



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:15 AM UTC

PDB ID : 8I4N / pdb_00008i4n
Title : Crystal structure of 6-phosphogluconate dehydrogenase from *Corynebacterium glutamicum*
Authors : Yu, H.; Kim, K.-J.
Deposited on : 2023-01-20
Resolution : 2.41 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
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

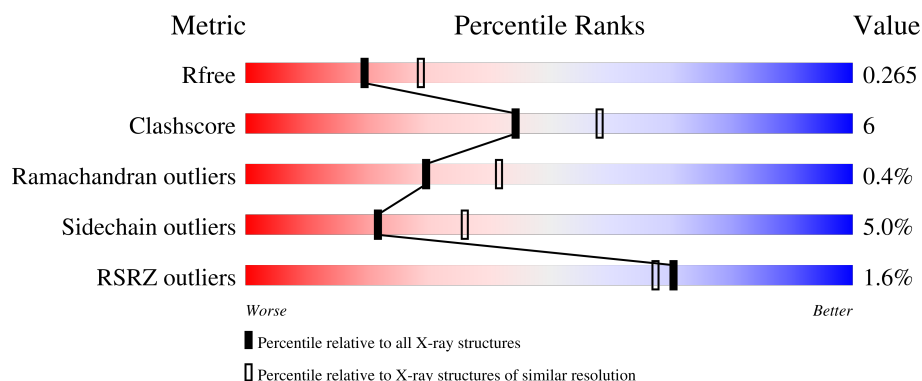
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	492	80%16%..
1	B	492	2% 80%15%..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7302 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 6-phosphogluconate dehydrogenase, decarboxylating.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3621	2271	628	713	9			
1	B	480	Total	C	N	O	S	0	0	0
			3617	2269	627	712	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	485	LEU	-	expression tag	UNP Q8NQI2
A	486	GLU	-	expression tag	UNP Q8NQI2
A	487	HIS	-	expression tag	UNP Q8NQI2
A	488	HIS	-	expression tag	UNP Q8NQI2
A	489	HIS	-	expression tag	UNP Q8NQI2
A	490	HIS	-	expression tag	UNP Q8NQI2
A	491	HIS	-	expression tag	UNP Q8NQI2
A	492	HIS	-	expression tag	UNP Q8NQI2
B	485	LEU	-	expression tag	UNP Q8NQI2
B	486	GLU	-	expression tag	UNP Q8NQI2
B	487	HIS	-	expression tag	UNP Q8NQI2
B	488	HIS	-	expression tag	UNP Q8NQI2
B	489	HIS	-	expression tag	UNP Q8NQI2
B	490	HIS	-	expression tag	UNP Q8NQI2
B	491	HIS	-	expression tag	UNP Q8NQI2
B	492	HIS	-	expression tag	UNP Q8NQI2

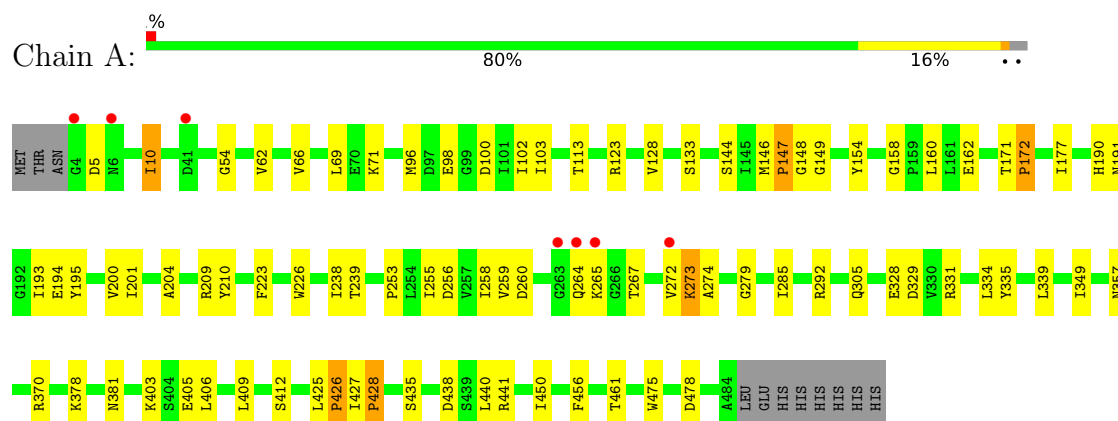
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		
2	B	29	Total	O	0	0
			29	29		

