



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:22 PM UTC

PDB ID : 1PYS / pdb_00001pys
Title : PHENYLALANYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS
Authors : Safro, M.; Mosyak, L.; Goldgur, Y.; Reshetnikova, L.; Delarue, M.
Deposited on : 1996-11-14
Resolution : 2.90 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

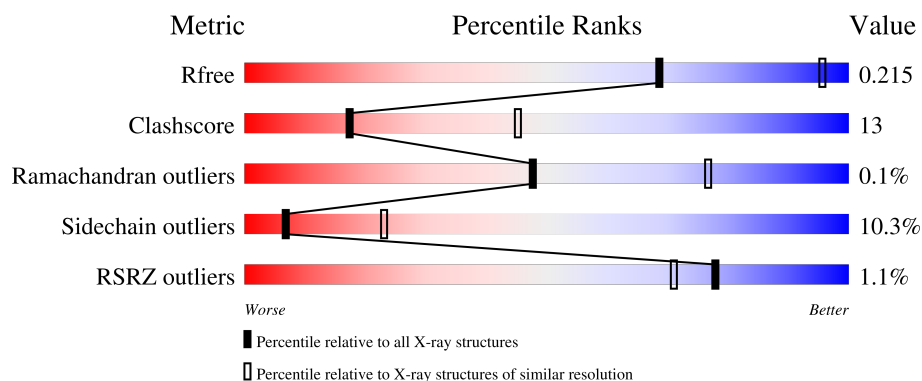
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	350	
2	B	785	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10968 atoms, of which 2385 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 PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	266	Total	C	H	N	O	S	16	0	0
			2550	1388	427	363	365	7			

- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	785	Total	C	H	N	O	S	46	0	0
			7421	3925	1294	1091	1101	10			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

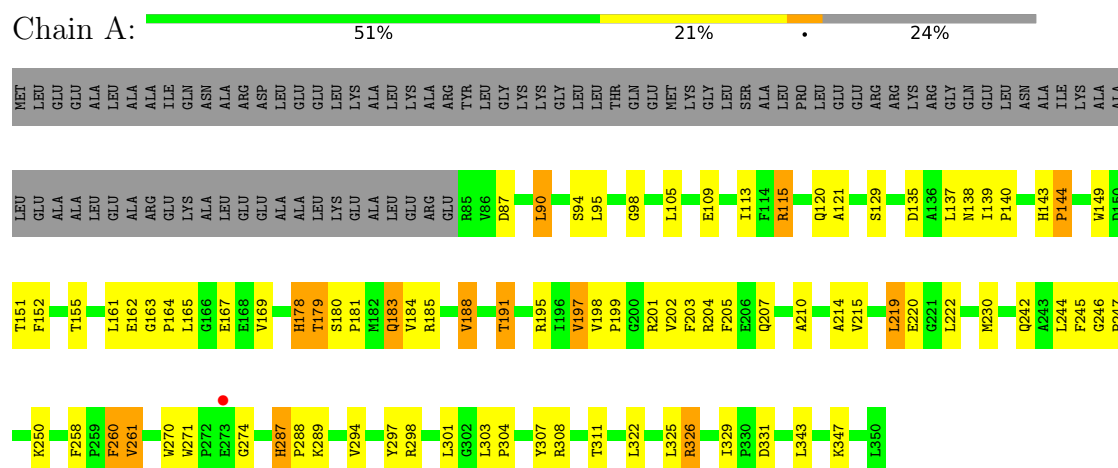
- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	80	Total	H	O	0	0
			240	160	80		
4	B	252	Total	H	O	0	0
			756	504	252		

