



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:10 AM UTC

PDB ID : 1KCX / pdb_00001kcx
Title : X-ray structure of NYSGRC target T-45
Authors : Deo, R.C.; Schmidt, E.F.; Strittmatter, S.M.; Burley, S.K.; New York SGX
Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2001-11-11
Resolution : 2.12 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

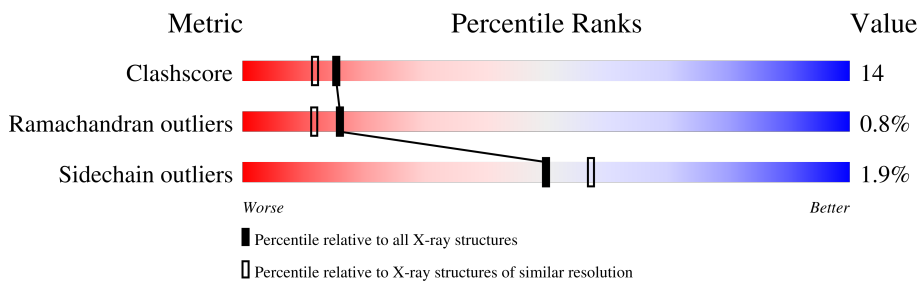
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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))
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	518	 70% 19% 8%
1	B	518	 69% 19% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8086 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 DIHYDROPYRIMIDINASE RELATED PROTEIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3641	2312	616	695	18			
1	B	476	Total	C	N	O	S	0	0	0
			3641	2312	616	695	18			

- Molecule 2 is water.

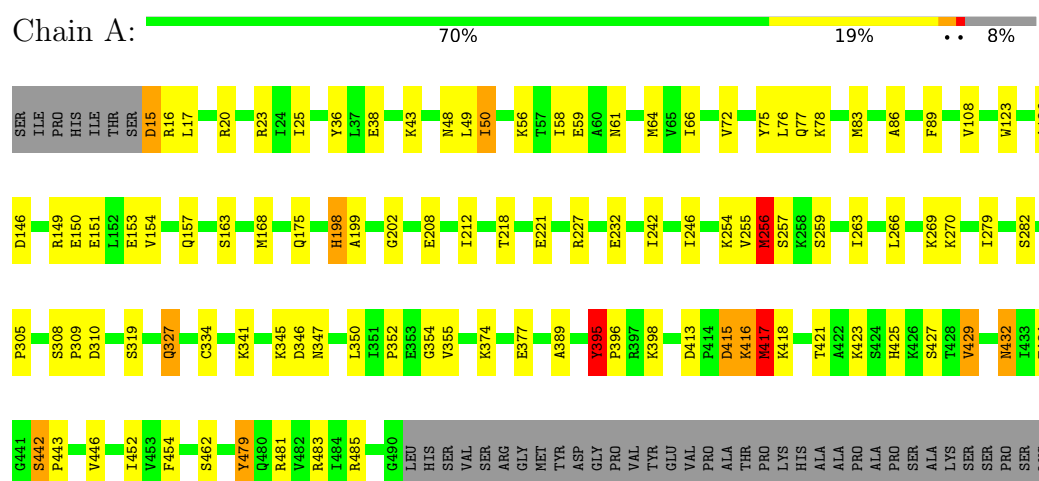
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	421	Total	O	0	0
			421	421		
2	B	383	Total	O	0	0
			383	383		

