



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:28 pm BST

PDB ID : 3ZNI  
Title : Structure of phosphoTyr363-Cbl-b - UbcH5B-Ub - ZAP-70 peptide complex  
Authors : Dou, H.; Buetow, L.; Sibbet, G.J.; Cameron, K.; Huang, D.T.  
Deposited on : 2013-02-14  
Resolution : 2.21 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

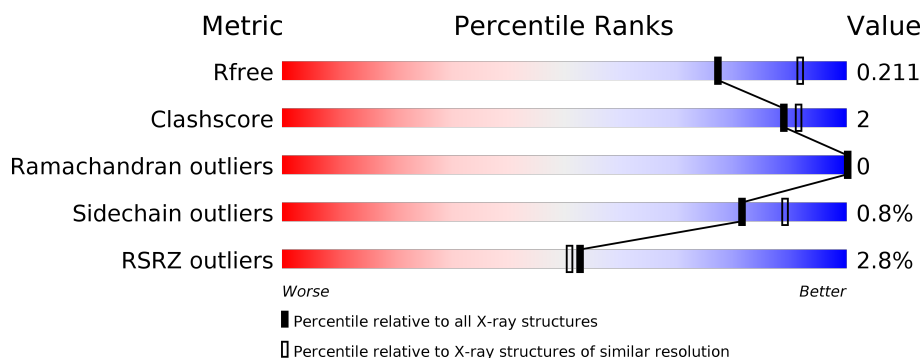
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.21 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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  $\geq 3$ , 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	394	<div> <div style="width: 100%;"></div> <div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> </div> </div>
1	E	394	<div> <div style="width: 100%;"></div> <div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> </div> </div>
1	I	394	<div> <div style="width: 100%;"></div> <div> <div style="width: 91%;"></div> <div style="width: 7%;"></div> </div> </div>
1	M	394	<div> <div style="width: 100%;"></div> <div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> </div> </div>
2	B	12	<div> <div style="width: 25%;"></div> <div style="width: 75%;"></div> <div style="width: 25%;"></div> </div>
2	F	12	<div> <div style="width: 8%;"></div> <div style="width: 67%;"></div> <div style="width: 33%;"></div> </div>

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Mol	Chain	Length	Quality of chain
2	J	12	<div><div></div><div>67%</div><div>33%</div></div>
2	N	12	<div><div>25%</div><div></div><div>75%</div><div>25%</div></div>
3	C	146	<div><div>%</div><div></div><div>97%</div><div>.</div></div>
3	G	146	<div><div>2%</div><div></div><div>95%</div><div>5% .</div></div>
3	K	146	<div><div>4%</div><div></div><div>99%</div><div>.</div></div>
3	O	146	<div><div>%</div><div></div><div>97%</div><div>.</div></div>
4	D	81	<div><div></div><div>86%</div><div>9% 5%</div></div>
4	H	81	<div><div>6%</div><div></div><div>86%</div><div>9% 5%</div></div>
4	L	81	<div><div>5%</div><div></div><div>88%</div><div>7% 5%</div></div>
4	P	81	<div><div>%</div><div></div><div>88%</div><div>6% . 5%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 20546 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 E3 UBIQUITIN-PROTEIN LIGASE CBL-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	P	S	0	2	0
			3098	1987	522	565	1	23			
1	E	390	Total	C	N	O	P	S	0	1	0
			3120	2002	526	568	1	23			
1	I	386	Total	C	N	O	P	S	0	1	0
			3072	1969	517	563	1	22			
1	M	390	Total	C	N	O	P	S	0	3	0
			3128	2006	531	568	1	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP Q13191
A	35	SER	-	expression tag	UNP Q13191
A	360	PHE	TYR	engineered mutation	UNP Q13191
E	34	GLY	-	expression tag	UNP Q13191
E	35	SER	-	expression tag	UNP Q13191
E	360	PHE	TYR	engineered mutation	UNP Q13191
I	34	GLY	-	expression tag	UNP Q13191
I	35	SER	-	expression tag	UNP Q13191
I	360	PHE	TYR	engineered mutation	UNP Q13191
M	34	GLY	-	expression tag	UNP Q13191
M	35	SER	-	expression tag	UNP Q13191
M	360	PHE	TYR	engineered mutation	UNP Q13191