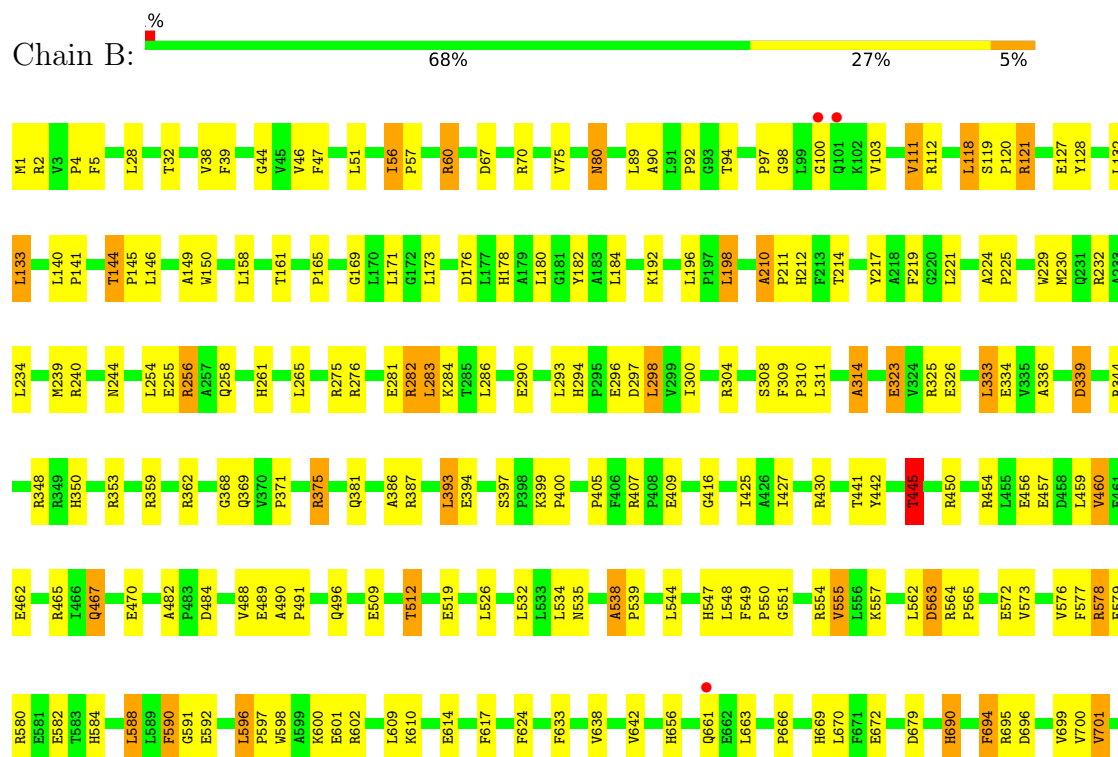
3 Residue-property plots

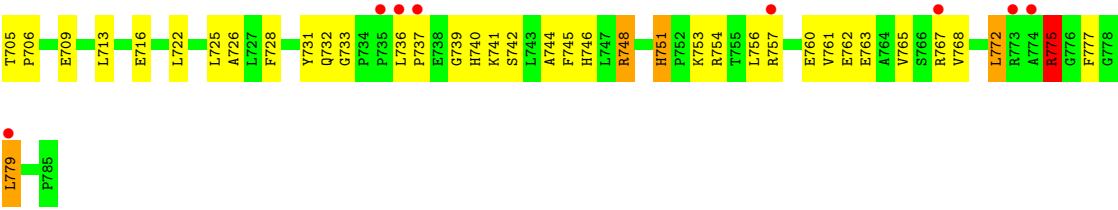
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 2: PHENYLALANYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	176.00Å 176.00Å 141.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.90 10.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (10.00-2.90) 90.5 (10.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.88Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.177 , 0.236 0.165 , 0.215	Depositor DCC
R_{free} test set	5281 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	43.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 58.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10968	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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

