



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 16, 2018 – 11:58 PM EDT

PDB ID : 6DDC  
Title : Crystal structure of the single mutant (D52N) of NT5C2-537X in the basal state, Northeast Structural Genomics Consortium Target  
Authors : Forouhar, F.; Dieck, C.L.; Tzoneva, G.; Carpenter, Z.; Ambesi-Impiombato, A.; Sanchez-Martin, M.; Kirschner-Schwabe, R.; Lew, S.; Seetharaman, J.; Ferrando, A.A.; Tong, L.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2018-05-09  
Resolution : 2.91 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

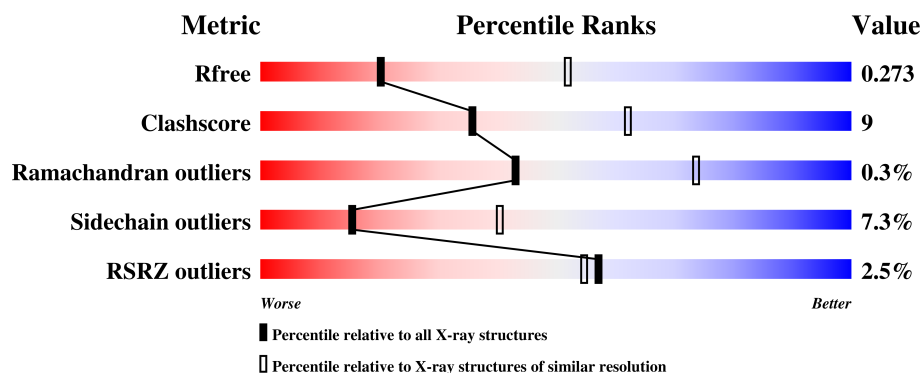
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	111664	1983 (2.94-2.90)
Clashscore	122126	2200 (2.94-2.90)
Ramachandran outliers	120053	2150 (2.94-2.90)
Sidechain outliers	120020	2152 (2.94-2.90)
RSRZ outliers	108989	1928 (2.94-2.90)

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. 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	554	<div> <div>2%</div> <div>63%</div> <div>21%</div> <div>•</div> <div>14%</div> </div>
1	B	554	<div> <div>3%</div> <div>66%</div> <div>18%</div> <div>•</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	602	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8038 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 Cytosolic purine 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	475	Total	C	N	O	S	0	0	0
			3873	2504	641	708	20			
1	B	474	Total	C	N	O	S	0	0	0
			3868	2501	643	705	19			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	GLY	-	expression tag	UNP P49902
A	-16	SER	-	expression tag	UNP P49902
A	-15	SER	-	expression tag	UNP P49902
A	-14	HIS	-	expression tag	UNP P49902
A	-13	HIS	-	expression tag	UNP P49902
A	-12	HIS	-	expression tag	UNP P49902
A	-11	HIS	-	expression tag	UNP P49902
A	-10	HIS	-	expression tag	UNP P49902
A	-9	HIS	-	expression tag	UNP P49902
A	-8	SER	-	expression tag	UNP P49902
A	-7	SER	-	expression tag	UNP P49902
A	-6	GLY	-	expression tag	UNP P49902
A	-5	LEU	-	expression tag	UNP P49902
A	-4	VAL	-	expression tag	UNP P49902
A	-3	PRO	-	expression tag	UNP P49902
A	-2	ARG	-	expression tag	UNP P49902
A	-1	GLY	-	expression tag	UNP P49902
A	0	SER	-	expression tag	UNP P49902
A	52	ASN	ASP	engineered mutation	UNP P49902
B	-17	GLY	-	expression tag	UNP P49902
B	-16	SER	-	expression tag	UNP P49902
B	-15	SER	-	expression tag	UNP P49902
B	-14	HIS	-	expression tag	UNP P49902
B	-13	HIS	-	expression tag	UNP P49902
B	-12	HIS	-	expression tag	UNP P49902