- Molecule 2 is a protein called TYROSINE-PROTEIN KINASE ZAP-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			69	40	9	19	1			
2	F	8	Total	C	N	O	P	0	0	0
			63	37	8	17	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	8	Total	C	N	O	P	0	0	0
			63	37	8	17	1			
2	N	9	Total	C	N	O	P	0	0	0
			68	40	9	18	1			

- Molecule 3 is a protein called UBIQUITIN-CONJUGATING ENZYME E2 D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	146	Total	C	N	O	S	0	0	0
			1162	748	198	210	6			
3	G	146	Total	C	N	O	S	0	0	0
			1172	753	202	211	6			
3	K	146	Total	C	N	O	S	0	1	0
			1179	756	205	212	6			
3	O	146	Total	C	N	O	S	0	3	0
			1187	762	207	212	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	22	ARG	SER	engineered mutation	UNP P62837
C	85	LYS	CYS	engineered mutation	UNP P62837
G	22	ARG	SER	engineered mutation	UNP P62837
G	85	LYS	CYS	engineered mutation	UNP P62837
K	22	ARG	SER	engineered mutation	UNP P62837
K	85	LYS	CYS	engineered mutation	UNP P62837
O	22	ARG	SER	engineered mutation	UNP P62837
O	85	LYS	CYS	engineered mutation	UNP P62837

- Molecule 4 is a protein called POLYUBIQUITIN-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	77	Total	C	N	O	S	0	0	0
			599	375	104	119	1			
4	H	77	Total	C	N	O	S	0	0	0
			595	374	105	115	1			
4	L	77	Total	C	N	O	S	0	0	0
			583	368	101	113	1			
4	P	77	Total	C	N	O	S	0	0	0
			600	377	104	118	1			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP P0CG48
D	-3	SER	-	expression tag	UNP P0CG48
D	-2	GLY	-	expression tag	UNP P0CG48
D	-1	GLY	-	expression tag	UNP P0CG48
D	0	SER	-	expression tag	UNP P0CG48
H	-4	GLY	-	expression tag	UNP P0CG48
H	-3	SER	-	expression tag	UNP P0CG48
H	-2	GLY	-	expression tag	UNP P0CG48
H	-1	GLY	-	expression tag	UNP P0CG48
H	0	SER	-	expression tag	UNP P0CG48
L	-4	GLY	-	expression tag	UNP P0CG48
L	-3	SER	-	expression tag	UNP P0CG48
L	-2	GLY	-	expression tag	UNP P0CG48
L	-1	GLY	-	expression tag	UNP P0CG48
L	0	SER	-	expression tag	UNP P0CG48
P	-4	GLY	-	expression tag	UNP P0CG48
P	-3	SER	-	expression tag	UNP P0CG48
P	-2	GLY	-	expression tag	UNP P0CG48
P	-1	GLY	-	expression tag	UNP P0CG48
P	0	SER	-	expression tag	UNP P0CG48

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	2	Total Zn 2 2	0	0
5	A	2	Total Zn 2 2	0	0
5	M	2	Total Zn 2 2	0	0
5	E	2	Total Zn 2 2	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	1	Total Ca 1 1	0	0
6	A	1	Total Ca 1 1	0	0
6	M	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Ca	0	0
			1	1		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	E	1	Total	C	O	0	0
			4	2	2		
7	I	1	Total	C	O	0	0
			4	2	2		
7	M	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	125	Total	O	0	0
			125	125		
8	B	1	Total	O	0	0
			1	1		
8	C	67	Total	O	0	0
			67	67		
8	D	14	Total	O	0	0
			14	14		

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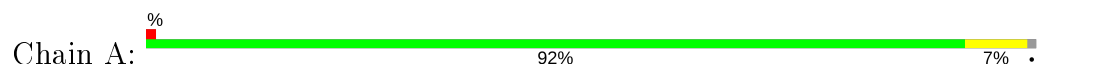
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	171	Total 171	O 171	0	0
8	F	1	Total 1	O 1	0	0
8	G	49	Total 49	O 49	0	0
8	H	7	Total 7	O 7	0	0
8	I	98	Total 98	O 98	0	0
8	J	2	Total 2	O 2	0	0
8	K	37	Total 37	O 37	0	0
8	L	7	Total 7	O 7	0	0
8	M	111	Total 111	O 111	0	0
8	O	60	Total 60	O 60	0	0
8	P	10	Total 10	O 10	0	0