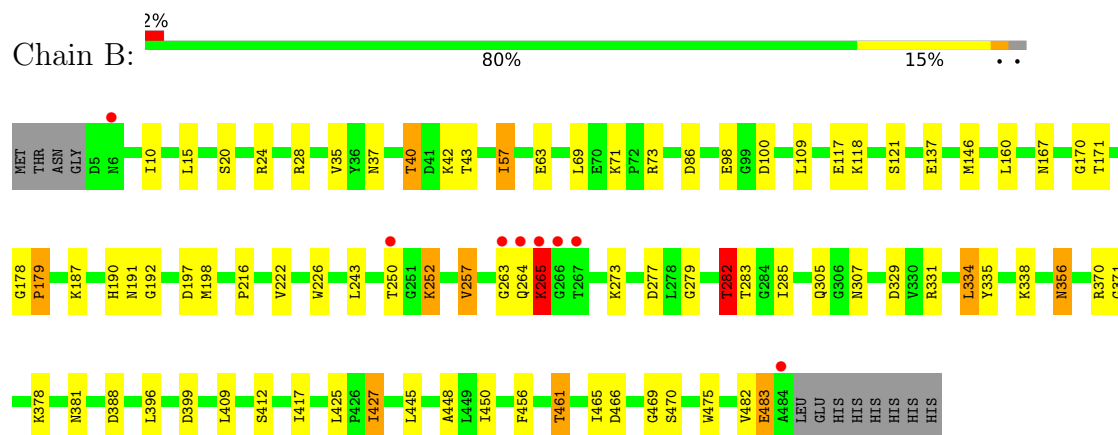
3 Residue-property plots

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: 6-phosphogluconate dehydrogenase, decarboxylating



- Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.90Å 120.30Å 152.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.99 – 2.41 33.99 – 2.41	Depositor EDS
% Data completeness (in resolution range)	94.5 (33.99-2.41) 94.8 (33.99-2.41)	Depositor EDS
R_{merge}	0.97	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.42Å)	Xtriage
Refinement program	REFMAC 7.1.000	Depositor
R, R_{free}	0.200 , 0.267 0.210 , 0.265	Depositor DCC
R_{free} test set	2167 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	34.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7302	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

