



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:35 PM BST

PDB ID : 6DDB  
Title : Crystal structure of the double mutant (D52N/R367Q) 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 : 2.80 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](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	:	2.13.1
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)	:	2.13.1

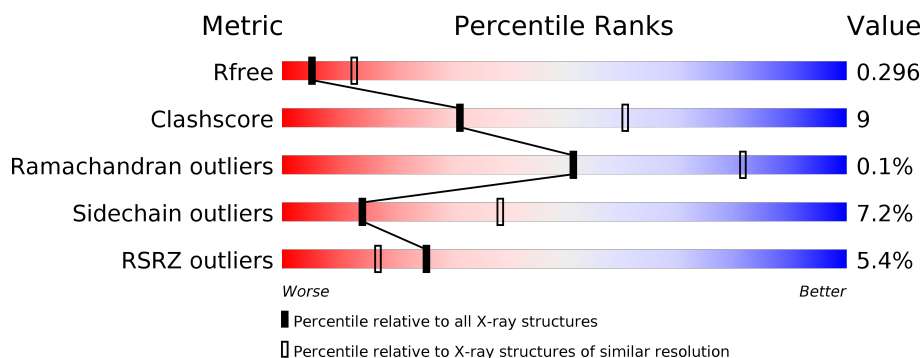
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	554	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>19%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	554	<div> <div>5%</div> <div> <div></div> <div>64%</div> <div>18%</div> <div>•</div> <div>16%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7819 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	467	Total	C	N	O	S	0	0	0
			3812	2466	630	697	19			
1	B	467	Total	C	N	O	S	0	0	0
			3812	2466	630	697	19			

There are 40 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
A	367	GLN	ARG	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

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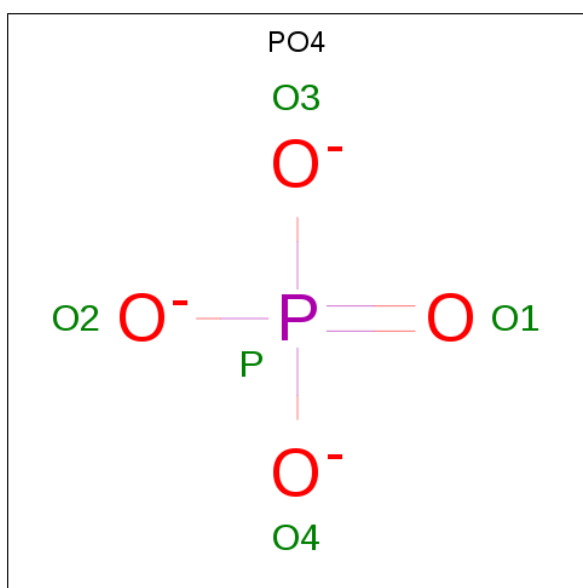
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-12	HIS	-	expression tag	UNP P49902
B	-11	HIS	-	expression tag	UNP P49902
B	-10	HIS	-	expression tag	UNP P49902
B	-9	HIS	-	expression tag	UNP P49902
B	-8	SER	-	expression tag	UNP P49902
B	-7	SER	-	expression 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
B	367	GLN	ARG	engineered mutation	UNP P49902