3 Residue-property plots

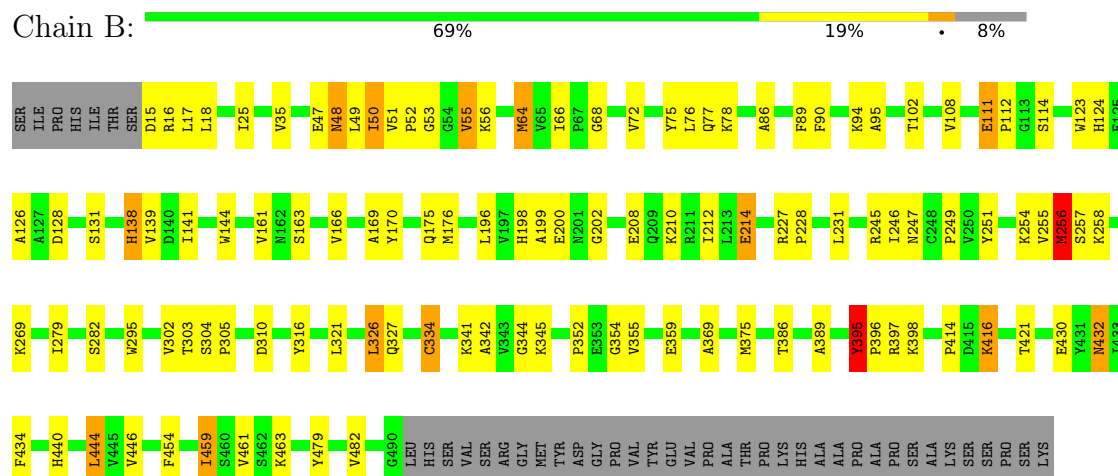
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: DIHYDROPYRIMIDINASE RELATED PROTEIN-1



• Molecule 1: DIHYDROPYRIMIDINASE RELATED PROTEIN-1



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.40Å 152.11Å 157.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.12	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.12)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.204 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8086	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

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	0.72	7/3719 (0.2%)	1.11	29/5042 (0.6%)
1	B	0.53	2/3719 (0.1%)	1.01	19/5042 (0.4%)
All	All	0.63	9/7438 (0.1%)	1.06	48/10084 (0.5%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	417	MET	SD-CE	18.65	2.26	1.79
1	A	417	MET	CG-SD	14.50	2.17	1.80
1	A	416	LYS	CG-CD	11.28	1.86	1.52
1	B	256	MET	SD-CE	-10.84	1.52	1.79
1	A	256	MET	SD-CE	-10.39	1.53	1.79
1	A	416	LYS	CB-CG	8.39	1.77	1.52
1	A	418	LYS	CA-C	-8.04	1.44	1.53
1	B	64	MET	SD-CE	-7.19	1.61	1.79
1	A	416	LYS	CD-CE	6.05	1.70	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	MET	CA-C-N	-16.33	97.97	122.47
1	A	417	MET	C-N-CA	-16.33	97.97	122.47
1	A	417	MET	N-CA-C	14.30	141.25	110.80
1	A	415	ASP	N-CA-C	11.18	127.92	112.72
1	A	86	ALA	N-CA-C	8.99	122.06	111.71
1	A	418	LYS	N-CA-C	8.75	124.33	107.44
1	B	86	ALA	N-CA-C	8.29	120.31	111.28
1	B	479	TYR	N-CA-C	7.82	122.64	113.18
1	A	479	TYR	N-CA-C	7.72	122.53	113.18
1	B	310	ASP	CA-C-N	7.42	128.08	119.47
1	B	310	ASP	C-N-CA	7.42	128.08	119.47
1	B	199	ALA	N-CA-C	7.16	120.44	108.20
1	B	395	TYR	N-CA-C	7.08	125.47	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	395	TYR	CA-C-N	-6.74	111.64	119.32
1	B	395	TYR	C-N-CA	-6.74	111.64	119.32
1	A	417	MET	O-C-N	-6.41	114.06	122.59
1	A	417	MET	CG-SD-CE	6.38	114.94	100.90
1	A	199	ALA	N-CA-C	6.32	119.50	107.75
1	A	395	TYR	N-CA-C	6.31	123.75	109.81
1	A	138	HIS	N-CA-C	-6.26	100.09	110.17
1	A	157	GLN	N-CA-C	6.24	118.16	111.36
1	B	254	LYS	N-CA-C	6.17	119.87	111.17
1	A	416	LYS	CB-CG-CD	6.14	125.42	111.30
1	A	327	GLN	N-CA-C	5.93	121.17	113.88
1	A	48	ASN	N-CA-C	5.85	117.29	108.46
1	A	310	ASP	CA-C-N	5.79	125.47	119.56
1	A	310	ASP	C-N-CA	5.79	125.47	119.56
1	A	254	LYS	N-CA-C	5.76	119.29	111.17
1	B	76	LEU	N-CA-C	5.59	118.14	111.71
1	A	442	SER	N-CA-C	5.54	113.00	108.07
1	B	131	SER	N-CA-C	5.49	117.98	110.24
1	B	302	VAL	N-CA-C	5.45	115.43	108.12
1	A	416	LYS	CD-CE-NZ	5.44	129.30	111.90
1	B	326	LEU	N-CA-C	-5.41	100.58	109.40
1	B	386	THR	N-CA-C	5.39	117.58	111.11
1	B	53	GLY	N-CA-C	5.38	119.15	112.64
1	A	395	TYR	CA-C-N	-5.36	113.15	119.84
1	A	395	TYR	C-N-CA	-5.36	113.15	119.84
1	A	168	MET	N-CA-C	-5.35	106.76	113.72
1	B	257	SER	N-CA-C	5.35	117.81	109.52
1	A	198	HIS	N-CA-C	-5.34	97.82	107.75
1	B	55	VAL	N-CA-C	5.30	115.48	107.80
1	A	76	LEU	N-CA-C	5.29	117.80	111.71
1	B	444	LEU	N-CA-C	-5.26	106.92	113.55
1	B	138	HIS	N-CA-C	-5.24	101.73	110.17
1	A	429	VAL	N-CA-C	5.04	115.55	110.05
1	A	257	SER	N-CA-C	5.04	117.32	109.52
1	A	232	GLU	N-CA-C	-5.01	105.29	111.40