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	1.32	9/3685 (0.2%)	1.69	30/5001 (0.6%)
1	B	1.38	12/3681 (0.3%)	1.67	34/4996 (0.7%)
All	All	1.35	21/7366 (0.3%)	1.68	64/9997 (0.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	PRO	N-CA	18.36	1.68	1.47
1	B	425	LEU	C-N	17.47	1.49	1.33
1	B	179	PRO	N-CA	16.91	1.68	1.47
1	A	428	PRO	N-CA	16.66	1.68	1.47
1	A	426	PRO	N-CA	16.15	1.68	1.47
1	B	445	LEU	C-N	15.30	1.50	1.34
1	B	146	MET	C-N	14.50	1.50	1.33
1	B	252	LYS	C-N	13.59	1.49	1.33
1	B	171	THR	C-N	13.42	1.49	1.33
1	B	57	ILE	C-N	13.13	1.50	1.33
1	A	149	GLY	C-N	12.49	1.49	1.33
1	B	399	ASP	C-N	12.46	1.49	1.33
1	B	427	ILE	C-N	11.56	1.50	1.33
1	A	171	THR	C-N	9.48	1.44	1.33
1	A	425	LEU	C-N	9.18	1.44	1.33
1	B	71	LYS	C-N	8.23	1.49	1.34
1	A	71	LYS	C-N	8.22	1.49	1.34
1	B	178	GLY	C-N	7.78	1.44	1.33
1	A	146	MET	C-N	6.84	1.49	1.33
1	B	216	PRO	C-O	-5.49	1.16	1.24
1	A	253	PRO	C-O	-5.14	1.17	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	GLY	CA-C-N	16.67	136.95	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	178	GLY	C-N-CA	16.67	136.95	119.78
1	A	171	THR	CA-C-N	16.61	137.71	119.93
1	A	171	THR	C-N-CA	16.61	137.71	119.93
1	A	427	ILE	CA-C-N	14.15	137.53	119.84
1	A	427	ILE	C-N-CA	14.15	137.53	119.84
1	A	425	LEU	CA-C-N	14.11	136.34	119.98
1	A	425	LEU	C-N-CA	14.11	136.34	119.98
1	B	445	LEU	CA-C-N	12.46	132.03	119.82
1	B	445	LEU	C-N-CA	12.46	132.03	119.82
1	B	57	ILE	CA-C-N	12.06	132.18	119.76
1	B	57	ILE	C-N-CA	12.06	132.18	119.76
1	B	171	THR	CA-C-N	11.91	132.40	119.90
1	B	171	THR	C-N-CA	11.91	132.40	119.90
1	A	149	GLY	CA-C-N	11.77	131.88	119.76
1	A	149	GLY	C-N-CA	11.77	131.88	119.76
1	B	252	LYS	CA-C-N	10.94	131.64	119.83
1	B	252	LYS	C-N-CA	10.94	131.64	119.83
1	B	399	ASP	CA-C-N	9.87	130.13	119.28
1	B	399	ASP	C-N-CA	9.87	130.13	119.28
1	A	146	MET	CA-C-N	9.76	132.03	119.84
1	A	146	MET	C-N-CA	9.76	132.03	119.84
1	B	427	ILE	CA-C-N	9.60	129.22	119.24
1	B	427	ILE	C-N-CA	9.60	129.22	119.24
1	A	113	THR	CA-CB-OG1	-9.54	95.29	109.60
1	B	146	MET	CA-C-N	9.36	130.70	120.13
1	B	146	MET	C-N-CA	9.36	130.70	120.13
1	A	426	PRO	CB-CA-C	9.06	123.49	111.71
1	B	179	PRO	CA-N-CD	-8.01	100.78	112.00
1	B	425	LEU	CA-C-N	7.61	131.64	120.46
1	B	425	LEU	C-N-CA	7.61	131.64	120.46
1	A	172	PRO	CA-N-CD	-7.44	101.58	112.00
1	B	277	ASP	CB-CA-C	7.44	123.40	110.01
1	A	428	PRO	CA-N-CD	-7.29	101.79	112.00
1	A	172	PRO	N-CA-C	-6.83	100.13	111.26
1	B	399	ASP	CB-CA-C	-6.67	99.52	109.60
1	B	399	ASP	O-C-N	-6.36	116.51	121.47
1	A	149	GLY	O-C-N	-5.94	115.83	121.77
1	A	195	TYR	N-CA-C	-5.94	104.89	111.36
1	A	274	ALA	N-CA-C	-5.92	104.41	111.69
1	A	426	PRO	N-CA-C	-5.92	101.36	110.95
1	A	426	PRO	CA-N-CD	-5.87	103.79	112.00
1	A	54	GLY	CA-C-O	-5.85	116.42	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	478	ASP	CA-CB-CG	5.70	118.30	112.60
1	B	257	VAL	N-CA-CB	-5.69	105.95	112.21
1	B	282	THR	CB-CA-C	5.68	121.72	110.42
1	B	378	LYS	CA-C-N	5.67	128.15	120.38
1	B	378	LYS	C-N-CA	5.67	128.15	120.38
1	B	388	ASP	N-CA-C	-5.41	105.04	111.69
1	A	378	LYS	CA-C-N	5.39	128.90	120.82
1	A	378	LYS	C-N-CA	5.39	128.90	120.82
1	B	179	PRO	N-CA-C	-5.32	102.75	111.21
1	B	427	ILE	O-C-N	-5.24	115.13	121.10
1	B	252	LYS	O-C-N	-5.22	115.69	121.53
1	A	147	PRO	CA-C-N	5.19	125.18	121.65
1	A	147	PRO	C-N-CA	5.19	125.18	121.65
1	A	204	ALA	CA-C-N	5.16	127.14	120.44
1	A	204	ALA	C-N-CA	5.16	127.14	120.44
1	B	40	THR	CA-C-N	5.09	127.35	120.38
1	B	40	THR	C-N-CA	5.09	127.35	120.38
1	B	371	GLY	CA-C-O	-5.07	116.91	121.47
1	B	469	GLY	CA-C-O	-5.06	117.25	122.26
1	A	201	ILE	CA-C-N	5.05	125.69	119.99
1	A	201	ILE	C-N-CA	5.05	125.69	119.99