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

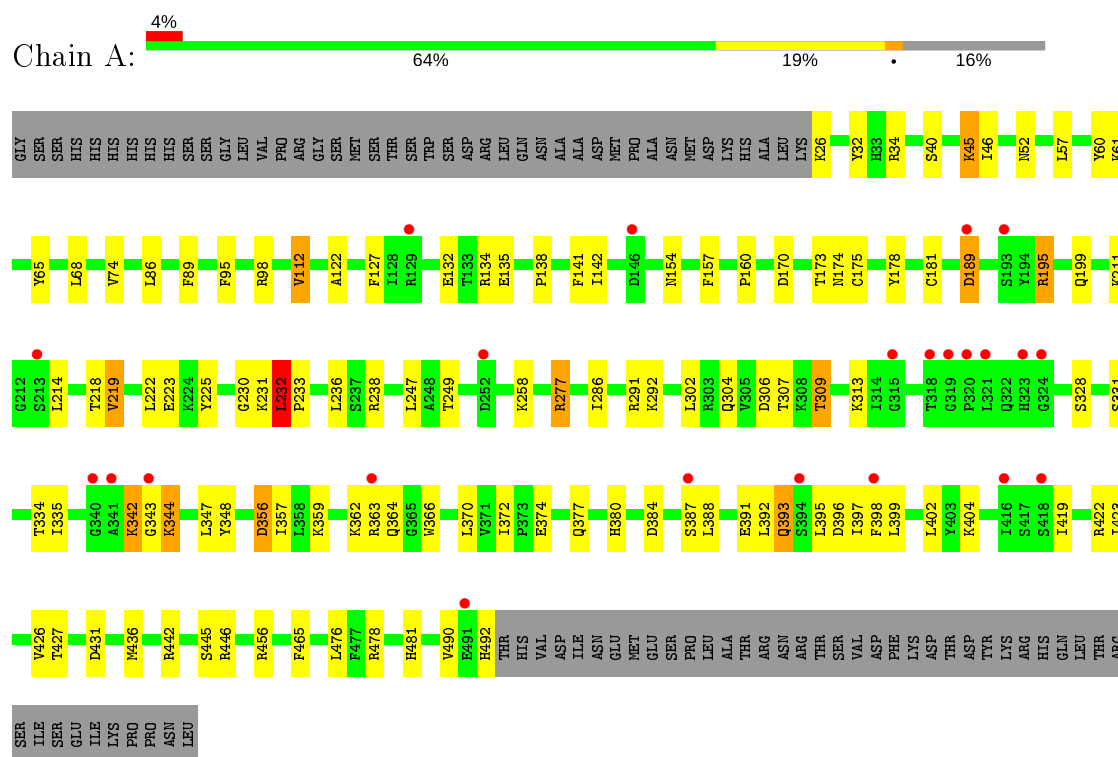
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	B	84	Total	O	0	0
			84	84		

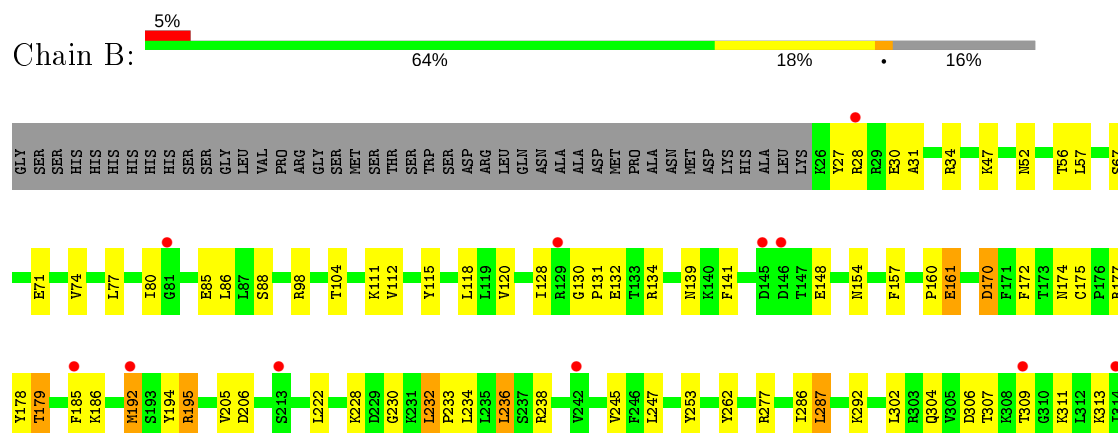
### 3 Residue-property plots [i](#)

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: Cytosolic purine 5'-nucleotidase



- Molecule 1: Cytosolic purine 5'-nucleotidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.13Å 123.12Å 90.31Å 90.00° 115.50° 90.00°	Depositor
Resolution (Å)	49.12 – 2.80 49.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.12-2.80) 98.7 (49.13-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.53 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, $R_{free}$	0.217 , 0.291 0.217 , 0.296	Depositor DCC
$R_{free}$ test set	3453 reflections (10.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.0	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 65.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7819	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8731e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, MN

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	0.43	0/3912	0.59	1/5285 (0.0%)
1	B	0.42	0/3912	0.58	0/5285
All	All	0.43	0/7824	0.59	1/10570 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	232	LEU	CA-CB-CG	6.52	130.30	115.30

