, A.; Dong, L.; Savitsky, P.; Cooper, C.D.O.; Chaikuad, A.; Goubin, S.; Shrestha, L.; Li, Q.; Mukhopadhyay, S.; Yang, J.; Xia, X.; Shintre, C.A.; Barr, A.J.; Berridge, G.; Chalk, R.; Bray, J.E.; Von Delft, F.; Bullock, A.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.; Burgess-Brown, N.; Carpenter, E.P.
Deposited on	:	2012-11-01
Resolution	:	3.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

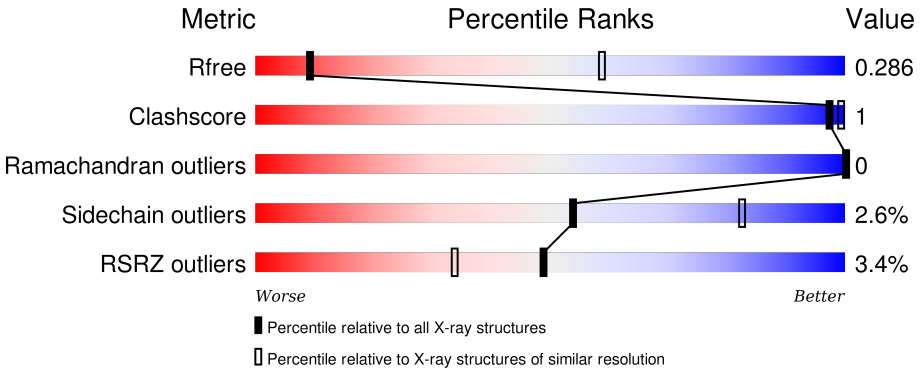
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.80 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}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	482	% 83% 5% 12%
1	B	482	5% 83% • 14%
1	D	482	3% 81% 5% 14%
1	E	482	3% 82% • 14%
2	F	4	50% 25% 25%

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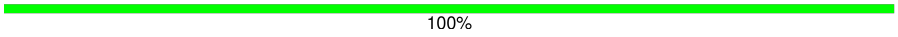
Mol	Chain	Length	Quality of chain
2	G	4	
2	H	4	
2	I	4	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12513 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 CAAX PRENYL PROTEASE 1 HOMOLOG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	1	0
			3153	2096	489	561	7			
1	B	416	Total	C	N	O	S	0	1	0
			3061	2026	482	546	7			
1	D	415	Total	C	N	O	S	0	1	0
			3156	2101	490	557	8			
1	E	414	Total	C	N	O	S	0	1	0
			3045	2015	473	550	7			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	THR	VARIANT	UNP O75844
A	336	ALA	GLU	ENGINEERED MUTATION	UNP O75844
A	476	ALA	-	EXPRESSION TAG	UNP O75844
A	477	GLU	-	EXPRESSION TAG	UNP O75844
A	478	ASN	-	EXPRESSION TAG	UNP O75844
A	479	LEU	-	EXPRESSION TAG	UNP O75844
A	480	TYR	-	EXPRESSION TAG	UNP O75844
A	481	PHE	-	EXPRESSION TAG	UNP O75844
A	482	GLN	-	EXPRESSION TAG	UNP O75844
B	137	ALA	THR	VARIANT	UNP O75844
B	336	ALA	GLU	ENGINEERED MUTATION	UNP O75844
B	476	ALA	-	EXPRESSION TAG	UNP O75844
B	477	GLU	-	EXPRESSION TAG	UNP O75844
B	478	ASN	-	EXPRESSION TAG	UNP O75844
B	479	LEU	-	EXPRESSION TAG	UNP O75844
B	480	TYR	-	EXPRESSION TAG	UNP O75844
B	481	PHE	-	EXPRESSION TAG	UNP O75844
B	482	GLN	-	EXPRESSION TAG	UNP O75844
D	137	ALA	THR	VARIANT	UNP O75844
D	336	ALA	GLU	ENGINEERED MUTATION	UNP O75844
D	476	ALA	-	EXPRESSION TAG	UNP O75844