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	3621	0	3545	45	0
1	B	3617	0	3542	47	0
2	A	35	0	0	1	0
2	B	29	0	0	0	0
All	All	7302	0	7087	86	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 6.

All (86) 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:428:PRO:N	1:A:428:PRO:CA	1.68	1.44
1:A:426:PRO:N	1:A:426:PRO:CA	1.68	1.35
1:B:179:PRO:N	1:B:179:PRO:CA	1.68	1.32
1:A:172:PRO:CA	1:A:172:PRO:N	1.68	1.28
1:A:96:MET:HE2	1:A:100:ASP:HB3	1.67	0.77
1:B:334:LEU:HD12	1:B:334:LEU:O	1.85	0.77
1:B:250:THR:HG23	1:B:252:LYS:H	1.51	0.74
1:B:334:LEU:HD12	1:B:334:LEU:C	2.14	0.73
1:A:172:PRO:N	1:A:172:PRO:C	2.46	0.72
1:A:426:PRO:N	1:A:426:PRO:C	2.48	0.70
1:B:63:GLU:OE2	1:B:63:GLU:HA	1.91	0.69
1:A:123:ARG:HG2	1:A:123:ARG:O	1.94	0.68
1:B:179:PRO:N	1:B:179:PRO:C	2.50	0.66
1:A:370:ARG:HH11	1:A:381:ASN:HD21	1.46	0.61
1:B:73:ARG:HB2	1:B:100:ASP:CG	2.25	0.61
1:B:15:LEU:HD12	1:B:43:THR:HA	1.83	0.60
1:A:62:VAL:O	1:A:66:VAL:HG23	2.04	0.58
1:A:209:ARG:NH2	1:A:256:ASP:OD2	2.37	0.57
1:A:450:ILE:HG23	1:B:198:MET:HE2	1.86	0.56
1:B:37:ASN:HD22	1:B:42:LYS:HB2	1.69	0.56
1:B:335:TYR:CD1	1:B:409:LEU:HD11	2.40	0.56
1:B:10:ILE:HB	1:B:160:LEU:HD23	1.88	0.56
1:A:133:SER:OG	1:A:144:SER:HB3	2.07	0.55
1:A:264:GLN:HE22	1:B:279:GLY:HA2	1.72	0.55
1:B:15:LEU:HD11	1:B:35:VAL:HB	1.89	0.54
1:A:428:PRO:N	1:A:428:PRO:C	2.61	0.53
1:A:255:ILE:HA	1:A:258:ILE:HD12	1.91	0.53
1:A:123:ARG:HG2	1:A:123:ARG:HH21	1.75	0.52
1:B:370:ARG:HH11	1:B:381:ASN:HD21	1.56	0.51
1:A:226:TRP:CD2	1:A:331:ARG:HG3	2.47	0.50
1:B:356:ASN:N	1:B:356:ASN:ND2	2.60	0.50
1:B:73:ARG:NH1	1:B:100:ASP:OD2	2.44	0.49
1:A:200:VAL:HB	1:A:334:LEU:CD1	2.43	0.49
1:A:273:LYS:HG2	1:B:273:LYS:HG2	1.94	0.49
1:A:456:PHE:HA	1:A:475:TRP:CD1	2.48	0.49
1:A:223:PHE:HD2	1:A:239:THR:HG22	1.78	0.48
1:A:128:VAL:HA	1:A:148:GLY:O	2.13	0.48
1:A:259:VAL:HG23	1:A:259:VAL:O	2.14	0.48
1:A:223:PHE:CD2	1:A:239:THR:HG22	2.49	0.48
1:B:40:THR:HG22	1:B:40:THR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ASN:ND2	1:B:42:LYS:HB2	2.29	0.48
1:B:69:LEU:HB2	1:B:73:ARG:HD3	1.96	0.47
1:B:482:VAL:HG23	1:B:482:VAL:O	2.14	0.46
1:A:5:ASP:OD1	1:A:5:ASP:N	2.43	0.46