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	3812	0	3753	72	0
1	B	3812	0	3753	77	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
4	A	89	0	0	6	0
4	B	84	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7819	0	7506	136	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 (136) 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:302:LEU:HD22	1:B:334:THR:HG21	1.67	0.75
1:B:309:THR:HG23	1:B:311:LYS:H	1.54	0.72
1:A:195:ARG:NH2	1:A:199:GLN:OE1	2.23	0.71
1:A:74:VAL:HG13	1:A:86:LEU:HB3	1.74	0.69
1:A:195:ARG:HH21	1:A:199:GLN:HB2	1.58	0.67
1:A:395:LEU:HD22	1:A:419:ILE:HG23	1.79	0.65
1:B:85:GLU:OE2	1:B:177:ARG:NH2	2.30	0.65
1:A:219:VAL:HG21	1:A:258:LYS:HD3	1.78	0.64
1:B:395:LEU:HB3	1:B:419:ILE:HD11	1.79	0.64
1:B:247:LEU:HD23	1:B:286:ILE:HG23	1.80	0.63
1:A:189:ASP:N	1:A:189:ASP:OD1	2.18	0.62
1:B:175:CYS:HB3	1:B:178:TYR:HD2	1.64	0.62
1:B:234:LEU:HD23	1:B:469:LEU:HD11	1.80	0.62
1:A:98:ARG:NE	1:A:374:GLU:OE2	2.26	0.62
1:B:304:GLN:HB2	1:B:316:THR:HG23	1.80	0.62
1:B:393:GLN:O	1:B:397:ILE:HG12	1.99	0.61
1:A:391:GLU:OE2	1:A:422:ARG:NH2	2.34	0.60
1:B:74:VAL:HG13	1:B:86:LEU:HB3	1.83	0.60
1:A:219:VAL:HA	1:A:222:LEU:HD21	1.83	0.60
1:B:228:LYS:NZ	4:B:704:HOH:O	2.34	0.59
1:A:57:LEU:HD23	1:A:465:PHE:CZ	2.38	0.59
1:A:356:ASP:HB3	1:A:359:LYS:HE3	1.85	0.58
1:A:34:ARG:NH2	3:A:603:PO4:O1	2.32	0.58
1:A:363:ARG:NH2	1:B:134:ARG:O	2.27	0.58
1:A:175:CYS:HB3	1:A:178:TYR:HD2	1.68	0.57
1:A:32:TYR:HH	1:A:380:HIS:CE1	2.22	0.57
1:A:247:LEU:HD11	1:A:249:THR:HB	1.85	0.57
1:A:304:GLN:HG2	1:A:313:LYS:HD2	1.86	0.57
1:A:492:HIS:HB3	1:B:386:SER:HB2	1.86	0.57
1:B:391:GLU:OE2	1:B:422:ARG:NH2	2.37	0.57
1:B:112:VAL:HG12	1:B:118:LEU:HD12	1.87	0.57
1:B:306:ASP:OD2	1:B:309:THR:HG22	2.04	0.56
1:A:395:LEU:HD13	1:A:423:ILE:HG13	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HD2	4:A:708:HOH:O	2.04	0.55
1:A:112:VAL:HG11	1:A:142:ILE:HD11	1.89	0.55
1:B:356:ASP:HB3	1:B:359:LYS:HG3	1.88	0.55
1:A:423:ILE:O	1:A:427:THR:HG23	2.08	0.54
1:A:61:LYS:NZ	1:A:223:GLU:O	2.41	0.54
1:A:393:GLN:O	1:A:397:ILE:HG12	2.07	0.54
1:B:185:PHE:HB2	1:B:192:MET:HE3	1.90	0.54
1:B:364:GLN:OE1	1:B:364:GLN:N	2.38	0.54