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	3641	0	3603	102	0
1	B	3641	0	3603	94	0
2	A	421	0	0	8	1
2	B	383	0	0	5	0
All	All	8086	0	7206	196	1

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 14.

All (196) 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:416:LYS:CB	1:A:416:LYS:CG	1.77	1.58
1:A:416:LYS:CG	1:A:416:LYS:CD	1.86	1.54
1:A:417:MET:SD	1:A:417:MET:CG	2.17	1.33
1:A:417:MET:SD	1:A:417:MET:CE	2.26	1.24
1:A:417:MET:SD	1:A:442:SER:OG	2.11	1.07
1:A:416:LYS:HE3	1:A:417:MET:CG	1.89	1.03
1:A:416:LYS:CE	1:A:417:MET:HG3	1.88	1.01
1:B:166:VAL:HB	1:B:176:MET:HE1	1.48	0.94
1:A:416:LYS:HE3	1:A:417:MET:HG3	0.95	0.93
1:A:218:THR:HB	1:A:346:ASP:O	1.69	0.92
1:B:389:ALA:HB1	1:B:395:TYR:HA	1.49	0.91
1:A:416:LYS:HG3	1:A:417:MET:SD	2.11	0.91
1:B:432:ASN:HD22	1:B:434:PHE:H	1.23	0.86
1:A:432:ASN:HD22	1:A:434:PHE:H	1.24	0.84
1:B:111:GLU:HB3	1:B:112:PRO:CD	2.08	0.84
1:B:416:LYS:O	1:B:416:LYS:HG3	1.79	0.82
1:B:166:VAL:HB	1:B:176:MET:CE	2.10	0.81
1:A:413:ASP:O	1:A:417:MET:HE1	1.83	0.79
1:A:266:LEU:HD11	1:A:270:LYS:HE3	1.65	0.77
1:A:416:LYS:O	1:A:417:MET:SD	2.44	0.76
1:B:111:GLU:HB3	1:B:112:PRO:HD2	1.68	0.75
1:A:255:VAL:C	1:A:256:MET:HE3	2.12	0.73
1:A:416:LYS:HD2	1:A:417:MET:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ALA:HB1	1:A:395:TYR:HA	1.73	0.70
1:A:50:ILE:HG22	1:A:50:ILE:O	1.92	0.70
1:A:25:ILE:HB	1:A:66:ILE:HG22	1.75	0.69
1:B:138:HIS:HD2	1:B:163:SER:OG	1.76	0.69
1:B:255:VAL:C	1:B:256:MET:HE3	2.18	0.68
1:A:256:MET:HG3	1:A:282:SER:HB3	1.77	0.67
1:B:210:LYS:O	1:B:214:GLU:HG2	1.95	0.66
1:A:149:ARG:O	1:A:153:GLU:HG3	1.96	0.66
1:B:166:VAL:CB	1:B:176:MET:HE1	2.21	0.66
1:A:421:THR:HG21	1:A:423:LYS:HZ3	1.61	0.66
1:B:432:ASN:ND2	1:B:434:PHE:H	1.93	0.66
1:B:141:ILE:HD13	1:B:144:TRP:HZ3	1.60	0.65
1:B:341:LYS:HA	1:B:352:PRO:HD2	1.77	0.65
1:A:432:ASN:ND2	1:A:434:PHE:H	1.94	0.64
1:A:395:TYR:O	1:A:398:LYS:O	2.15	0.64
1:B:64:MET:HE1	1:B:414:PRO:HB3	1.81	0.63
1:A:16:ARG:HD3	1:A:36:TYR:OH	1.99	0.63
1:B:395:TYR:O	1:B:398:LYS:O	2.17	0.62
1:B:72:VAL:O	1:B:138:HIS:HE1	1.82	0.62
1:B:111:GLU:CB	1:B:112:PRO:CD	2.79	0.61
1:B:25:ILE:HB	1:B:66:ILE:HG22	1.83	0.61
1:A:416:LYS:C	1:A:417:MET:SD	2.84	0.60