1:B:187:LYS:HE2	1:B:191:ASN:HD21	1.81	0.46
1:A:403:LYS:HE3	1:B:307:ASN:O	2.15	0.46
1:B:263:GLY:HA3	1:B:265:LYS:HD3	1.98	0.46
1:A:264:GLN:O	1:A:264:GLN:HG2	2.12	0.46
1:A:10:ILE:HB	1:A:160:LEU:HD13	1.98	0.45
1:A:191:ASN:HD22	1:A:267:THR:HG21	1.81	0.45
1:B:167:ASN:HD21	1:B:170:GLY:HA2	1.81	0.45
1:A:154:TYR:CE1	1:A:158:GLY:HA2	2.51	0.45
1:A:335:TYR:CD1	1:A:409:LEU:HD11	2.51	0.45
1:B:456:PHE:HA	1:B:475:TRP:CD1	2.51	0.45
1:B:192:GLY:O	1:B:285:ILE:HG12	2.17	0.45
1:A:339:LEU:HD23	1:A:406:LEU:HD21	1.99	0.44
1:A:193:ILE:O	1:A:193:ILE:HG22	2.17	0.44
1:A:279:GLY:HA2	1:B:264:GLN:NE2	2.32	0.44
1:A:405:GLU:O	1:A:409:LEU:HG	2.17	0.44
1:A:209:ARG:HD3	1:A:210:TYR:CZ	2.53	0.44
1:B:57:ILE:HG22	1:B:57:ILE:O	2.17	0.44
1:B:335:TYR:HD1	1:B:409:LEU:HD11	1.82	0.44
1:A:329:ASP:HA	1:A:412:SER:HB3	2.00	0.43
1:A:441:ARG:NH2	2:A:502:HOH:O	2.52	0.43
1:B:226:TRP:CD2	1:B:331:ARG:HG3	2.53	0.43
1:B:483:GLU:H	1:B:483:GLU:HG3	1.52	0.43
1:B:282:THR:HG23	1:B:285:ILE:HB	2.01	0.42
1:B:329:ASP:HA	1:B:412:SER:HB3	2.02	0.42
1:B:396:LEU:HD23	1:B:396:LEU:HA	1.91	0.42
1:B:282:THR:CG2	1:B:282:THR:O	2.68	0.42
1:A:272:VAL:CG2	1:A:285:ILE:HG22	2.50	0.42
1:B:263:GLY:C	1:B:265:LYS:HD3	2.44	0.42
1:B:243:LEU:HD23	1:B:243:LEU:HA	1.91	0.41
1:B:20:SER:O	1:B:24:ARG:HG3	2.20	0.41
1:A:158:GLY:O	1:A:162:GLU:HG3	2.20	0.41
1:A:147:PRO:HD2	1:A:177:ILE:HG12	2.02	0.41
1:A:260:ASP:HB3	1:B:448:ALA:HB2	2.01	0.41
1:B:252:LYS:HE2	1:B:252:LYS:HB3	1.86	0.41
1:B:461:THR:HG21	1:B:470:SER:HB3	2.01	0.41
1:B:118:LYS:N	1:B:118:LYS:HD3	2.34	0.41
1:B:482:VAL:O	1:B:482:VAL:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:ASP:HA	1:A:441:ARG:HG2	2.02	0.41
1:A:103:ILE:HA	1:A:128:VAL:O	2.22	0.40
1:A:328:GLU:OE1	1:A:328:GLU:HA	2.20	0.40
1:B:109:LEU:HD12	1:B:109:LEU:HA	1.85	0.40
1:B:265:LYS:HB2	1:B:265:LYS:HE2	1.59	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	479/492 (97%)	454 (95%)	22 (5%)	3 (1%)	21	30
1	B	478/492 (97%)	456 (95%)	21 (4%)	1 (0%)	43	57
All	All	957/984 (97%)	910 (95%)	43 (4%)	4 (0%)	30	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	GLU
1	A	265	LYS
1	A	273	LYS
1	B	265	LYS