### 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 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.

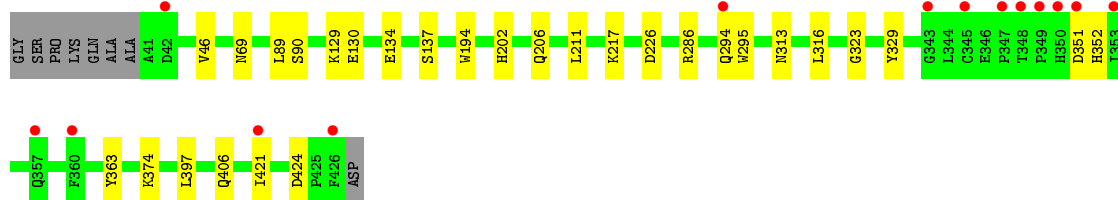
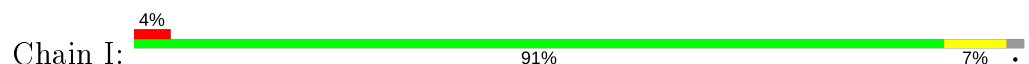
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE CBL-B



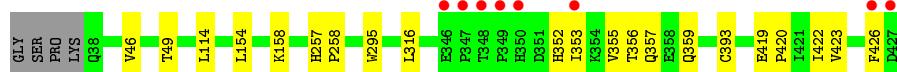
- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE CBL-B



- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE CBL-B

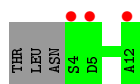


- Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE CBL-B

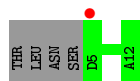


- Molecule 2: TYROSINE-PROTEIN KINASE ZAP-70

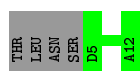




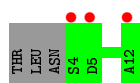
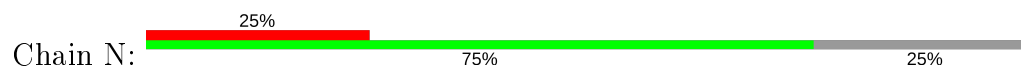
- Molecule 2: TYROSINE-PROTEIN KINASE ZAP-70



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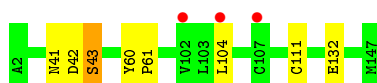
- Molecule 2: TYROSINE-PROTEIN KINASE ZAP-70



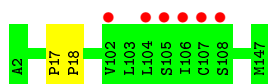
- Molecule 3: UBIQUITIN-CONJUGATING ENZYME E2 D2



- Molecule 3: UBIQUITIN-CONJUGATING ENZYME E2 D2

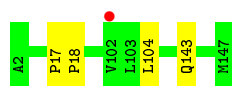


- Molecule 3: UBIQUITIN-CONJUGATING ENZYME E2 D2



- Molecule 3: UBIQUITIN-CONJUGATING ENZYME E2 D2





● Molecule 4: POLYUBIQUITIN-C

Chain D: 86% 9% 5%



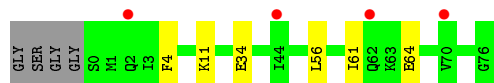
● Molecule 4: POLYUBIQUITIN-C

Chain H: 6% 86% 9% 5%



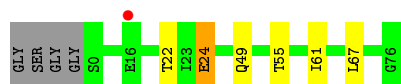
● Molecule 4: POLYUBIQUITIN-C

Chain L: 5% 88% 7% 5%



● Molecule 4: POLYUBIQUITIN-C

Chain P: % 88% 6% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.97Å 131.80Å 122.00Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	30.54 – 2.21 30.54 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.54-2.21) 99.6 (30.54-2.21)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.22Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.175 , 0.211 0.176 , 0.211	Depositor DCC
$R_{free}$ test set	7485 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.2	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	20546	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, CA, PTR, EDO