1:A:295:TRP:CZ2	1:A:345:LYS:HA	2.36	0.60
1:B:77:GLN:HE22	1:B:126:ALA:CB	2.15	0.60
1:A:415:ASP:O	1:A:416:LYS:HB3	2.00	0.60
1:B:304:SER:HA	1:B:305:PRO:C	2.28	0.59
1:A:416:LYS:CD	1:A:417:MET:HB3	2.32	0.59
1:A:416:LYS:CG	1:A:416:LYS:CA	2.76	0.59
1:B:16:ARG:CZ	1:B:52:PRO:HG2	2.33	0.59
1:A:17:LEU:HD13	1:A:56:LYS:HD3	1.85	0.58
1:A:304:SER:HA	1:A:305:PRO:C	2.27	0.58
1:B:112:PRO:HA	2:B:556:HOH:O	2.04	0.58
1:A:417:MET:HE2	1:A:442:SER:O	2.04	0.57
1:B:245:ARG:NE	1:B:245:ARG:HA	2.19	0.57
1:A:255:VAL:O	1:A:256:MET:HE3	2.04	0.57
1:B:256:MET:HE2	1:B:282:SER:HB3	1.86	0.57
1:B:258:LYS:HG2	1:B:316:TYR:CD2	2.39	0.57
1:A:138:HIS:HD2	1:A:163:SER:OG	1.88	0.57
1:B:342:ALA:C	1:B:344:GLY:H	2.13	0.56
1:B:256:MET:HE1	1:B:279:ILE:HG12	1.86	0.56
1:A:256:MET:HE1	1:A:279:ILE:HG12	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:MET:CE	1:B:414:PRO:HD3	2.36	0.56
1:B:200:GLU:OE2	1:B:227:ARG:NH1	2.39	0.55
1:A:395:TYR:O	1:A:396:PRO:C	2.49	0.55
1:B:421:THR:HB	2:B:624:HOH:O	2.07	0.55
1:B:49:LEU:C	1:B:50:ILE:HG13	2.32	0.55
1:A:327:GLN:N	1:A:327:GLN:CD	2.65	0.55
1:B:256:MET:HG3	1:B:282:SER:HB3	1.89	0.55
1:A:266:LEU:CD1	1:A:270:LYS:HE3	2.36	0.54
1:B:139:VAL:HG23	1:B:161:VAL:HG11	1.90	0.54
1:B:200:GLU:CD	1:B:227:ARG:NH1	2.67	0.53
1:A:208:GLU:O	1:A:212:ILE:HG12	2.09	0.53
1:B:295:TRP:CZ2	1:B:345:LYS:HA	2.44	0.53
1:A:256:MET:HE2	1:A:282:SER:OG	2.08	0.52
1:B:47:GLU:O	1:B:48:ASN:CB	2.56	0.52
1:B:459:ILE:HD12	1:B:461:VAL:HG13	1.91	0.52
1:A:83:MET:HE3	1:A:352:PRO:HG3	1.91	0.52
1:B:432:ASN:HD22	1:B:432:ASN:C	2.17	0.52
1:B:369:ALA:HB1	1:B:375:MET:HG2	1.90	0.52
1:A:72:VAL:O	1:A:138:HIS:HE1	1.93	0.52
1:A:256:MET:HE2	1:A:282:SER:CB	2.40	0.51
1:A:256:MET:HE2	1:A:282:SER:HB3	1.93	0.51
1:B:255:VAL:O	1:B:256:MET:HE3	2.10	0.51
1:B:166:VAL:CG1	1:B:176:MET:HE1	2.39	0.51
1:B:397:ARG:HG3	1:B:398:LYS:HG2	1.93	0.51
1:A:432:ASN:HD22	1:A:432:ASN:C	2.18	0.51
1:A:49:LEU:O	1:A:50:ILE:HB	2.11	0.50
1:A:334:CYS:O	1:A:354:GLY:HA3	2.11	0.50
1:B:395:TYR:CG	1:B:396:PRO:N	2.79	0.50
1:B:64:MET:CE	1:B:414:PRO:HB3	2.42	0.50
1:A:50:ILE:O	1:A:50:ILE:CG2	2.60	0.50
1:B:256:MET:HE2	1:B:282:SER:CB	2.42	0.49
1:A:270:LYS:HD2	2:A:880:HOH:O	2.12	0.49