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Chain	Residue	Modelled	Actual	Comment	Reference
D	477	GLU	-	EXPRESSION TAG	UNP O75844
D	478	ASN	-	EXPRESSION TAG	UNP O75844
D	479	LEU	-	EXPRESSION TAG	UNP O75844
D	480	TYR	-	EXPRESSION TAG	UNP O75844
D	481	PHE	-	EXPRESSION TAG	UNP O75844
D	482	GLN	-	EXPRESSION TAG	UNP O75844
E	137	ALA	THR	VARIANT	UNP O75844
E	336	ALA	GLU	ENGINEERED MUTATION	UNP O75844
E	476	ALA	-	EXPRESSION TAG	UNP O75844
E	477	GLU	-	EXPRESSION TAG	UNP O75844
E	478	ASN	-	EXPRESSION TAG	UNP O75844
E	479	LEU	-	EXPRESSION TAG	UNP O75844
E	480	TYR	-	EXPRESSION TAG	UNP O75844
E	481	PHE	-	EXPRESSION TAG	UNP O75844
E	482	GLN	-	EXPRESSION TAG	UNP O75844

- Molecule 2 is a protein called PRELAMIN-A/C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	S	0	0	0
			19	11	3	4	1			
2	G	4	Total	C	N	O	S	0	0	0
			28	16	4	6	2			
2	H	4	Total	C	N	O	S	0	0	0
			28	16	4	6	2			
2	I	3	Total	C	N	O	S	0	0	0
			19	11	3	4	1			

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

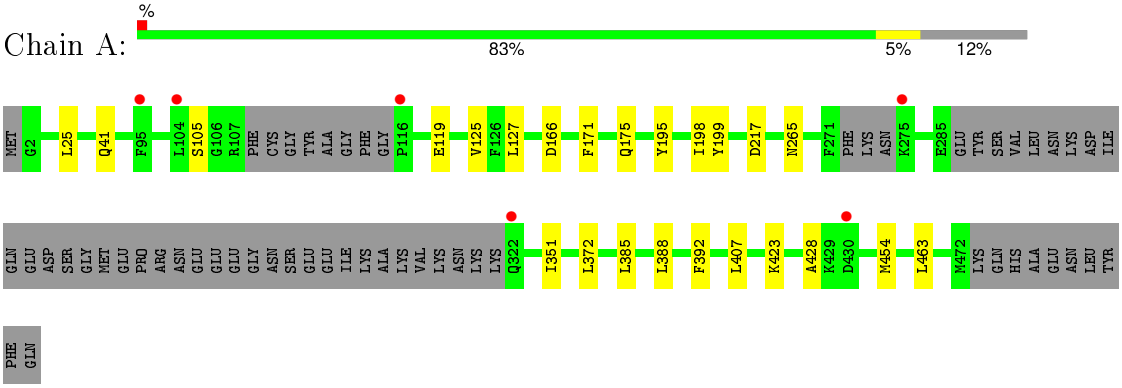
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

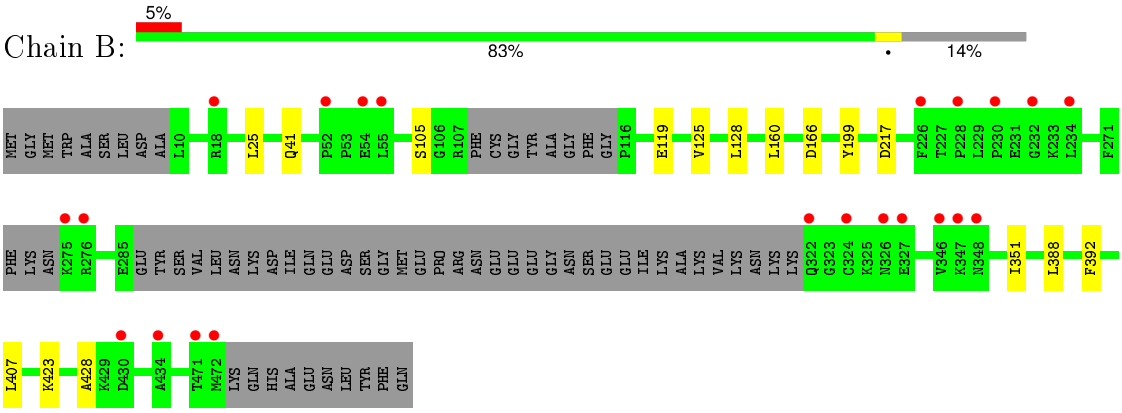
- Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG