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	0.27	0/3164	0.41	0/4291
1	E	0.29	0/3183	0.43	0/4310
1	I	0.26	0/3136	0.41	0/4252
1	M	0.27	0/3198	0.41	0/4331
2	B	0.22	0/53	0.43	0/71
2	F	0.24	0/47	0.38	0/63
2	J	0.21	0/47	0.39	0/63
2	N	0.24	0/52	0.40	0/70
3	C	0.27	0/1198	0.44	0/1634
3	G	0.26	0/1208	0.45	0/1646
3	K	0.25	0/1218	0.44	0/1660
3	O	0.28	0/1232	0.48	0/1678
4	D	0.24	0/605	0.46	0/816
4	H	0.24	0/601	0.46	0/810
4	L	0.25	0/589	0.44	0/796
4	P	0.26	0/606	0.44	0/816
All	All	0.27	0/20137	0.43	0/27307

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	3098	0	2967	14	0
1	E	3120	0	3022	8	0
1	I	3072	0	2937	16	0
1	M	3128	0	3024	13	0
2	B	69	0	50	0	0
2	F	63	0	45	0	0
2	J	63	0	45	0	0
2	N	68	0	47	0	0
3	C	1162	0	1139	3	0
3	G	1172	0	1156	5	0
3	K	1179	0	1162	1	0
3	O	1187	0	1176	2	0
4	D	599	0	612	3	0
4	H	595	0	615	3	0
4	L	583	0	593	5	0
4	P	600	0	619	3	0
5	A	2	0	0	0	0
5	E	2	0	0	0	0
5	I	2	0	0	0	0
5	M	2	0	0	0	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
6	I	1	0	0	0	0
6	M	1	0	0	0	0
7	A	4	0	6	0	0
7	E	4	0	6	0	0
7	I	4	0	6	0	0
7	M	4	0	6	0	0
8	A	125	0	0	1	0
8	B	1	0	0	0	0
8	C	67	0	0	0	0
8	D	14	0	0	0	0
8	E	171	0	0	0	0
8	F	1	0	0	0	0
8	G	49	0	0	0	0
8	H	7	0	0	0	0
8	I	98	0	0	0	0
8	J	2	0	0	0	0
8	K	37	0	0	0	0
8	L	7	0	0	0	0
8	M	111	0	0	0	0
8	O	60	0	0	0	0
8	P	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	20546	0	19233	74	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 2.