1:A:417:MET:HE1	1:A:442:SER:H	1.78	0.49
1:B:77:GLN:HE21	1:B:89:PHE:HD2	1.58	0.49
1:B:208:GLU:O	1:B:212:ILE:HG12	2.13	0.49
1:B:75:TYR:HB3	1:B:78:LYS:HB2	1.94	0.49
1:A:56:LYS:HE2	1:A:452:ILE:HD12	1.95	0.49
1:B:108:VAL:HG22	1:B:123:TRP:CG	2.48	0.49
1:B:327:GLN:N	1:B:327:GLN:CD	2.70	0.48
1:A:417:MET:CE	1:A:442:SER:O	2.61	0.48
1:B:228:PRO:HG2	1:B:231:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:PHE:CD1	1:B:463:LYS:HG3	2.49	0.48
1:B:16:ARG:HD3	1:B:55:VAL:HG22	1.96	0.48
1:B:198:HIS:HE1	1:B:200:GLU:OE2	1.97	0.48
1:B:342:ALA:C	1:B:344:GLY:N	2.70	0.47
1:A:442:SER:HB2	1:A:443:PRO:CD	2.44	0.47
1:B:303:THR:HB	1:B:355:VAL:HG13	1.96	0.47
1:B:295:TRP:CH2	1:B:342:ALA:HA	2.50	0.47
1:A:437:MET:HE3	2:A:665:HOH:O	2.13	0.46
1:A:198:HIS:HD2	2:A:569:HOH:O	1.99	0.46
1:B:77:GLN:HE22	1:B:126:ALA:HB1	1.81	0.46
1:B:395:TYR:CD1	1:B:395:TYR:C	2.91	0.46
1:A:64:MET:HE1	1:A:377:GLU:HB3	1.97	0.46
1:A:294:ASN:C	1:A:294:ASN:OD1	2.57	0.46
1:B:175:GLN:OE1	1:B:202:GLY:HA3	2.15	0.46
1:B:77:GLN:NE2	1:B:89:PHE:CD2	2.84	0.46
1:A:15:ASP:HB2	2:A:828:HOH:O	2.15	0.46
1:B:111:GLU:HB2	1:B:114:SER:OG	2.15	0.46
1:A:59:GLU:HB3	1:A:61:ASN:OD1	2.16	0.46
1:A:417:MET:CG	1:A:442:SER:OG	2.63	0.46
1:B:169:ALA:HB2	1:B:200:GLU:HB2	1.97	0.46
1:A:49:LEU:O	1:A:50:ILE:CB	2.63	0.45
1:A:75:TYR:HB3	1:A:78:LYS:HB2	1.97	0.45
1:B:16:ARG:NH1	1:B:52:PRO:HG2	2.31	0.45
1:B:68:GLY:HA3	1:B:102:THR:OG1	2.16	0.45
1:B:64:MET:HE3	1:B:414:PRO:HD3	1.98	0.45
1:B:141:ILE:HD13	1:B:144:TRP:CZ3	2.47	0.45
1:B:246:ILE:O	1:B:247:ASN:HB3	2.17	0.45
1:B:200:GLU:OE1	1:B:227:ARG:NH1	2.48	0.45
1:A:416:LYS:HD3	2:A:922:HOH:O	2.15	0.45
1:A:242:ILE:HG22	1:A:246:ILE:HD12	1.99	0.45
1:B:395:TYR:O	1:B:396:PRO:C	2.58	0.45
1:A:269:LYS:HE3	2:B:738:HOH:O	2.17	0.45
1:A:481:ARG:O	1:A:485:ARG:HG3	2.17	0.45
1:B:51:VAL:HA	1:B:52:PRO:HD3	1.89	0.45
1:A:256:MET:CE	1:A:279:ILE:HG12	2.47	0.44
1:A:413:ASP:HB3	1:A:417:MET:CE	2.47	0.44
1:B:94:LYS:HG2	1:B:459:ILE:HD13	1.98	0.44
1:B:95:ALA:O	1:B:359:GLU:HG3	2.17	0.44
1:B:75:TYR:HB2	1:B:334:CYS:HB3	2.00	0.44
1:B:196:LEU:HG	1:B:251:TYR:CD1	2.53	0.44
1:A:58:ILE:HD11	1:A:452:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ASN:O	1:B:247:ASN:CG	2.61	0.44