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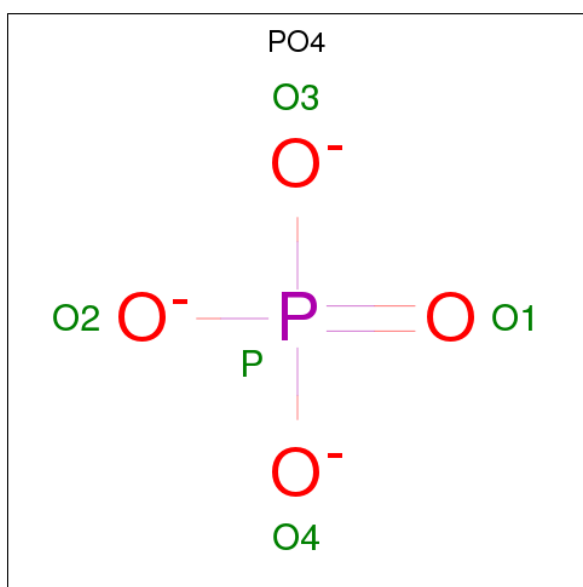
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P49902
B	-10	HIS	-	expression tag	UNP P49902
B	-9	HIS	-	expression tag	UNP P49902
B	-8	SER	-	expression tag	UNP P49902
B	-7	SER	-	expression tag	UNP P49902
B	-6	GLY	-	expression tag	UNP P49902
B	-5	LEU	-	expression tag	UNP P49902
B	-4	VAL	-	expression tag	UNP P49902
B	-3	PRO	-	expression tag	UNP P49902
B	-2	ARG	-	expression tag	UNP P49902
B	-1	GLY	-	expression tag	UNP P49902
B	0	SER	-	expression tag	UNP P49902
B	52	ASN	ASP	engineered mutation	UNP P49902

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		
4	B	123	Total	O	0	0
			123	123		



T493	HIS	P503	ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	VAL	L504	ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	ASP	A505	ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	ILE	T506	ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	ASN	R507	ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	GLU		ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	MET		ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	GLU		ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU
	SER		ASN	ARG	THR	SER	VAL	ASP	PHE	LYS	ASP	THR	ASP	TYR	LYS	ARG	HIS	GLN	LEU	THR	ARG	SER	ILE	SER	GLU	ILE	LYS	PRO	PRO	ASN	LEU



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.56Å 124.15Å 90.74Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	39.42 – 2.91 44.83 – 2.91	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.42-2.91) 96.4 (44.83-2.91)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.181 , 0.264 0.180 , 0.273	Depositor DCC
$R_{free}$ test set	3067 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.93% 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: PO4, 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	0.45	0/3973	0.59	0/5365
1	B	0.42	0/3968	0.57	0/5358
All	All	0.44	0/7941	0.58	0/10723

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	3873	0	3820	75	0
1	B	3868	0	3820	71	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	2	0
3	B	10	0	0	1	0
4	A	152	0	0	5	0
4	B	123	0	0	7	0
All	All	8038	0	7640	134	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 9.