All (74) 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:65:LEU:O	1:A:140:ARG:NH2	2.16	0.78
1:E:46:VAL:HG11	1:E:89:LEU:HD11	1.68	0.75
3:G:132:GLU:HG2	1:I:90:SER:HA	1.69	0.73
4:D:14:THR:O	4:D:33:LYS:NZ	2.23	0.71
1:I:46:VAL:HG11	1:I:89:LEU:HD11	1.76	0.66
1:I:352:HIS:ND1	1:I:424:ASP:OD2	2.29	0.65
1:E:65:LEU:O	1:E:140:ARG:NH2	2.32	0.62
1:M:353:ILE:HD11	1:M:423:VAL:HG22	1.81	0.62
1:M:356:THR:HG23	1:M:359:GLN:H	1.65	0.61
4:L:11:LYS:NZ	4:L:34:GLU:OE2	2.34	0.60
1:I:294:GLN:NE2	1:I:313:ASN:OD1	2.36	0.58
1:M:355:VAL:HG12	1:M:426:PHE:HB2	1.86	0.58
4:L:4:PHE:HE2	4:L:64:GLU:HG3	1.69	0.57
1:A:214:MET:SD	8:A:2078:HOH:O	2.58	0.57
1:M:154:LEU:HD11	1:M:158:LYS:HE3	1.89	0.55
1:I:323:GLY:HA3	1:I:329:TYR:CD2	2.43	0.54
4:D:26:VAL:HG21	4:D:56:LEU:HD21	1.91	0.53
1:M:356:THR:OG1	1:M:357:GLN:N	2.42	0.52
1:A:376:CYS:HB3	1:A:396:CYS:SG	2.51	0.51
1:I:134:GLU:HB2	1:I:137:SER:HB3	1.93	0.50
1:M:295:TRP:CD2	1:M:316:LEU:HD22	2.47	0.49
4:H:62:GLN:NE2	4:H:65:SER:OG	2.44	0.49
1:A:323:GLY:HA3	1:A:329:TYR:CD2	2.48	0.49
1:I:363:PTR:HE1	1:I:374:LYS:HE2	1.95	0.48
1:I:217:LYS:NZ	1:I:226:ASP:OD1	2.36	0.47
1:I:129:LYS:HB3	1:I:130:GLU:H	1.52	0.46
1:I:202:HIS:CE1	1:I:206:GLN:HG3	2.50	0.46
1:E:376:CYS:HB3	1:E:396:CYS:SG	2.55	0.46
1:I:295:TRP:CD2	1:I:316:LEU:HD22	2.51	0.46
1:M:352:HIS:CD2	1:M:422:ILE:HB	2.51	0.46
1:M:352:HIS:HD2	1:M:422:ILE:HB	1.80	0.46
3:C:60:TYR:CD1	3:C:61:PRO:HA	2.51	0.45
1:A:327:GLY:HA2	1:A:330:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:41:ASN:OD1	3:G:42:ASP:N	2.49	0.45
3:G:60:TYR:CD1	3:G:61:PRO:HA	2.52	0.45
4:L:11:LYS:HE2	4:L:11:LYS:HB3	1.76	0.45
1:M:257:HIS:HA	1:M:258:PRO:HD3	1.79	0.45
4:P:22:THR:OG1	4:P:24:GLU:HG3	2.17	0.45
4:H:23:ILE:HB	4:H:52:ASP:HA	1.97	0.45
4:L:4:PHE:CE2	4:L:64:GLU:HG3	2.51	0.45
1:A:302:GLY:HA2	1:A:303:ASP:HA	1.50	0.44
3:C:13:LEU:HD21	3:C:100:SER:HB2	1.99	0.44
4:P:22:THR:HA	4:P:55:THR:HA	2.00	0.44
3:G:43:SER:HB2	3:G:111:CYS:SG	2.58	0.43
1:I:194:TRP:CZ2	1:I:217:LYS:HB2	2.53	0.43
1:E:85:LEU:HD21	1:E:110:TYR:HE2	1.84	0.43
1:E:269:VAL:HG13	1:E:284:ILE:HD11	2.00	0.43
3:G:104:LEU:HA	3:G:104:LEU:HD23	1.90	0.43
1:E:295:TRP:CD2	1:E:316:LEU:HD22	2.54	0.43
4:P:61:ILE:HD13	4:P:67:LEU:HD21	2.00	0.42
1:M:295:TRP:CE2	1:M:316:LEU:HD22	2.55	0.42
3:C:66:LYS:HE2	1:I:69:ASN:ND2	2.35	0.42
1:I:194:TRP:CD1	1:I:217:LYS:HD2	2.55	0.42
1:A:160:ILE:C	1:A:162:PRO:HD3	2.40	0.42
1:E:194:TRP:CG	1:E:217:LYS:HD2	2.55	0.42