Chain A:



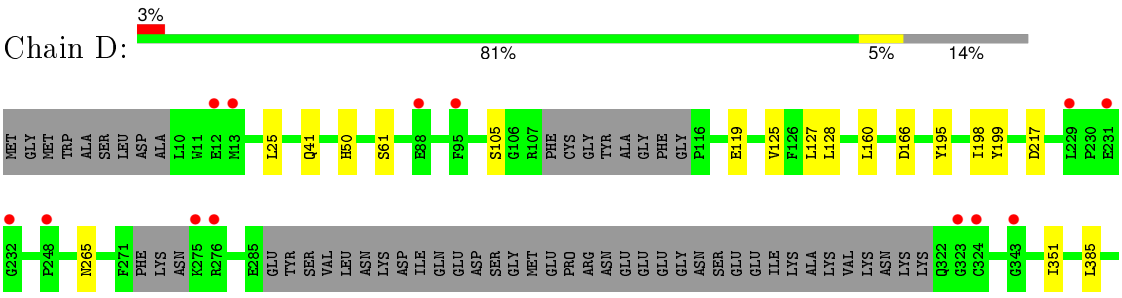
- Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG

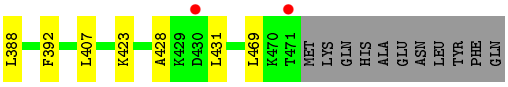
Chain B:



- Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG

Chain D:





• Molecule 1: CAAX PRENYL PROTEASE 1 HOMOLOG

Chain E:

• Molecule 2: PRELAMIN-A/C

Chain F:

• Molecule 2: PRELAMIN-A/C

Chain G:

There are no outlier residues recorded for this chain.

• Molecule 2: PRELAMIN-A/C

Chain H:

• Molecule 2: PRELAMIN-A/C

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.32Å 95.54Å 132.03Å 76.26° 79.67° 72.30°	Depositor
Resolution (Å)	38.50 – 3.80 37.94 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (38.50-3.80) 92.6 (37.94-3.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 3.76Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.263 , 0.281 0.276 , 0.286	Depositor DCC
R_{free} test set	1420 reflections (5.56%)	DCC
Wilson B-factor (Å^2)	153.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 139.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 26941 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	12513	wwPDB-VP
Average B, all atoms (Å^2)	173.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN

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	0/3247	0.53	0/4447
1	B	0.42	0/3154	0.53	0/4320
1	D	0.41	0/3253	0.53	0/4446
1	E	0.42	0/3136	0.53	0/4299
2	F	0.48	0/18	0.62	0/23
2	G	0.52	0/27	0.48	0/33
2	H	0.53	0/27	0.49	0/33
2	I	0.39	0/18	0.52	0/23
All	All	0.42	0/12880	0.53	0/17624

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	3153	0	2871	8	0
1	B	3061	0	2709	5	0
1	D	3156	0	2908	9	0
1	E	3045	0	2712	7	0
2	F	19	0	15	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	28	0	24	0	0
2	H	28	0	24	1	0
2	I	19	0	15	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	12513	0	11278	29	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 1.

