



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:41 PM UTC

PDB ID : 6DDC / pdb_00006ddc
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

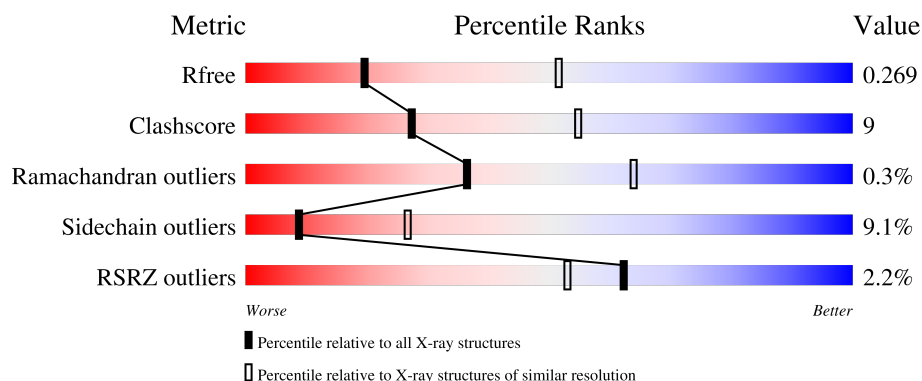
1 Overall quality at a glance

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}	180053	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	554	% 62% 22% • 14%
1	B	554	2% 64% 18% • 14%

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

Continued on next page...

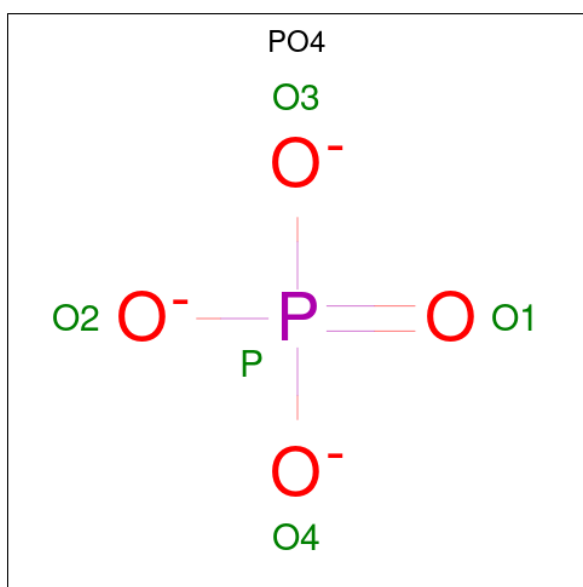
Continued from previous page...

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 (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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		

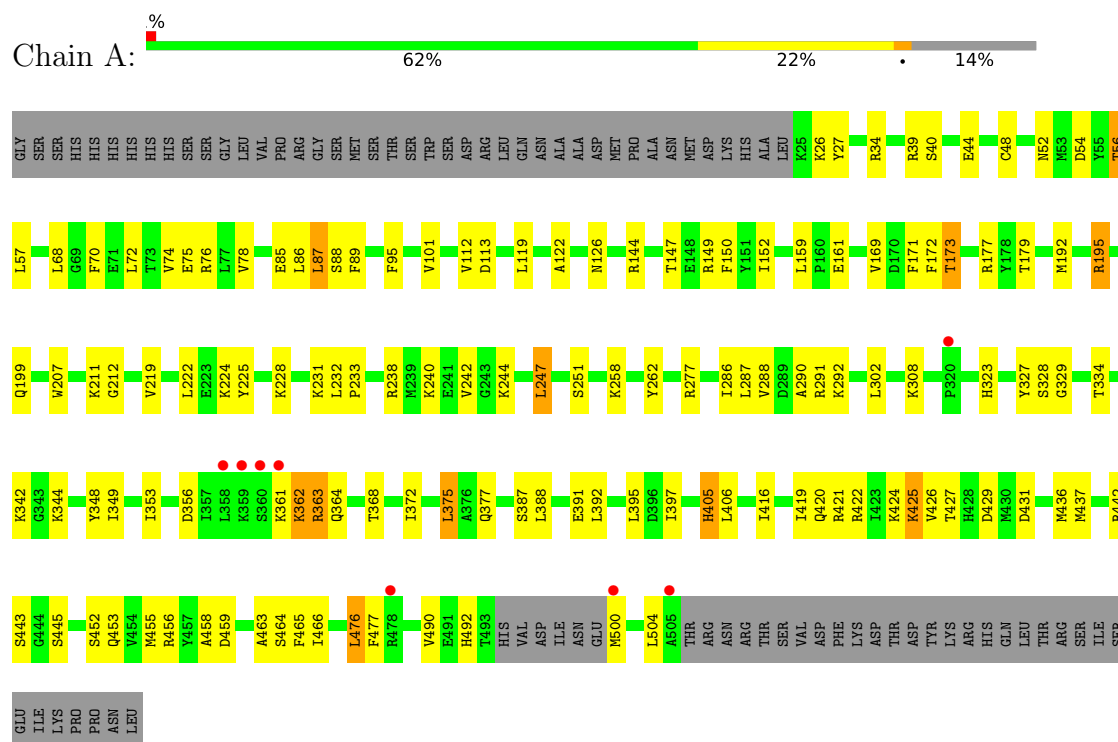
- Molecule 4 is water.