1:B:169:ALA:O	1:B:170:TYR:HB2	2.18	0.44
1:B:334:CYS:O	1:B:354:GLY:HA3	2.18	0.43
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.56	0.43
1:A:446:VAL:HB	1:A:454:PHE:HB3	2.00	0.43
1:B:124:HIS:CE1	1:B:128:ASP:OD2	2.71	0.43
1:B:444:LEU:HD23	1:B:444:LEU:HA	1.88	0.43
1:A:38:GLU:HB3	1:A:43:LYS:NZ	2.34	0.43
1:A:77:GLN:HE22	1:A:126:ALA:HB1	1.84	0.43
1:A:256:MET:HE3	1:A:256:MET:N	2.34	0.43
1:B:200:GLU:CD	1:B:227:ARG:HH12	2.24	0.43
1:B:141:ILE:HG21	1:B:144:TRP:CZ3	2.54	0.43
1:A:83:MET:CE	1:A:352:PRO:HG3	2.48	0.43
1:A:175:GLN:OE1	1:A:202:GLY:HA3	2.19	0.43
1:B:17:LEU:HD12	1:B:56:LYS:O	2.19	0.43
1:B:321:LEU:HD12	1:B:326:LEU:O	2.19	0.43
1:A:319:SER:OG	1:A:374:LYS:HE3	2.18	0.42
1:A:23:ARG:NH1	1:A:25:ILE:HD11	2.34	0.42
1:A:413:ASP:HB3	1:A:417:MET:HE3	2.01	0.42
1:A:38:GLU:HB3	1:A:43:LYS:HG3	2.00	0.42
1:A:77:GLN:HE21	1:A:89:PHE:HD2	1.66	0.42
1:A:355:VAL:HA	2:A:933:HOH:O	2.19	0.42
1:A:347:ASN:HB3	1:A:350:LEU:HD12	2.02	0.42
1:A:108:VAL:HG22	1:A:123:TRP:CG	2.55	0.42
1:B:77:GLN:NE2	1:B:89:PHE:HD2	2.16	0.42
1:B:77:GLN:HG2	2:B:814:HOH:O	2.19	0.42
1:A:227:ARG:NH2	2:A:600:HOH:O	2.52	0.42
1:B:18:LEU:HD12	1:B:35:VAL:O	2.20	0.42
1:A:341:LYS:HA	1:A:352:PRO:HD2	2.02	0.42
1:A:417:MET:SD	1:A:442:SER:CB	3.05	0.42
1:A:145:TYR:OH	1:A:151:GLU:OE2	2.33	0.41
1:A:266:LEU:O	1:A:269:LYS:HG2	2.20	0.41
1:A:425:HIS:CD2	1:A:425:HIS:C	2.98	0.41
1:A:479:TYR:O	1:A:483:ARG:HG3	2.20	0.41
1:A:138:HIS:CD2	1:A:163:SER:OG	2.71	0.41
1:A:417:MET:CE	1:A:442:SER:H	2.33	0.41
1:A:427:SER:OG	1:A:429:VAL:HG22	2.19	0.41
1:A:308:SER:HA	1:A:309:PRO:HD3	1.90	0.41
1:A:417:MET:CE	1:A:442:SER:OG	2.69	0.41
1:A:395:TYR:CG	1:A:396:PRO:N	2.84	0.41
1:A:423:LYS:HE2	2:A:766:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:SER:O	1:A:263:ILE:HG12	2.21	0.41
1:A:150:GLU:O	1:A:154:VAL:HG23	2.21	0.41
1:B:108:VAL:HG13	1:B:123:TRP:CE3	2.56	0.41
1:B:430:GLU:HG3	2:B:702:HOH:O	2.21	0.41
1:A:221:GLU:OE1	1:A:221:GLU:N	2.53	0.40
1:B:94:LYS:HG2	1:B:459:ILE:CD1	2.51	0.40
1:B:245:ARG:NE	1:B:245:ARG:CA	2.84	0.40
1:B:249:PRO:HD3	1:B:482:VAL:HG21	2.03	0.40
1:B:446:VAL:HB	1:B:454:PHE:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:758:HOH:O	2:A:758:HOH:O[4_555]	2.09	0.11