All (29) 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:E:127:LEU:HD13	1:E:385:LEU:HD21	1.79	0.63
1:D:105:SER:HB2	1:D:125:VAL:HG13	1.83	0.60
1:B:105:SER:HB2	1:B:125:VAL:HG13	1.82	0.60
1:A:105:SER:HB2	1:A:125:VAL:HG13	1.85	0.58
1:E:55:LEU:HA	1:E:58:ILE:HD12	1.87	0.57
1:A:265:ASN:HD21	2:F:662:SER:HB2	1.71	0.55
1:D:388:LEU:O	1:D:392:PHE:HB2	2.08	0.54
1:A:388:LEU:O	1:A:392:PHE:HB2	2.09	0.53
1:B:388:LEU:O	1:B:392:PHE:HB2	2.08	0.53
1:E:388:LEU:O	1:E:392:PHE:HB2	2.09	0.53
1:E:265:ASN:HD21	2:I:662:SER:HB2	1.74	0.51
1:A:195:TYR:HB3	1:A:198:ILE:HD12	1.94	0.50
1:E:125:VAL:HA	1:E:128:LEU:HD12	1.94	0.49
1:D:195:TYR:HB3	1:D:198:ILE:HD12	1.95	0.48
1:D:127:LEU:HD13	1:D:385:LEU:HD21	1.96	0.48
1:D:265:ASN:HD21	2:H:662:SER:HB2	1.79	0.47
1:D:431:LEU:HD23	1:D:469:LEU:HD21	1.99	0.45
1:B:351:ILE:HG21	1:B:407:LEU:HD21	1.98	0.44
1:A:127:LEU:HD13	1:A:385:LEU:HD21	2.00	0.43
1:D:351:ILE:HG21	1:D:407:LEU:HD21	2.00	0.43
1:A:351:ILE:HG21	1:A:407:LEU:HD21	2.00	0.42
1:A:423:LYS:HA	1:A:428:ALA:HB2	2.02	0.42
1:B:423:LYS:HA	1:B:428:ALA:HB2	2.02	0.42
1:E:423:LYS:HA	1:E:428:ALA:HB2	2.02	0.41
1:D:125:VAL:HA	1:D:128:LEU:HD12	2.01	0.41
1:D:423:LYS:HA	1:D:428:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:PHE:O	1:A:175:GLN:HG2	2.20	0.41
1:B:125:VAL:HA	1:B:128:LEU:HD12	2.02	0.40
1:E:105:SER:HB2	1:E:125:VAL:HG13	2.04	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	417/482 (86%)	405 (97%)	12 (3%)	0	100	100
1	B	409/482 (85%)	396 (97%)	13 (3%)	0	100	100
1	D	408/482 (85%)	396 (97%)	12 (3%)	0	100	100
1	E	407/482 (84%)	396 (97%)	11 (3%)	0	100	100
2	F	1/4 (25%)	0	1 (100%)	0	100	100
2	G	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
2	H	2/4 (50%)	1 (50%)	1 (50%)	0	100	100
2	I	1/4 (25%)	0	1 (100%)	0	100	100
All	All	1647/1944 (85%)	1595 (97%)	52 (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	A	295/424 (70%)	286 (97%)	9 (3%)	47 80
1	B	277/424 (65%)	270 (98%)	7 (2%)	55 83
1	D	303/424 (72%)	294 (97%)	9 (3%)	48 80
1	E	282/424 (66%)	277 (98%)	5 (2%)	66 88
2	F	2/4 (50%)	2 (100%)	0	100 100
2	G	3/4 (75%)	3 (100%)	0	100 100
2	H	3/4 (75%)	3 (100%)	0	100 100
2	I	2/4 (50%)	2 (100%)	0	100 100
All	All	1167/1712 (68%)	1137 (97%)	30 (3%)	54 82