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	0.71	0/2191	1.09	18/2971 (0.6%)
2	B	0.66	0/6280	1.12	52/8536 (0.6%)
All	All	0.67	0/8471	1.12	70/11507 (0.6%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	10.76	131.72	109.34
1	A	163	GLY	CA-C-N	9.40	129.01	119.24
1	A	163	GLY	C-N-CA	9.40	129.01	119.24
2	B	256	ARG	N-CA-C	7.79	122.89	112.30
2	B	144	THR	CA-C-N	7.75	128.20	119.83
2	B	144	THR	C-N-CA	7.75	128.20	119.83
1	A	329	ILE	CA-C-N	7.42	127.05	119.19
1	A	329	ILE	C-N-CA	7.42	127.05	119.19
2	B	133	LEU	N-CA-C	-7.28	99.51	110.28
2	B	592	GLU	N-CA-C	7.25	119.19	111.28
2	B	161	THR	CA-C-N	7.11	127.72	119.47
2	B	161	THR	C-N-CA	7.11	127.72	119.47
2	B	326	GLU	N-CA-C	6.87	118.76	111.28
2	B	336	ALA	N-CA-C	6.77	119.05	108.96
1	A	135	ASP	N-CA-C	6.75	118.29	111.07
2	B	666	PRO	N-CA-C	-6.67	102.56	110.70
1	A	94	SER	N-CA-C	6.64	119.58	109.62
1	A	151	THR	N-CA-C	6.62	120.07	110.28
2	B	56	ILE	CA-C-N	6.61	127.01	119.93
2	B	56	ILE	C-N-CA	6.61	127.01	119.93
2	B	775	ARG	N-CA-C	-6.39	105.52	113.38
2	B	427	ILE	CB-CA-C	-6.36	103.86	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	300	ILE	N-CA-C	-6.35	98.72	107.99
2	B	118	LEU	N-CA-C	6.33	120.01	109.95
1	A	138	ASN	N-CA-C	6.22	120.18	112.47
2	B	150	TRP	CA-C-N	6.18	126.15	120.03
2	B	150	TRP	C-N-CA	6.18	126.15	120.03
2	B	416	GLY	N-CA-C	-6.18	106.17	115.32
2	B	387	ARG	N-CA-C	-6.08	99.33	109.24
2	B	538	ALA	CA-C-N	6.05	126.22	119.32
2	B	538	ALA	C-N-CA	6.05	126.22	119.32
2	B	70	ARG	N-CA-C	-5.99	100.39	109.85
1	A	311	THR	N-CA-C	-5.93	100.76	109.18
2	B	690	HIS	CA-C-N	5.92	125.93	119.90
2	B	690	HIS	C-N-CA	5.92	125.93	119.90
2	B	397	SER	CA-C-N	-5.88	113.91	120.14
2	B	397	SER	C-N-CA	-5.88	113.91	120.14
1	A	260	PHE	N-CA-C	5.78	119.31	112.72
2	B	563	ASP	N-CA-C	-5.76	100.31	109.23
2	B	5	PHE	N-CA-C	5.74	118.03	111.02
2	B	573	VAL	N-CA-C	-5.68	100.16	108.11
2	B	617	PHE	N-CA-C	5.61	118.32	111.82
1	A	140	PRO	N-CA-C	5.58	119.45	111.13
1	A	214	ALA	N-CA-C	-5.54	106.69	113.50
2	B	482	ALA	CA-C-N	5.50	126.71	119.84
2	B	482	ALA	C-N-CA	5.50	126.71	119.84
2	B	210	ALA	CA-C-N	5.46	125.17	119.82
2	B	210	ALA	C-N-CA	5.46	125.17	119.82
1	A	246	GLY	CA-C-N	5.45	124.97	119.19
1	A	246	GLY	C-N-CA	5.45	124.97	119.19
2	B	445	THR	CA-C-N	5.41	125.95	120.38
2	B	445	THR	C-N-CA	5.41	125.95	120.38
1	A	287	HIS	CA-C-N	5.38	125.46	119.32
1	A	287	HIS	C-N-CA	5.38	125.46	119.32
2	B	60	ARG	N-CA-C	-5.34	106.35	112.92
2	B	339	ASP	CA-C-N	5.32	124.51	118.97
2	B	339	ASP	C-N-CA	5.32	124.51	118.97
1	A	161	LEU	N-CA-C	-5.27	100.59	109.07
2	B	535	ASN	CA-C-N	5.13	125.03	119.85
2	B	535	ASN	C-N-CA	5.13	125.03	119.85
2	B	596	LEU	CA-C-N	5.12	124.56	119.24
2	B	596	LEU	C-N-CA	5.12	124.56	119.24
2	B	158	LEU	N-CA-C	5.11	118.04	110.48
2	B	314	ALA	N-CA-C	5.10	117.95	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	751	HIS	CA-C-N	5.10	126.22	119.84
2	B	751	HIS	C-N-CA	5.10	126.22	119.84
1	A	245	PHE	N-CA-C	5.09	120.12	112.94
2	B	445	THR	CB-CA-C	5.08	116.00	110.15
2	B	739	GLY	N-CA-C	-5.04	107.31	115.08
2	B	121	ARG	N-CA-C	5.00	116.81	111.36

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	2123	427	2075	45	0
2	B	6127	1294	6180	164	1
3	A	1	0	0	0	0
4	A	80	160	0	3	0
4	B	252	504	0	18	2
All	All	8583	2385	8255	205	2

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 13.