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	368/379 (97%)	355 (96%)	13 (4%)	32	51
1	B	368/379 (97%)	344 (94%)	24 (6%)	15	25
All	All	736/758 (97%)	699 (95%)	37 (5%)	22	36

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	69	LEU
1	A	98	GLU
1	A	102	ILE
1	A	190	HIS
1	A	238	ILE
1	A	292	ARG
1	A	305	GLN
1	A	349	ILE
1	A	357	ASN
1	A	435	SER
1	A	440	LEU
1	A	461	THR
1	B	28	ARG
1	B	86	ASP
1	B	98	GLU
1	B	117	GLU
1	B	121	SER
1	B	137	GLU
1	B	190	HIS
1	B	197	ASP
1	B	222	VAL
1	B	257	VAL
1	B	265	LYS
1	B	282	THR
1	B	283	THR
1	B	305	GLN
1	B	334	LEU
1	B	338	LYS
1	B	356	ASN
1	B	417	ILE
1	B	427	ILE
1	B	450	ILE
1	B	461	THR
1	B	465	ILE

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Mol	Chain	Res	Type
1	B	466	ASP
1	B	483	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	141	ASN
1	A	167	ASN
1	A	176	HIS
1	A	191	ASN
1	A	199	GLN
1	A	300	GLN
1	A	305	GLN
1	A	325	GLN
1	A	381	ASN
1	A	422	GLN
1	B	37	ASN
1	B	167	ASN
1	B	184	HIS
1	B	191	ASN
1	B	206	HIS
1	B	300	GLN
1	B	325	GLN
1	B	356	ASN
1	B	381	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	481/492 (97%)	-0.07	7 (1%) 72 69	25, 40, 63, 103	0
1	B	480/492 (97%)	0.04	8 (1%) 69 66	23, 39, 69, 117	0
All	All	961/984 (97%)	-0.01	15 (1%) 70 67	23, 40, 66, 117	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	GLN	5.0
1	B	265	LYS	3.9
1	A	264	GLN	3.7
1	A	265	LYS	3.3
1	A	263	GLY	3.1
1	A	41	ASP	2.7
1	B	263	GLY	2.6
1	A	4	GLY	2.6
1	B	266	GLY	2.4
1	B	484	ALA	2.4
1	A	6	ASN	2.3
1	B	250	THR	2.1
1	B	267	THR	2.1
1	B	6	ASN	2.1
1	A	272	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.