All (134) 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:B:92:ASP:OD2	1:B:94:THR:OG1	2.01	0.78
1:A:39:ARG:NH1	1:A:456:ARG:O	2.18	0.75
1:A:292:LYS:NZ	1:A:348:TYR:OH	2.20	0.75
1:B:485:PRO:O	1:B:489:THR:OG1	2.05	0.74
1:A:247:LEU:HD23	1:A:286:ILE:HG23	1.69	0.73
1:A:52:ASN:HB3	1:A:56:THR:OG1	1.90	0.71
1:A:397:ILE:HG12	1:B:26:LYS:HB3	1.72	0.70
1:B:407:ASP:OD2	4:B:701:HOH:O	2.10	0.69
1:A:453:GLN:HB3	1:A:456:ARG:HH21	1.59	0.68
1:B:399:LEU:HD13	1:B:419:ILE:HG21	1.76	0.67
1:B:52:ASN:OD1	1:B:292:LYS:NZ	2.27	0.66
1:A:224:LYS:HD3	1:A:225:TYR:CZ	2.35	0.62
1:B:206:ASP:OD2	4:B:702:HOH:O	2.16	0.61
1:B:304:GLN:HG2	1:B:313:LYS:HD2	1.82	0.61
1:B:247:LEU:HD23	1:B:286:ILE:HG23	1.83	0.59
1:A:388:LEU:HD22	1:A:426:VAL:HG13	1.82	0.59
1:A:425:LYS:NZ	1:A:429:ASP:OD1	2.26	0.59
1:B:95:PHE:HA	1:B:436:MET:HB2	1.84	0.59
1:A:302:LEU:HD13	1:A:334:THR:HG21	1.83	0.58
1:A:362:LYS:O	1:A:362:LYS:HE3	2.04	0.57
1:A:72:LEU:HA	1:A:75:GLU:HG2	1.86	0.57
1:A:361:LYS:HD3	1:A:363:ARG:HB2	1.88	0.56
1:A:416:ILE:HD12	1:B:476:LEU:HD12	1.88	0.56
1:A:52:ASN:ND2	3:A:602:PO4:O1	2.39	0.56
1:A:504:LEU:HD12	1:B:466:ILE:HB	1.87	0.55
1:B:190:LEU:HD12	1:B:190:LEU:H	1.72	0.55
1:B:292:LYS:NZ	1:B:348:TYR:OH	2.33	0.55
1:A:453:GLN:HB3	1:A:456:ARG:NH2	2.22	0.54
1:B:42:ALA:HB3	1:B:45:LYS:HE3	1.90	0.54
1:B:391:GLU:OE2	1:B:422:ARG:NH2	2.42	0.53
1:A:344:LYS:HG2	1:A:364:GLN:HG2	1.90	0.53
1:B:398:PHE:O	1:B:402:LEU:HG	2.10	0.52
1:A:476:LEU:HD12	1:B:416:ILE:HD12	1.91	0.52
1:B:423:ILE:O	1:B:427:THR:HG23	2.09	0.52
1:B:64:GLU:N	1:B:64:GLU:OE1	2.41	0.52
1:B:232:LEU:HB3	1:B:233:PRO:HD3	1.90	0.52
1:A:74:VAL:O	1:A:78:VAL:HG23	2.10	0.52
1:B:372:ILE:O	1:B:375:LEU:HB2	2.10	0.51
1:A:34:ARG:HH12	1:B:489:THR:HB	1.76	0.51
1:A:442:ARG:NH2	1:A:445:SER:O	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LYS:HB2	4:B:746:HOH:O	2.11	0.50
1:A:68:LEU:HD22	1:A:225:TYR:CZ	2.47	0.50
1:A:26:LYS:HG2	1:A:27:TYR:N	2.27	0.50
1:B:424:LYS:HB3	1:B:424:LYS:NZ	2.27	0.49
1:A:405:HIS:ND1	4:A:705:HOH:O	2.35	0.49
1:A:95:PHE:HA	1:A:436:MET:HB2	1.92	0.49
1:B:204:ALA:O	1:B:208:VAL:HG23	2.12	0.49
1:B:74:VAL:HG13	1:B:86:LEU:HB3	1.93	0.49
1:B:102:PHE:HD1	1:B:109:LEU:HD23	1.77	0.49
1:A:119:LEU:HD13	1:A:443:SER:HB3	1.95	0.49
1:A:416:ILE:O	1:A:420:GLN:HB2	2.13	0.49
1:A:54:ASP:N	3:A:602:PO4:O3	2.40	0.49
1:A:149:ARG:HG2	1:A:150:PHE:CZ	2.47	0.49
1:A:34:ARG:HH22	1:B:489:THR:CB	2.26	0.49
1:A:445:SER:HA	1:B:481:HIS:NE2	2.27	0.49
1:A:231:LYS:HG3	4:A:813:HOH:O	2.13	0.48
1:A:361:LYS:HE2	1:A:363:ARG:NH2	2.29	0.48
1:B:145:ASP:OD1	1:B:145:ASP:N	2.46	0.48
1:A:195:ARG:NH2	1:A:199:GLN:OE1	2.47	0.48
1:B:361:LYS:HE2	1:B:363:ARG:HB2	1.95	0.48
1:A:48:CYS:HA	1:A:244:LYS:O	2.14	0.47
1:B:306:ASP:HB3	1:B:309:THR:HG23	1.95	0.47
1:B:118:LEU:HD11	1:B:142:ILE:HG23	1.96	0.47
1:A:169:VAL:O	1:A:173:THR:HB	2.13	0.47
1:B:303:ARG:HB2	1:B:328:SER:HB3	1.96	0.47
1:B:362:LYS:HE3	1:B:362:LYS:HB2	1.74	0.47
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.96	0.47
1:A:40:SER:HA	1:A:477:PHE:O	2.14	0.47
1:B:291:ARG:HH21	1:B:291:ARG:HB3	1.80	0.47
1:A:391:GLU:OE2	1:A:422:ARG:NH2	2.37	0.46