All (205) 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)
2:B:286:LEU:HD21	2:B:323:GLU:HG3	1.42	1.00
2:B:239:MET:HE3	2:B:254:LEU:HD11	1.58	0.83
1:A:191:THR:HG23	2:B:484:ASP:OD2	1.86	0.74
2:B:80:ASN:H	2:B:80:ASN:HD22	1.35	0.74
2:B:282:ARG:NH1	2:B:290:GLU:HG2	2.02	0.74
1:A:242:GLN:OE1	1:A:247:PRO:HA	1.90	0.72
2:B:701:VAL:CG1	2:B:705:THR:HB	2.20	0.72
2:B:362:ARG:HH11	2:B:362:ARG:HG2	1.55	0.71
1:A:155:THR:HB	2:B:534:LEU:HD21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:ARG:HH11	2:B:602:ARG:HG3	1.57	0.70
2:B:733:GLY:O	2:B:736:LEU:HB2	1.91	0.70
1:A:195:ARG:NH1	4:A:427:HOH:O	2.24	0.69
2:B:445:THR:HG22	4:B:912:HOH:O	1.94	0.68
1:A:179:THR:OG1	1:A:220:GLU:HG3	1.94	0.67
2:B:751:HIS:HB3	2:B:754:ARG:O	1.95	0.66
2:B:146:LEU:N	4:B:826:HOH:O	2.29	0.66
2:B:255:GLU:OE2	2:B:375:ARG:HD2	1.96	0.66
2:B:281:GLU:HG2	2:B:310:PRO:HG2	1.78	0.66
2:B:563:ASP:O	2:B:565:PRO:HD3	1.96	0.66
2:B:425:ILE:HD11	2:B:442:TYR:CZ	2.32	0.65
1:A:250:LYS:HG3	1:A:270:TRP:CB	2.27	0.65
1:A:184:VAL:O	1:A:188:VAL:HG13	1.97	0.65
2:B:584:HIS:HD2	2:B:672:GLU:OE2	1.80	0.64
2:B:46:VAL:HA	4:B:826:HOH:O	1.96	0.64
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.79	0.64
2:B:713:LEU:HD22	2:B:772:LEU:HD13	1.80	0.63
2:B:212:HIS:HE1	2:B:394:GLU:OE2	1.81	0.63
2:B:121:ARG:HH11	2:B:121:ARG:HG3	1.64	0.61
2:B:80:ASN:HD22	2:B:80:ASN:N	1.98	0.61
1:A:183:GLN:HB2	1:A:222:LEU:HD22	1.84	0.60
2:B:144:THR:HB	4:B:1021:HOH:O	2.00	0.60
2:B:701:VAL:HG13	2:B:705:THR:HB	1.83	0.60
2:B:80:ASN:HD21	2:B:132:LEU:H	1.50	0.59
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.37	0.59
2:B:694:PHE:HD1	2:B:694:PHE:N	2.00	0.59
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.83	0.59
1:A:199:PRO:HB3	1:A:219:LEU:HD12	1.85	0.58
2:B:768:VAL:O	2:B:772:LEU:HB2	2.04	0.58
1:A:165:LEU:HD12	1:A:301:LEU:HD23	1.86	0.58
2:B:578:ARG:O	2:B:579:GLU:HB2	2.03	0.57
2:B:557:LYS:HE2	2:B:663:LEU:O	2.05	0.57
2:B:496:GLN:HG3	4:B:962:HOH:O	2.04	0.57
2:B:368:GLY:O	2:B:371:PRO:HD2	2.04	0.56
2:B:713:LEU:HD11	2:B:775:ARG:HG3	1.86	0.56
2:B:694:PHE:N	2:B:694:PHE:CD1	2.71	0.56
2:B:47:PHE:N	4:B:826:HOH:O	2.39	0.56
2:B:239:MET:CE	2:B:254:LEU:HD21	2.35	0.55
1:A:120:GLN:HE21	2:B:489:GLU:HG2	1.71	0.55
2:B:192:LYS:H	2:B:381:GLN:HE22	1.55	0.55
2:B:751:HIS:HB2	2:B:756:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LEU:HD11	1:A:303:LEU:HD11	1.89	0.55
1:A:115:ARG:HG2	4:A:421:HOH:O	2.07	0.54
2:B:210:ALA:N	2:B:211:PRO:HD3	2.22	0.54