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

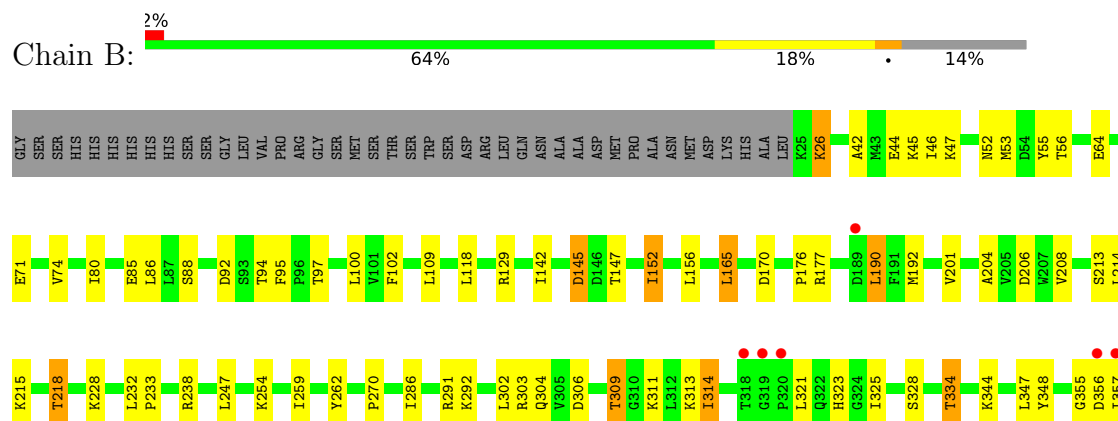
3 Residue-property plots

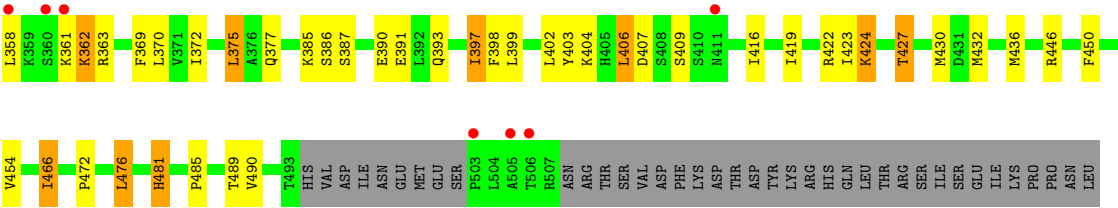
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, α , β , γ	144.56Å 124.15Å 90.74Å 90.00° 116.25° 90.00°	Depositor
Resolution (Å)	39.42 – 2.91 39.42 – 2.91	Depositor EDS
% Data completeness (in resolution range)	96.3 (39.42-2.91) 96.3 (39.42-2.91)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.90Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.181 , 0.264 0.178 , 0.269	Depositor DCC
R_{free} test set	3067 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8038	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.36	0/3973	0.56	0/5365
1	B	0.34	0/3968	0.54	0/5358
All	All	0.35	0/7941	0.55	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	78	0
1	B	3868	0	3820	74	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	8	0
All	All	8038	0	7640	140	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 (140) 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:292:LYS:NZ	1:B:348:TYR:OH	2.33	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:H	1:B:190:LEU:HD12	1.72	0.55
1:A:122:ALA:HB3	1:A:437:MET:HE1	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:NH2	1:A:445:SER:O	2.39	0.50
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:95:PHE:HA	1:A:436:MET:HB2	1.92	0.49
1:A:405:HIS:ND1	4:A:705:HOH:O	2.35	0.49
1:B:74:VAL:HG13	1:B:86:LEU:HB3	1.93	0.49
1:B:204:ALA:O	1:B:208:VAL:HG23	2.12	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:54:ASP:N	3:A:602:PO4:O3	2.40	0.49
1:A:416:ILE:O	1:A:420:GLN:HB2	2.13	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:40:SER:HA	1:A:477:PHE:O	2.14	0.47
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.96	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:172:PHE:CE2	1:A:192:MET:HE1	2.51	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:B:430:MET:HE3	4:B:813:HOH:O	2.15	0.45
1:A:26:LYS:HB2	1:B:397:ILE:HG13	1.97	0.45
1:A:113:ASP:HB3	1:A:119:LEU:HD21	1.97	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:290:ALA:O	1:A:291:ARG:HB2	2.16	0.45
1:B:214:LEU:O	1:B:218:THR:OG1	2.35	0.45
1:B:52:ASN:HB3	1:B:56:THR:OG1	2.17	0.44
1:B:399:LEU:HA	1:B:399:LEU:HD12	1.73	0.44
1:A:27:TYR:CE2	1:B:404:LYS:HA	2.52	0.44
1:B:152:ILE:H	1:B:152:ILE:HD12	1.83	0.44
1:B:314:ILE:H	1:B:314:ILE:HG13	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:B:432:MET:SD	1:B:436:MET:HE2	2.58	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:46:ILE:HD13	1:B:46:ILE:HA	1.90	0.43
1:B:370:LEU:HD23	1:B:372:ILE:HD11	2.01	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:75:GLU:HG3	1:A:76:ARG:N	2.34	0.42
1:A:219:VAL:HG11	1:A:258:LYS:HD3	2.02	0.42
1:B:55:TYR:CD1	1:B:156:LEU:HD13	2.55	0.42
1:B:228:LYS:HE2	1:B:262:TYR:O	2.20	0.42
1:B:311:LYS:HD2	1:B:311:LYS:HA	1.95	0.42
1:B:302:LEU:HD13	1:B:334:THR:HG21	2.02	0.42
1:B:385:LYS:C	1:B:387:SER:H	2.28	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:287:LEU:HD21	1:A:329:GLY:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:VAL:O	1:A:328:SER:HA	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
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:101:VAL:HG13	1:A:150:PHE:HB3	2.02	0.41
1:A:126:ASN:OD1	4:A:702:HOH:O	2.22	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:HA	1:B:422:ARG:HD2	1.89	0.40
1:A:421:ARG:HG2	4:A:742:HOH:O	2.21	0.40
1:A:500:MET:HE2	1:A:500:MET:HA	2.02	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