1:A:154:LEU:HD11	1:A:158:LYS:HE3	2.01	0.41
4:D:39:ASP:O	4:D:72:ARG:HD3	2.20	0.41
3:O:17:PRO:HA	3:O:18:PRO:HD3	1.80	0.41
1:E:175:LYS:HD3	1:E:175:LYS:HA	1.80	0.41
1:A:294:GLN:HE22	1:A:312:HIS:CE1	2.38	0.41
1:A:269:VAL:HG13	1:A:284:ILE:HD11	2.02	0.41
1:A:330:LEU:O	1:A:338:ASN:HB2	2.21	0.41
1:I:351:ASP:OD1	1:I:421:ILE:HG22	2.21	0.41
1:M:49:THR:HG21	1:M:114:LEU:HD23	2.02	0.41
1:A:175:LYS:HA	1:A:175:LYS:HD3	1.88	0.41
4:H:61:ILE:HD13	4:H:67:LEU:HD21	2.02	0.41
3:K:17:PRO:HA	3:K:18:PRO:HD3	1.93	0.41
1:A:322:ASP:OD1	1:A:325:ARG:NH1	2.52	0.41
4:L:56:LEU:HB3	4:L:61:ILE:HB	2.02	0.41
1:A:295:TRP:CD2	1:A:316:LEU:HD22	2.56	0.40
3:O:104:LEU:HD23	3:O:104:LEU:HA	1.87	0.40
1:I:295:TRP:CE2	1:I:316:LEU:HD22	2.57	0.40
1:M:46:VAL:O	1:M:49:THR:HB	2.21	0.40
1:M:419:GLU:HA	1:M:420:PRO:HD3	1.95	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	389/394 (99%)	380 (98%)	9 (2%)	0	100	100
1	E	388/394 (98%)	381 (98%)	7 (2%)	0	100	100
1	I	384/394 (98%)	376 (98%)	8 (2%)	0	100	100
1	M	390/394 (99%)	381 (98%)	9 (2%)	0	100	100
2	B	6/12 (50%)	6 (100%)	0	0	100	100
2	F	5/12 (42%)	5 (100%)	0	0	100	100
2	J	5/12 (42%)	5 (100%)	0	0	100	100
2	N	6/12 (50%)	6 (100%)	0	0	100	100
3	C	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
3	G	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
3	K	145/146 (99%)	143 (99%)	2 (1%)	0	100	100
3	O	147/146 (101%)	143 (97%)	4 (3%)	0	100	100
4	D	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
4	H	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
4	L	75/81 (93%)	73 (97%)	2 (3%)	0	100	100
4	P	75/81 (93%)	74 (99%)	1 (1%)	0	100	100
All	All	2453/2532 (97%)	2402 (98%)	51 (2%)	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	325/352 (92%)	324 (100%)	1 (0%)	92	96
1	E	332/352 (94%)	328 (99%)	4 (1%)	71	82
1	I	325/352 (92%)	321 (99%)	4 (1%)	71	82
1	M	332/352 (94%)	331 (100%)	1 (0%)	92	96
2	B	6/9 (67%)	6 (100%)	0	100	100
2	F	5/9 (56%)	5 (100%)	0	100	100
2	J	5/9 (56%)	5 (100%)	0	100	100
2	N	5/9 (56%)	5 (100%)	0	100	100
3	C	127/130 (98%)	127 (100%)	0	100	100
3	G	129/130 (99%)	128 (99%)	1 (1%)	81	89
3	K	130/130 (100%)	130 (100%)	0	100	100
3	O	131/130 (101%)	130 (99%)	1 (1%)	81	89
4	D	67/70 (96%)	66 (98%)	1 (2%)	65	76
4	H	66/70 (94%)	65 (98%)	1 (2%)	65	76
4	L	63/70 (90%)	63 (100%)	0	100	100
4	P	67/70 (96%)	65 (97%)	2 (3%)	41	51
All	All	2115/2244 (94%)	2099 (99%)	16 (1%)	81	89