2:B:353:ARG:C	2:B:353:ARG:HD3	2.33	0.54
1:A:250:LYS:HG3	1:A:270:TRP:HB3	1.89	0.54
2:B:255:GLU:HB2	4:B:915:HOH:O	2.06	0.54
2:B:772:LEU:HD23	2:B:779:LEU:HD11	1.88	0.54
2:B:90:ALA:HB2	2:B:118:LEU:HD11	1.90	0.54
2:B:467:GLN:HA	2:B:467:GLN:HE21	1.72	0.54
2:B:214:THR:HA	2:B:393:LEU:O	2.07	0.54
2:B:728:PHE:CZ	2:B:744:ALA:HB1	2.43	0.53
2:B:624:PHE:CE1	2:B:642:VAL:HG13	2.43	0.53
1:A:326:ARG:HB2	1:A:326:ARG:HH11	1.73	0.53
1:A:115:ARG:HG3	4:A:430:HOH:O	2.07	0.52
2:B:368:GLY:C	2:B:371:PRO:HD2	2.34	0.52
2:B:258:GLN:HE22	2:B:369:GLN:NE2	2.07	0.52
2:B:751:HIS:HB2	2:B:756:LEU:HD21	1.92	0.52
2:B:165:PRO:HB3	2:B:362:ARG:HB3	1.91	0.52
2:B:221:LEU:HD23	2:B:386:ALA:HB2	1.92	0.52
1:A:210:ALA:HA	1:A:331:ASP:OD1	2.10	0.51
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.45	0.51
2:B:496:GLN:HG2	4:B:961:HOH:O	2.09	0.51
2:B:512:THR:HB	2:B:572:GLU:OE2	2.10	0.51
2:B:602:ARG:HG3	2:B:602:ARG:NH1	2.23	0.51
2:B:407:ARG:HD3	2:B:456:GLU:OE2	2.09	0.51
2:B:282:ARG:HH12	2:B:290:GLU:HG2	1.75	0.51
2:B:261:HIS:HE1	4:B:801:HOH:O	1.93	0.51
2:B:344:ARG:O	2:B:348:ARG:HD3	2.11	0.51
2:B:362:ARG:HG2	2:B:362:ARG:NH1	2.22	0.51
2:B:298:LEU:HB3	2:B:314:ALA:HB3	1.92	0.51
2:B:737:PRO:O	2:B:740:HIS:HB2	2.11	0.50
2:B:224:ALA:H	2:B:244:ASN:HB2	1.76	0.50
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.93	0.50
2:B:580:ARG:HG2	2:B:580:ARG:HH11	1.76	0.50
2:B:564:ARG:HD2	2:B:564:ARG:N	2.27	0.50
1:A:87:ASP:HB3	1:A:90:LEU:HD22	1.94	0.50
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.47	0.50
2:B:141:PRO:HB2	2:B:144:THR:HG23	1.93	0.49
2:B:286:LEU:HD21	2:B:323:GLU:CG	2.29	0.49
2:B:121:ARG:HG3	2:B:121:ARG:NH1	2.28	0.49
2:B:283:LEU:HB2	2:B:293:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ARG:HH11	1:A:204:ARG:HG3	1.77	0.49
1:A:343:LEU:HD13	2:B:509:GLU:O	2.12	0.49
2:B:325:ARG:HB2	2:B:325:ARG:NH1	2.28	0.49
2:B:97:PRO:HG2	2:B:98:GLY:H	1.77	0.48
2:B:120:PRO:HG2	2:B:128:TYR:HD2	1.77	0.48
2:B:229:TRP:CH2	2:B:230:MET:HE3	2.48	0.48
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.96	0.48
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.97	0.48
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.47	0.48
2:B:350:HIS:CD2	4:B:1028:HOH:O	2.66	0.48
2:B:212:HIS:CE1	2:B:394:GLU:OE2	2.64	0.47
2:B:169:GLY:HA2	2:B:254:LEU:O	2.15	0.47
2:B:51:LEU:HD11	2:B:67:ASP:HB2	1.96	0.47
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.45	0.47
2:B:578:ARG:O	2:B:578:ARG:HG3	2.14	0.47