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	41	GLN
1	A	119	GLU
1	A	166	ASP
1	A	199	TYR
1	A	217	ASP
1	A	372	LEU
1	A	454	MET
1	A	463	LEU
1	B	25	LEU
1	B	41	GLN
1	B	119	GLU
1	B	160	LEU
1	B	166	ASP
1	B	199	TYR
1	B	217	ASP
1	D	25	LEU
1	D	41	GLN
1	D	50	HIS
1	D	61	SER
1	D	119	GLU
1	D	160	LEU
1	D	166	ASP
1	D	199	TYR
1	D	217	ASP
1	E	41	GLN
1	E	119	GLU

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Mol	Chain	Res	Type
1	E	160	LEU
1	E	166	ASP
1	E	217	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	265	ASN
1	B	41	GLN
1	D	50	HIS
1	E	41	GLN
1	E	265	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 carbohydrates 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

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	424/482 (87%)	-0.05	6 (1%) 78 63	99, 170, 240, 260	0
1	B	416/482 (86%)	0.09	22 (5%) 30 20	103, 178, 252, 261	0
1	D	415/482 (86%)	-0.03	15 (3%) 46 32	103, 167, 222, 242	0
1	E	414/482 (85%)	-0.01	14 (3%) 49 34	105, 198, 239, 257	0
2	F	3/4 (75%)	-0.31	0 100 100	175, 175, 180, 181	0
2	G	4/4 (100%)	-0.61	0 100 100	206, 208, 211, 214	0
2	H	4/4 (100%)	-0.48	0 100 100	174, 174, 178, 181	0
2	I	3/4 (75%)	-0.20	0 100 100	217, 217, 220, 235	0
All	All	1683/1944 (86%)	-0.01	57 (3%) 49 34	99, 176, 237, 261	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	193	GLY	5.1
1	E	51	VAL	5.1
1	D	13	MET	4.9
1	E	194	ASP	4.9
1	E	50	HIS	4.8
1	B	324	CYS	4.8
1	B	472	MET	4.3
1	D	275	LYS	4.2
1	B	232	GLY	4.1
1	E	275	LYS	4.1
1	E	52	PRO	3.5
1	B	347	LYS	3.5
1	D	324	CYS	3.4
1	B	348	ASN	3.4
1	A	275	LYS	3.3
1	B	430	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	327	GLU	3.2
1	E	13	MET	3.1
1	E	195	TYR	3.0
1	D	471	THR	3.0
1	E	420	ALA	3.0
1	B	228	PRO	2.9
1	D	248	PRO	2.9
1	D	323	GLY	2.9
1	B	52	PRO	2.9
1	E	231	GLU	2.7
1	D	232	GLY	2.7
1	D	88	GLU	2.7
1	B	55	LEU	2.7
1	E	379	TYR	2.7
1	B	275	LYS	2.7
1	B	234	LEU	2.6
1	E	254	VAL	2.6
1	B	230	PRO	2.6
1	B	326	ASN	2.6
1	D	430	ASP	2.6
1	A	116	PRO	2.6
1	E	192	GLY	2.6
1	B	471	THR	2.5
1	B	226	PHE	2.5
1	B	54	GLU	2.5
1	D	231	GLU	2.5
1	B	322	GLN	2.4
1	D	276	ARG	2.4
1	B	346	VAL	2.3
1	D	95	PHE	2.3
1	D	229	LEU	2.2
1	B	18	ARG	2.2
1	A	322	GLN	2.2
1	A	430	ASP	2.2
1	E	324	CYS	2.1
1	B	276	ARG	2.1
1	D	343	GLY	2.1
1	A	104	LEU	2.1
1	A	95	PHE	2.1
1	D	12	GLU	2.1
1	B	434	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	B	600	1/1	0.97	0.24	1.83	154,154,154,154	0
3	ZN	D	600	1/1	0.98	0.23	1.74	130,130,130,130	0
3	ZN	A	600	1/1	0.95	0.24	1.24	141,141,141,141	0
3	ZN	E	600	1/1	0.93	0.17	-0.52	187,187,187,187	0

6.5 Other polymers (i)

There are no such residues in this entry.