1:B:85:GLU:OE2	1:B:177:ARG:NH2	2.39	0.46
1:A:368:THR:N	1:A:459:ASP:OD2	2.47	0.46
1:B:357:ILE:HG23	1:B:358:LEU:HD22	1.97	0.46
1:A:464:SER:HB3	1:A:466:ILE:HG22	1.98	0.46
1:A:113:ASP:HB3	1:A:119:LEU:HD21	1.97	0.45
1:A:26:LYS:HB2	1:B:397:ILE:HG13	1.97	0.45
1:A:290:ALA:O	1:A:291:ARG:HB2	2.16	0.45
1:B:347:LEU:HD11	1:B:369:PHE:HB2	1.96	0.45
1:A:287:LEU:HA	1:A:327:TYR:O	2.16	0.45
1:A:424:LYS:HE3	1:A:424:LYS:HB3	1.69	0.45
1:B:165:LEU:HD13	1:B:201:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:HIS:HB3	1:B:386:SER:HB3	1.99	0.45
1:B:176:PRO:O	4:B:703:HOH:O	2.21	0.45
1:A:453:GLN:HG2	4:A:771:HOH:O	2.16	0.45
1:B:214:LEU:O	1:B:218:THR:OG1	2.35	0.45
1:B:399:LEU:HD12	1:B:399:LEU:HA	1.73	0.44
1:B:52:ASN:HB3	1:B:56:THR:OG1	2.17	0.44
1:A:27:TYR:CE2	1:B:404:LYS:HA	2.52	0.44
1:B:152:ILE:HD12	1:B:152:ILE:H	1.83	0.44
1:B:314:ILE:HG13	1:B:314:ILE:H	1.61	0.44
1:B:393:GLN:O	1:B:397:ILE:HD12	2.17	0.44
1:B:52:ASN:ND2	3:B:602:PO4:O1	2.49	0.44
1:A:207:TRP:O	1:A:212:GLY:N	2.50	0.44
1:A:395:LEU:HD22	1:A:419:ILE:HG13	2.00	0.44
1:A:74:VAL:HG13	1:A:86:LEU:HB3	2.00	0.44
1:A:222:LEU:HD13	1:A:262:TYR:HB2	2.00	0.43
1:A:445:SER:HA	1:B:481:HIS:CD2	2.52	0.43
1:A:368:THR:OG1	1:A:458:ALA:HA	2.18	0.43
1:B:403:TYR:HA	1:B:406:LEU:HD22	2.00	0.43
1:B:47:LYS:HD3	4:B:753:HOH:O	2.19	0.43
1:A:372:ILE:O	1:A:375:LEU:HB2	2.19	0.43
1:B:370:LEU:HD23	1:B:372:ILE:HD11	2.01	0.43
1:B:46:ILE:HA	1:B:46:ILE:HD13	1.90	0.43
1:A:349:ILE:HG21	1:A:465:PHE:CB	2.49	0.42
1:A:85:GLU:O	1:A:88:SER:HB2	2.19	0.42
1:A:361:LYS:HE2	1:A:363:ARG:CZ	2.50	0.42
1:B:304:GLN:HE21	1:B:313:LYS:HE3	1.84	0.42
1:A:219:VAL:HG11	1:A:258:LYS:HD3	2.02	0.42
1:A:75:GLU:HG3	1:A:76:ARG:N	2.34	0.42
1:B:228:LYS:HE2	1:B:262:TYR:O	2.20	0.42
1:B:311:LYS:HA	1:B:311:LYS:HD2	1.95	0.42
1:B:55:TYR:CD1	1:B:156:LEU:HD13	2.55	0.42
1:B:302:LEU:HD13	1:B:334:THR:HG21	2.02	0.42
1:B:450:PHE:HB2	4:B:732:HOH:O	2.19	0.42
1:A:78:VAL:HG21	1:A:87:LEU:HD22	2.02	0.42
1:A:54:ASP:OD1	1:A:251:SER:OG	2.38	0.42
1:A:288:VAL:O	1:A:328:SER:HA	2.20	0.41
1:A:287:LEU:HD21	1:A:329:GLY:O	2.20	0.41
1:B:419:ILE:O	1:B:423:ILE:HG13	2.20	0.41
1:A:375:LEU:HB3	1:A:463:ALA:HB2	2.02	0.41
1:A:392:LEU:HD21	1:A:427:THR:HG23	2.00	0.41
1:B:71:GLU:HG2	4:B:795:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:HZ	1:A:89:PHE:HB3	1.85	0.41
1:B:291:ARG:HB3	1:B:291:ARG:NH2	2.35	0.41
1:B:466:ILE:HD12	1:B:466:ILE:HA	1.82	0.41
1:A:57:LEU:HD23	1:A:465:PHE:CZ	2.56	0.41
1:B:361:LYS:HG2	1:B:363:ARG:H	1.86	0.41
1:A:126:ASN:OD1	4:A:702:HOH:O	2.22	0.41
1:A:101:VAL:HG13	1:A:150:PHE:HB3	2.02	0.41
1:A:406:LEU:HB3	1:B:472:PRO:HG3	2.03	0.41
1:B:97:THR:O	1:B:100:LEU:HG	2.20	0.40
1:B:422:ARG:HD2	1:B:422:ARG:HA	1.89	0.40
1:A:421:ARG:HG2	4:A:742:HOH:O	2.21	0.40
1:A:342:LYS:HB3	1:A:364:GLN:OE1	2.21	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	471/554 (85%)	446 (95%)	24 (5%)	1 (0%)	49	80
1	B	470/554 (85%)	448 (95%)	20 (4%)	2 (0%)	36	68
All	All	941/1108 (85%)	894 (95%)	44 (5%)	3 (0%)	43	74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	270	PRO
1	B	355	GLY
1	A	171	PHE