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	345	CYS
4	D	49	GLN
1	E	183	ARG
1	E	303	ASP
1	E	314	LYS
1	E	355	VAL
3	G	43	SER
4	H	60	ASN
1	I	211	LEU
1	I	286	ARG
1	I	397	LEU
1	I	406	GLN
1	M	393	CYS
3	O	143	GLN

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Mol	Chain	Res	Type
4	P	24	GLU
4	P	49	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
4	H	62	GLN
1	M	352	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	PTR	E	363	1	15,16,17	1.34	1 (6%)	19,22,24	0.44	0
2	PTR	J	7	2	15,16,17	1.34	1 (6%)	19,22,24	0.53	0
1	PTR	I	363	1	15,16,17	1.29	1 (6%)	19,22,24	0.61	0
1	PTR	M	363	1	15,16,17	1.33	1 (6%)	19,22,24	0.45	0
2	PTR	B	7	2	15,16,17	1.28	1 (6%)	19,22,24	0.58	0
2	PTR	F	7	2	15,16,17	1.34	1 (6%)	19,22,24	0.63	0
2	PTR	N	7	2	15,16,17	1.35	1 (6%)	19,22,24	0.48	0
1	PTR	A	363	1	15,16,17	1.30	1 (6%)	19,22,24	0.61	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
1	PTR	E	363	1	-	1/10/11/13	0/1/1/1
2	PTR	J	7	2	-	0/10/11/13	0/1/1/1
1	PTR	I	363	1	-	2/10/11/13	0/1/1/1
1	PTR	M	363	1	-	1/10/11/13	0/1/1/1
2	PTR	B	7	2	-	1/10/11/13	0/1/1/1
2	PTR	F	7	2	-	1/10/11/13	0/1/1/1
2	PTR	N	7	2	-	0/10/11/13	0/1/1/1
1	PTR	A	363	1	-	1/10/11/13	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	7	PTR	OH-CZ	-4.35	1.30	1.40
1	E	363	PTR	OH-CZ	-4.34	1.30	1.40
2	F	7	PTR	OH-CZ	-4.32	1.30	1.40
2	J	7	PTR	OH-CZ	-4.29	1.30	1.40
1	A	363	PTR	OH-CZ	-4.25	1.31	1.40
1	M	363	PTR	OH-CZ	-4.15	1.31	1.40
1	I	363	PTR	OH-CZ	-4.13	1.31	1.40
2	B	7	PTR	OH-CZ	-4.01	1.31	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	363	PTR	C-CA-CB-CG
1	I	363	PTR	C-CA-CB-CG
1	M	363	PTR	C-CA-CB-CG
1	A	363	PTR	C-CA-CB-CG
1	I	363	PTR	N-CA-CB-CG
2	F	7	PTR	CE1-CZ-OH-P
2	B	7	PTR	CE1-CZ-OH-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	363	PTR	1	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	$\# Z  > 2$
7	EDO	A	1431	-	3,3,3	0.47	0	2,2,2	0.30	0
7	EDO	M	1431	-	3,3,3	0.45	0	2,2,2	0.30	0
7	EDO	I	1430	-	3,3,3	0.46	0	2,2,2	0.30	0
7	EDO	E	1431	-	3,3,3	0.55	0	2,2,2	0.12	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
7	EDO	A	1431	-	-	0/1/1/1	-
7	EDO	M	1431	-	-	1/1/1/1	-
7	EDO	I	1430	-	-	0/1/1/1	-
7	EDO	E	1431	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	M	1431	EDO	O1-C1-C2-O2