5.3.1 Protein backbone

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%)	43	71
1	B	470/554 (85%)	448 (95%)	20 (4%)	2 (0%)	30	58
All	All	941/1108 (85%)	894 (95%)	44 (5%)	3 (0%)	36	64

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%)	388 (92%)	36 (8%)	10	29
1	B	423/496 (85%)	382 (90%)	41 (10%)	8	24
All	All	847/992 (85%)	770 (91%)	77 (9%)	9	27

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	GLU
1	A	56	THR
1	A	87	LEU
1	A	112	VAL
1	A	144	ARG
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	240	LYS
1	A	242	VAL
1	A	247	LEU
1	A	277	ARG
1	A	308	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	HIS
1	A	353	ILE
1	A	356	ASP
1	A	362	LYS
1	A	363	ARG
1	A	375	LEU
1	A	377	GLN
1	A	387	SER
1	A	405	HIS
1	A	425	LYS
1	A	431	ASP
1	A	452	SER
1	A	455	MET
1	A	476	LEU
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	129	ARG
1	B	145	ASP
1	B	147	THR
1	B	152	ILE
1	B	165	LEU
1	B	170	ASP
1	B	190	LEU
1	B	192	MET
1	B	213	SER
1	B	215	LYS
1	B	218	THR
1	B	238	ARG
1	B	254	LYS
1	B	259	ILE
1	B	309	THR
1	B	314	ILE
1	B	321	LEU
1	B	323	HIS
1	B	325	ILE
1	B	334	THR
1	B	356	ASP
1	B	362	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	424	LYS
1	B	427	THR
1	B	446	ARG
1	B	454	VAL
1	B	466	ILE
1	B	476	LEU
1	B	481	HIS
1	B	490	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	HIS
1	A	143	GLN
1	B	108	ASN
1	B	117	ASN
1	B	126	ASN
1	B	322	GLN
1	B	352	HIS
1	B	380	HIS
1	B	411	ASN
1	B	420	GLN
1	B	453	GLN

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 [i](#)

There are no oligosaccharides 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	1.19	0	6,6,6	0.55	0
3	PO4	A	603	-	4,4,4	1.10	0	6,6,6	0.78	0
3	PO4	B	603	-	4,4,4	1.06	0	6,6,6	0.66	0
3	PO4	B	602	2	4,4,4	0.95	0	6,6,6	0.96	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	475/554 (85%)	-0.20	8 (1%) 69 60	15, 35, 77, 141	0
1	B	474/554 (85%)	-0.18	13 (2%) 56 46	12, 35, 87, 155	0
All	All	949/1108 (85%)	-0.19	21 (2%) 62 53	12, 35, 81, 155	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	506	THR	4.9
1	B	505	ALA	4.8
1	B	361	LYS	4.0
1	B	189	ASP	3.7
1	B	360	SER	3.2
1	B	358	LEU	3.1
1	A	505	ALA	3.1
1	B	503	PRO	2.9
1	A	361	LYS	2.7
1	A	358	LEU	2.6
1	A	360	SER	2.6
1	B	357	ILE	2.5
1	B	411	ASN	2.4
1	A	500	MET	2.3
1	A	320	PRO	2.3
1	B	319	GLY	2.3
1	B	356	ASP	2.3
1	B	318	THR	2.3
1	B	320	PRO	2.2
1	A	478	ARG	2.2
1	A	359	LYS	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	601	1/1	0.96	0.10	34,34,34,34	0
2	MG	B	601	1/1	0.98	0.06	28,28,28,28	0
3	PO4	A	603	5/5	0.98	0.06	10,30,41,43	0
3	PO4	B	602	5/5	0.98	0.06	39,39,52,60	0
3	PO4	A	602	5/5	0.99	0.05	32,36,42,49	0
3	PO4	B	603	5/5	0.99	0.04	10,16,28,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.