### 5.3.2 Protein sidechains ⓘ

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	424/496 (86%)	391 (92%)	33 (8%)	14	36
1	B	423/496 (85%)	394 (93%)	29 (7%)	17	43
All	All	847/992 (85%)	785 (93%)	62 (7%)	15	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	MET
1	A	44	GLU
1	A	112	VAL
1	A	113	ASP
1	A	147	THR
1	A	152	ILE
1	A	159	LEU
1	A	161	GLU
1	A	173	THR
1	A	177	ARG
1	A	179	THR
1	A	195	ARG
1	A	211	LYS
1	A	228	LYS
1	A	238	ARG
1	A	247	LEU
1	A	308	LYS
1	A	323	HIS
1	A	356	ASP
1	A	362	LYS
1	A	363	ARG
1	A	369	PHE
1	A	375	LEU
1	A	377	GLN
1	A	384	ASP
1	A	387	SER
1	A	425	LYS

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Mol	Chain	Res	Type
1	A	431	ASP
1	A	452	SER
1	A	455	MET
1	A	476	LEU
1	A	478	ARG
1	A	490	VAL
1	B	26	LYS
1	B	44	GLU
1	B	53	MET
1	B	80	ILE
1	B	88	SER
1	B	145	ASP
1	B	147	THR
1	B	165	LEU
1	B	170	ASP
1	B	192	MET
1	B	215	LYS
1	B	218	THR
1	B	238	ARG
1	B	291	ARG
1	B	309	THR
1	B	311	LYS
1	B	321	LEU
1	B	323	HIS
1	B	356	ASP
1	B	362	LYS
1	B	375	LEU
1	B	377	GLN
1	B	390	GLU
1	B	397	ILE
1	B	406	LEU
1	B	409	SER
1	B	446	ARG
1	B	476	LEU
1	B	490	VAL

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains [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 6 ligands modelled in this entry, 2 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	$\# Z  > 2$
3	PO4	A	602	2	4,4,4	0.95	0	6,6,6	0.45	0
3	PO4	A	603	-	4,4,4	0.85	0	6,6,6	0.65	0
3	PO4	B	602	2	4,4,4	0.72	0	6,6,6	0.80	0
3	PO4	B	603	-	4,4,4	0.85	0	6,6,6	0.55	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
3	PO4	A	602	2	-	0/0/0/0	0/0/0/0
3	PO4	A	603	-	-	0/0/0/0	0/0/0/0
3	PO4	B	602	2	-	0/0/0/0	0/0/0/0
3	PO4	B	603	-	-	0/0/0/0	0/0/0/0

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	PO4	2	0
3	B	602	PO4	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

### 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	475/554 (85%)	-0.14	10 (2%) 63 61	15, 35, 77, 141	0
1	B	474/554 (85%)	-0.13	14 (2%) 50 45	12, 35, 87, 155	0
All	All	949/1108 (85%)	-0.14	24 (2%) 57 55	12, 35, 81, 155	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	THR	5.6
1	B	360	SER	5.3
1	B	505	ALA	4.1
1	B	320	PRO	3.7
1	B	316	THR	3.7
1	A	415	ASP	3.6
1	A	417	SER	3.4
1	B	314	ILE	3.4
1	A	505	ALA	3.4
1	A	320	PRO	2.6
1	B	417	SER	2.5
1	B	321	LEU	2.5
1	B	318	THR	2.5
1	A	189	ASP	2.5
1	B	133	THR	2.4
1	B	189	ASP	2.3
1	A	360	SER	2.3
1	B	309	THR	2.2
1	A	361	LYS	2.1
1	A	420	GLN	2.1
1	B	398	PHE	2.1
1	A	416	ILE	2.0
1	A	418	SER	2.0
1	B	317	TYR	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. 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
2	MG	A	601	1/1	0.87	0.23	34,34,34,34	0
2	MG	B	601	1/1	0.96	0.22	28,28,28,28	0
3	PO4	B	602	5/5	0.97	0.17	39,39,52,60	0
3	PO4	A	603	5/5	0.98	0.13	10,30,41,43	0
3	PO4	A	602	5/5	0.98	0.16	32,36,42,49	0
3	PO4	B	603	5/5	0.99	0.10	10,16,28,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.