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	389/394 (98%)	-0.34	5 (1%) 77 75	24, 43, 80, 136	0
1	E	389/394 (98%)	-0.25	13 (3%) 46 44	24, 40, 78, 113	0
1	I	385/394 (97%)	-0.14	14 (3%) 42 40	26, 48, 85, 141	0
1	M	389/394 (98%)	-0.26	8 (2%) 63 61	30, 45, 85, 135	0
2	B	8/12 (66%)	1.26	3 (37%) 0 0	59, 67, 82, 94	0
2	F	7/12 (58%)	0.07	1 (14%) 2 2	42, 48, 63, 70	0
2	J	7/12 (58%)	0.22	0 100 100	52, 58, 69, 75	0
2	N	8/12 (66%)	1.77	3 (37%) 0 0	54, 64, 92, 105	0
3	C	146/146 (100%)	-0.37	2 (1%) 75 73	23, 35, 59, 77	0
3	G	146/146 (100%)	-0.36	3 (2%) 63 61	28, 43, 71, 83	0
3	K	146/146 (100%)	-0.29	6 (4%) 37 35	30, 44, 71, 89	0
3	O	146/146 (100%)	-0.35	1 (0%) 87 86	22, 34, 60, 84	0
4	D	77/81 (95%)	-0.16	0 100 100	24, 49, 77, 81	0
4	H	77/81 (95%)	0.16	5 (6%) 18 17	27, 53, 87, 102	0
4	L	77/81 (95%)	0.24	4 (5%) 27 25	33, 60, 88, 100	0
4	P	77/81 (95%)	-0.28	1 (1%) 77 75	29, 49, 72, 81	0
All	All	2474/2532 (97%)	-0.23	69 (2%) 53 51	22, 44, 81, 141	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	345	CYS	8.2
1	I	348	THR	6.0
1	M	348	THR	5.6
2	N	4	SER	5.4
1	I	347	PRO	5.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	N	12	ALA	5.4
1	E	40	ALA	4.7
1	E	344	LEU	4.3
1	E	351	ASP	3.7
1	A	350	HIS	3.6
1	M	347	PRO	3.5
1	M	346	GLU	3.5
1	M	350	HIS	3.4
1	E	355	VAL	3.3
1	A	349	PRO	3.3
2	B	12	ALA	3.2
3	K	104	LEU	3.2
1	M	353	ILE	3.1
1	E	345	CYS	3.1
1	M	349	PRO	3.1
1	E	357	GLN	3.0
4	L	70	VAL	3.0
4	H	16	GLU	2.9
4	H	1	MET	2.9
1	E	426	PHE	2.9
1	A	348	THR	2.9
1	E	356	THR	2.9
3	K	106	ILE	2.8
1	I	360	PHE	2.8
1	M	426	PHE	2.8
1	I	353	ILE	2.8
1	I	350	HIS	2.8
1	E	348	THR	2.7
2	B	5	ASP	2.7
1	E	38	GLN	2.7
1	I	349	PRO	2.6
2	N	5	ASP	2.6
1	M	427	ASP	2.6
1	I	351	ASP	2.6
3	K	102	VAL	2.5
3	K	105	SER	2.5
3	C	104	LEU	2.4
3	O	102	VAL	2.4
1	I	426	PHE	2.4
1	E	352	HIS	2.3
4	H	70	VAL	2.3
3	K	107	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	357	GLN	2.2
1	I	421	ILE	2.2
4	L	2	GLN	2.2
2	F	5	ASP	2.2
1	E	353	ILE	2.2
1	A	347	PRO	2.2
2	B	4	SER	2.2
4	L	62	GLN	2.1
3	G	104	LEU	2.1
3	K	108	SER	2.1
4	P	16	GLU	2.1
3	G	102	VAL	2.1
1	I	343	GLY	2.1
3	C	103	LEU	2.1
1	A	346	GLU	2.1
3	G	107	CYS	2.1
1	I	294	GLN	2.1
4	H	2	GLN	2.1
4	H	62	GLN	2.1
1	I	42	ASP	2.0
1	E	427	ASP	2.0
4	L	44	ILE	2.0

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	PTR	I	363	16/17	0.87	0.15	57,62,67,67	0
1	PTR	A	363	16/17	0.94	0.12	44,52,64,65	0
1	PTR	M	363	16/17	0.96	0.10	47,61,69,71	0
2	PTR	B	7	16/17	0.97	0.11	41,46,59,60	0
2	PTR	F	7	16/17	0.97	0.11	31,34,39,40	0
2	PTR	N	7	16/17	0.97	0.09	36,41,51,51	0
1	PTR	E	363	16/17	0.97	0.10	40,48,59,60	0
2	PTR	J	7	16/17	0.98	0.13	35,40,49,51	0

### 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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
7	EDO	E	1431	4/4	0.83	0.29	43,44,46,48	0
7	EDO	M	1431	4/4	0.92	0.19	49,51,56,59	0
7	EDO	A	1431	4/4	0.96	0.17	41,41,41,46	0
6	CA	E	1430	1/1	0.97	0.09	52,52,52,52	0
7	EDO	I	1430	4/4	0.97	0.13	42,44,47,50	0
6	CA	A	1430	1/1	0.97	0.07	51,51,51,51	0
6	CA	I	1429	1/1	0.97	0.04	61,61,61,61	0
6	CA	M	1430	1/1	0.97	0.08	55,55,55,55	0
5	ZN	A	1428	1/1	0.99	0.08	40,40,40,40	0
5	ZN	I	1427	1/1	0.99	0.06	51,51,51,51	0
5	ZN	E	1428	1/1	0.99	0.07	38,38,38,38	0
5	ZN	M	1428	1/1	0.99	0.08	42,42,42,42	0
5	ZN	I	1428	1/1	1.00	0.11	37,37,37,37	0
5	ZN	E	1429	1/1	1.00	0.11	31,31,31,31	0
5	ZN	A	1429	1/1	1.00	0.11	28,28,28,28	0
5	ZN	M	1429	1/1	1.00	0.12	37,37,37,37	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.