1:A:250:LYS:HG3	1:A:270:TRP:HB2	1.94	0.47
2:B:350:HIS:HD2	4:B:1028:HOH:O	1.98	0.47
2:B:551:GLY:O	2:B:555:VAL:HG13	2.14	0.47
2:B:669:HIS:HD2	4:B:991:HOH:O	1.97	0.47
2:B:590:PHE:CD1	2:B:591:GLY:N	2.83	0.47
2:B:596:LEU:HD23	2:B:596:LEU:HA	1.77	0.47
1:A:307:TYR:CD1	1:A:307:TYR:N	2.83	0.47
2:B:701:VAL:HG22	2:B:777:PHE:CE1	2.50	0.47
2:B:725:LEU:HD23	2:B:725:LEU:C	2.40	0.46
1:A:180:SER:N	1:A:181:PRO:HD2	2.30	0.46
1:A:109:GLU:O	1:A:113:ILE:HG13	2.15	0.46
1:A:121:ALA:HA	1:A:197:VAL:O	2.15	0.46
2:B:538:ALA:HB1	2:B:539:PRO:HD2	1.98	0.46
2:B:706:PRO:HG2	2:B:709:GLU:HB2	1.98	0.46
2:B:119:SER:O	2:B:120:PRO:C	2.59	0.46
2:B:762:GLU:O	2:B:765:VAL:HG22	2.16	0.46
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.30	0.45
2:B:713:LEU:CD1	2:B:775:ARG:HG3	2.46	0.45
2:B:297:ASP:OD2	2:B:350:HIS:CE1	2.69	0.45
1:A:137:LEU:O	1:A:139:ILE:HG13	2.16	0.45
2:B:598:TRP:CD1	2:B:598:TRP:H	2.30	0.45
2:B:2:ARG:O	2:B:4:PRO:HD3	2.17	0.45
2:B:669:HIS:CD2	4:B:991:HOH:O	2.68	0.45
2:B:757:ARG:HB2	2:B:760:GLU:HG3	1.99	0.45
2:B:128:TYR:CB	2:B:240:ARG:HD2	2.47	0.44
2:B:761:VAL:O	2:B:765:VAL:HG13	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.53	0.44
2:B:690:HIS:CE1	2:B:753:LYS:O	2.71	0.44
1:A:297:TYR:O	1:A:301:LEU:HD13	2.18	0.44
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.99	0.44
2:B:176:ASP:OD2	2:B:465:ARG:NH2	2.50	0.44
1:A:164:PRO:HD2	1:A:167:GLU:OE2	2.17	0.44
2:B:772:LEU:HD23	2:B:779:LEU:CD1	2.47	0.44
1:A:294:VAL:O	1:A:298:ARG:HG3	2.17	0.43
2:B:580:ARG:HG2	2:B:580:ARG:NH1	2.33	0.43
2:B:624:PHE:HE1	2:B:642:VAL:HG13	1.83	0.43
2:B:696:ASP:OD1	2:B:746:HIS:HD2	2.00	0.43
2:B:284:LYS:HA	2:B:290:GLU:HA	1.99	0.43
1:A:139:ILE:HD13	1:A:149:TRP:CZ3	2.53	0.43
2:B:144:THR:HA	2:B:145:PRO:HD3	1.77	0.43
2:B:39:PHE:CE2	2:B:232:ARG:HG3	2.54	0.43
2:B:563:ASP:C	2:B:565:PRO:HD3	2.44	0.43
1:A:203:PHE:CD1	1:A:203:PHE:N	2.87	0.43
1:A:287:HIS:CE1	1:A:289:LYS:HG3	2.53	0.43
2:B:489:GLU:O	2:B:490:ALA:C	2.61	0.43
2:B:779:LEU:HD12	2:B:779:LEU:HA	1.87	0.43
2:B:772:LEU:O	2:B:777:PHE:HB2	2.18	0.43
1:A:162:GLU:O	1:A:185:ARG:NH2	2.51	0.43
2:B:196:LEU:HD21	2:B:219:PHE:HZ	1.84	0.43
2:B:44:GLY:HA3	2:B:94:THR:OG1	2.18	0.43
2:B:610:LYS:HE2	2:B:614:GLU:OE2	2.18	0.43
2:B:731:TYR:O	2:B:742:SER:N	2.45	0.43
2:B:75:VAL:CG2	2:B:111:VAL:HG22	2.49	0.43
2:B:140:LEU:HD11	2:B:149:ALA:HB2	2.01	0.43
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.34	0.43
1:A:179:THR:C	1:A:181:PRO:HD2	2.44	0.42