1:B:448:THR:HB	4:B:738:HOH:O	2.07	0.53
1:B:321:LEU:HD21	1:B:339:LEU:HD23	1.91	0.53
1:A:214:LEU:O	1:A:218:THR:OG1	2.21	0.52
1:A:199:GLN:HG2	4:A:789:HOH:O	2.09	0.52
1:A:141:PHE:CD1	1:B:359:LYS:HE2	2.45	0.52
1:A:157:PHE:O	1:A:160:PRO:HD2	2.10	0.51
1:B:52:ASN:HD22	1:B:292:LYS:NZ	2.09	0.51
1:A:442:ARG:NH2	1:A:445:SER:O	2.44	0.51
1:A:52:ASN:HD22	1:A:292:LYS:NZ	2.09	0.51
1:A:306:ASP:OD2	1:A:309:THR:HG22	2.12	0.50
1:B:232:LEU:HB3	1:B:233:PRO:HD3	1.94	0.50
1:A:342:LYS:HG3	1:A:343:GLY:N	2.27	0.50
1:B:104:THR:HB	1:B:195:ARG:HD2	1.94	0.50
1:A:134:ARG:O	1:B:363:ARG:NH2	2.44	0.50
1:B:161:GLU:HB2	1:B:205:VAL:HG21	1.94	0.49
1:B:111:LYS:HB3	1:B:120:VAL:HB	1.94	0.49
1:A:174:ASN:ND2	4:A:707:HOH:O	2.42	0.49
1:B:409:SER:OG	1:B:410:SER:N	2.45	0.49
1:B:57:LEU:HD23	1:B:465:PHE:CZ	2.47	0.49
1:A:46:ILE:HD12	1:A:347:LEU:HB2	1.95	0.49
1:A:302:LEU:HD22	1:A:334:THR:HG21	1.94	0.49
1:A:348:TYR:HB2	1:A:366:TRP:HE3	1.78	0.48
1:B:157:PHE:O	1:B:160:PRO:HD2	2.13	0.48
1:A:231:LYS:HE2	4:A:728:HOH:O	2.14	0.48
1:A:478:ARG:NE	4:A:710:HOH:O	2.47	0.48
1:B:232:LEU:CD1	1:B:236:LEU:HD12	2.44	0.48
1:B:287:LEU:HD11	1:B:329:GLY:O	2.13	0.48
1:B:228:LYS:HE3	1:B:262:TYR:O	2.14	0.47
1:B:313:LYS:NZ	4:B:709:HOH:O	2.47	0.47
1:B:222:LEU:HD13	1:B:262:TYR:HB2	1.96	0.47
1:B:179:THR:OG1	1:B:186:LYS:HB2	2.15	0.47
1:A:344:LYS:HE2	1:A:344:LYS:H	1.79	0.47
1:B:316:THR:HG22	1:B:318:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:HD3	1:B:363:ARG:NH1	2.30	0.47
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.96	0.46
1:A:138:PRO:HD3	1:B:363:ARG:HH12	1.80	0.46
1:B:128:ILE:HG23	1:B:132:GLU:HG3	1.98	0.46
1:A:374:GLU:O	1:A:377:GLN:HG2	2.15	0.45
1:B:232:LEU:HD13	1:B:465:PHE:HZ	1.81	0.45
1:A:52:ASN:ND2	1:A:292:LYS:HZ1	2.14	0.45
1:A:98:ARG:HG2	1:A:154:ASN:O	2.17	0.45
1:A:388:LEU:HD22	1:A:426:VAL:HG13	1.98	0.45
1:A:68:LEU:HD22	1:A:225:TYR:CZ	2.51	0.45
1:B:185:PHE:CE2	1:B:194:TYR:HE1	2.35	0.45
1:B:52:ASN:ND2	1:B:292:LYS:NZ	2.65	0.45
1:A:26:LYS:NZ	1:B:396:ASP:OD1	2.45	0.45
1:A:52:ASN:HD22	1:A:292:LYS:HZ1	1.64	0.45
1:A:86:LEU:HG	1:A:89:PHE:CE2	2.52	0.45
1:A:398:PHE:CZ	1:A:402:LEU:HD21	2.52	0.45
1:B:74:VAL:HG11	1:B:86:LEU:O	2.17	0.44