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	474/518 (92%)	449 (95%)	22 (5%)	3 (1%)	21	18
1	B	474/518 (92%)	446 (94%)	23 (5%)	5 (1%)	11	7
All	All	948/1036 (92%)	895 (94%)	45 (5%)	8 (1%)	16	12

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	395	TYR
1	B	111	GLU
1	B	395	TYR

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Mol	Chain	Res	Type
1	A	417	MET
1	B	50	ILE
1	B	48	ASN
1	B	334	CYS

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	388/428 (91%)	381 (98%)	7 (2%)	51	59
1	B	388/428 (91%)	380 (98%)	8 (2%)	47	54
All	All	776/856 (91%)	761 (98%)	15 (2%)	50	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	146	ASP
1	A	256	MET
1	A	417	MET
1	A	432	ASN
1	A	440	HIS
1	A	462	SER
1	B	15	ASP
1	B	214	GLU
1	B	256	MET
1	B	269	LYS
1	B	416	LYS
1	B	432	ASN
1	B	440	HIS
1	B	459	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	77	GLN
1	A	91	GLN
1	A	124	HIS
1	A	138	HIS
1	A	198	HIS
1	A	209	GLN
1	A	247	ASN
1	A	432	ASN
1	A	477	HIS
1	A	480	GLN
1	B	29	GLN
1	B	61	ASN
1	B	77	GLN
1	B	124	HIS
1	B	138	HIS
1	B	175	GLN
1	B	198	HIS
1	B	209	GLN
1	B	432	ASN
1	B	477	HIS
1	B	480	GLN

5.3.3 RNA [i](#)

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.