1:B:421:ARG:HD3	1:B:421:ARG:HA	1.60	0.44
1:B:185:PHE:CE2	1:B:194:TYR:CE1	3.05	0.44
1:A:392:LEU:HD11	1:A:427:THR:HG22	1.99	0.44
1:B:342:LYS:HZ3	1:B:364:GLN:HA	1.82	0.44
1:B:104:THR:CB	1:B:195:ARG:HD2	2.47	0.44
1:A:359:LYS:HD2	1:B:141:PHE:CD1	2.53	0.43
1:B:348:TYR:HB2	1:B:366:TRP:HE3	1.82	0.43
1:A:492:HIS:ND1	1:B:382:TRP:O	2.38	0.43
1:B:28:ARG:HD3	1:B:34:ARG:NH1	2.34	0.43
1:A:370:LEU:HD23	1:A:372:ILE:HD11	2.00	0.43
1:A:32:TYR:OH	1:A:380:HIS:ND1	2.46	0.43
1:A:456:ARG:HB2	1:B:115:TYR:CE1	2.53	0.43
1:A:95:PHE:HA	1:A:436:MET:HB2	1.99	0.43
1:B:170:ASP:O	1:B:174:ASN:ND2	2.46	0.43
1:B:232:LEU:HD12	1:B:236:LEU:HD12	2.00	0.42
1:B:130:GLY:HA3	1:B:131:PRO:HD3	1.74	0.42
1:B:292:LYS:NZ	3:B:602:PO4:O2	2.45	0.42
1:B:98:ARG:HG2	1:B:154:ASN:O	2.18	0.42
1:A:141:PHE:CD2	1:B:359:LYS:HB3	2.55	0.42
1:A:45:LYS:HB3	1:A:45:LYS:NZ	2.35	0.42
1:B:236:LEU:HD23	1:B:245:VAL:HG11	2.01	0.42
1:A:404:LYS:HA	1:B:27:TYR:CE2	2.55	0.42
1:B:77:LEU:O	1:B:80:ILE:HG12	2.19	0.42
1:B:483:LEU:HB3	1:B:487:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLY:O	1:A:233:PRO:HD2	2.20	0.42
1:B:172:PHE:HB2	1:B:185:PHE:CE2	2.55	0.42
1:A:399:LEU:HA	1:A:399:LEU:HD12	1.91	0.41
1:B:192:MET:HE3	1:B:192:MET:HB3	1.93	0.41
1:A:211:LYS:HA	1:A:211:LYS:HD2	1.87	0.41
1:A:362:LYS:O	1:B:139:ASN:ND2	2.53	0.41
1:B:342:LYS:NZ	1:B:364:GLN:HA	2.35	0.41
1:B:52:ASN:HB3	1:B:56:THR:OG1	2.21	0.41
1:B:253:TYR:CD1	1:B:326:VAL:HG11	2.55	0.41
1:B:185:PHE:HD2	1:B:192:MET:SD	2.44	0.41
1:B:230:GLY:O	1:B:233:PRO:HD2	2.21	0.41
1:B:30:GLU:HG2	1:B:31:ALA:N	2.36	0.41
1:B:47:LYS:HB2	1:B:345:ASP:HB3	2.03	0.41
1:A:122:ALA:HB2	1:A:127:PHE:CE2	2.56	0.40
1:A:247:LEU:HD23	1:A:286:ILE:HG23	2.02	0.40
1:B:431:ASP:O	1:B:438:GLY:HA2	2.21	0.40
1:A:344:LYS:H	1:A:344:LYS:CD	2.34	0.40
1:A:86:LEU:HG	1:A:89:PHE:HE2	1.85	0.40
1:B:67:SER:O	1:B:71:GLU:HG3	2.22	0.40
1:A:384:ASP:HB3	4:A:713:HOH:O	2.20	0.40
1:A:60:TYR:HB3	1:A:65:TYR:CG	2.57	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	465/554 (84%)	441 (95%)	24 (5%)	0	100	100
1	B	465/554 (84%)	437 (94%)	27 (6%)	1 (0%)	47	78
All	All	930/1108 (84%)	878 (94%)	51 (6%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	444	GLY

### 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	417/496 (84%)	383 (92%)	34 (8%)	11	33
1	B	417/496 (84%)	391 (94%)	26 (6%)	18	47
All	All	834/992 (84%)	774 (93%)	60 (7%)	14	38

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	SER
1	A	45	LYS
1	A	112	VAL
1	A	132	GLU
1	A	135	GLU
1	A	170	ASP
1	A	173	THR
1	A	181	CYS
1	A	189	ASP
1	A	195	ARG
1	A	219	VAL
1	A	232	LEU
1	A	236	LEU
1	A	238	ARG
1	A	277	ARG
1	A	291	ARG
1	A	307	THR
1	A	309	THR
1	A	328	SER
1	A	331	SER
1	A	335	ILE
1	A	342	LYS

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Mol	Chain	Res	Type
1	A	344	LYS
1	A	356	ASP
1	A	357	ILE
1	A	364	GLN
1	A	387	SER
1	A	393	GLN
1	A	396	ASP
1	A	431	ASP
1	A	446	ARG
1	A	476	LEU
1	A	481	HIS
1	A	490	VAL
1	B	88	SER
1	B	148	GLU
1	B	161	GLU
1	B	170	ASP
1	B	179	THR
1	B	192	MET
1	B	195	ARG
1	B	206	ASP
1	B	232	LEU
1	B	236	LEU
1	B	238	ARG
1	B	277	ARG
1	B	287	LEU
1	B	307	THR
1	B	356	ASP
1	B	359	LYS
1	B	380	HIS
1	B	386	SER
1	B	390	GLU
1	B	396	ASP
1	B	419	ILE
1	B	446	ARG
1	B	455	MET
1	B	476	LEU
1	B	481	HIS
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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

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	B	603	-	4,4,4	0.80	0	6,6,6	0.55	0
3	PO4	A	603	-	4,4,4	0.95	0	6,6,6	0.46	0
3	PO4	B	602	2	4,4,4	0.90	0	6,6,6	0.53	0
3	PO4	A	602	2	4,4,4	1.00	0	6,6,6	0.52	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	PO4	1	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	467/554 (84%)	0.29	23 (4%)	29	20	17, 36, 76, 144	3 (0%)
1	B	467/554 (84%)	0.33	27 (5%)	23	15	17, 40, 81, 173	3 (0%)
All	All	934/1108 (84%)	0.31	50 (5%)	25	17	17, 38, 80, 173	6 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	GLY	11.5
1	B	324	GLY	8.4
1	A	324	GLY	8.3
1	B	323	HIS	7.7
1	A	323	HIS	7.4
1	B	316	THR	7.4
1	B	321	LEU	6.6
1	A	319	GLY	6.2
1	A	320	PRO	5.9
1	B	320	PRO	5.2
1	A	340	GLY	4.9
1	A	321	LEU	4.6
1	B	314	ILE	4.3
1	B	315	GLY	4.2
1	A	394	SER	4.1
1	A	491	GLU	3.5
1	B	242	VAL	3.3
1	B	491	GLU	3.3
1	A	193	SER	3.2
1	B	327	TYR	3.2
1	A	416	ILE	2.9
1	B	325	ILE	2.8
1	A	213	SER	2.8
1	A	343	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	185	PHE	2.6
1	B	129	ARG	2.6
1	A	341	ALA	2.6
1	A	129	ARG	2.5
1	A	398	PHE	2.5
1	B	81	GLY	2.5
1	B	317	TYR	2.5
1	B	192	MET	2.5
1	B	309	THR	2.4
1	B	481	HIS	2.4
1	A	252	ASP	2.4
1	A	318	THR	2.3
1	B	340	GLY	2.3
1	A	363	ARG	2.3
1	B	213	SER	2.3
1	B	326	VAL	2.2
1	A	315	GLY	2.2
1	B	145	ASP	2.2
1	A	146	ASP	2.2
1	A	189	ASP	2.2
1	A	418	SER	2.2
1	B	146	ASP	2.1
1	B	28	ARG	2.1
1	A	387	SER	2.0
1	B	417	SER	2.0
1	B	411	ASN	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, 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
3	PO4	B	603	5/5	0.97	0.21	48,54,60,64	0
3	PO4	A	603	5/5	0.97	0.21	29,44,46,48	0
2	MN	B	601	1/1	0.98	0.19	37,37,37,37	0
3	PO4	A	602	5/5	0.98	0.15	25,31,33,33	0
3	PO4	B	602	5/5	0.98	0.14	22,30,33,34	0
2	MN	A	601	1/1	0.98	0.10	31,31,31,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.