1:A:298:ARG:NH1	1:A:304:PRO:O	2.51	0.42
2:B:56:ILE:HA	2:B:57:PRO:HD3	1.91	0.42
2:B:601:GLU:H	2:B:601:GLU:CD	2.27	0.42
2:B:699:VAL:HG12	2:B:701:VAL:HG23	2.02	0.42
2:B:405:PRO:HA	2:B:442:TYR:O	2.20	0.42
2:B:596:LEU:HA	2:B:597:PRO:HD3	1.89	0.42
1:A:258:PHE:HB2	1:A:261:VAL:CG2	2.50	0.42
2:B:75:VAL:HG23	2:B:111:VAL:HG22	2.01	0.42
2:B:359:ARG:HH11	2:B:359:ARG:HG3	1.84	0.42
2:B:554:ARG:HG2	2:B:554:ARG:HH11	1.85	0.42
1:A:152:PHE:CE1	1:A:205:PHE:HD2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.88	0.42
2:B:217:TYR:CE2	2:B:219:PHE:CD1	3.07	0.42
2:B:309:PHE:HA	2:B:310:PRO:HD3	1.92	0.42
2:B:578:ARG:O	2:B:579:GLU:CB	2.66	0.42
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.87	0.41
2:B:726:ALA:O	2:B:745:PHE:HA	2.20	0.41
2:B:178:HIS:O	2:B:430:ARG:NH1	2.51	0.41
2:B:92:PRO:HA	2:B:103:VAL:HG12	2.02	0.41
2:B:462:GLU:OE1	2:B:465:ARG:NH1	2.54	0.41
2:B:450:ARG:HD2	2:B:450:ARG:HA	1.79	0.41
2:B:722:LEU:HD21	2:B:725:LEU:HB2	2.03	0.41
2:B:748:ARG:NH2	4:B:980:HOH:O	2.54	0.41
2:B:128:TYR:CG	2:B:240:ARG:HD2	2.55	0.41
1:A:98:GLY:O	1:A:347:LYS:HE2	2.20	0.41
2:B:234:LEU:HD23	2:B:234:LEU:HA	1.85	0.41
1:A:143:HIS:HA	1:A:144:PRO:HD3	1.96	0.41
1:A:178:HIS:HA	1:A:202:VAL:HG11	2.03	0.41
2:B:46:VAL:CA	4:B:826:HOH:O	2.62	0.41
2:B:275:ARG:HG3	2:B:276:ARG:O	2.19	0.41
2:B:333:LEU:HD23	2:B:333:LEU:HA	1.89	0.41
2:B:399:LYS:HA	2:B:400:PRO:HD3	1.91	0.41
1:A:260:PHE:CD1	1:A:260:PHE:N	2.88	0.41
2:B:368:GLY:HA3	4:B:797:HOH:O	2.21	0.41
2:B:544:LEU:HB3	2:B:577:PHE:CD1	2.56	0.40
2:B:547:HIS:HE1	4:B:992:HOH:O	2.04	0.40
1:A:203:PHE:CD2	1:A:215:VAL:HG22	2.57	0.40
2:B:178:HIS:HD2	2:B:182:TYR:O	2.05	0.40
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.95	0.40
2:B:144:THR:C	4:B:1021:HOH:O	2.64	0.40
2:B:633:PHE:O	2:B:656:HIS:HB2	2.21	0.40
2:B:732:GLN:HB3	2:B:741:LYS:HA	2.03	0.40
2:B:588:LEU:HD23	2:B:588:LEU:C	2.46	0.40

All (2) 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:B:304:ARG:HH22	4:B:988:HOH:H1[3_565]	1.25	0.35
4:B:1025:HOH:H2	4:B:1025:HOH:H2[4_555]	1.34	0.26

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	264/350 (75%)	251 (95%)	13 (5%)	0	100	100
2	B	783/785 (100%)	750 (96%)	32 (4%)	1 (0%)	48	77
All	All	1047/1135 (92%)	1001 (96%)	45 (4%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	100	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	214/277 (77%)	189 (88%)	25 (12%)	5	17
2	B	630/630 (100%)	568 (90%)	62 (10%)	7	25
All	All	844/907 (93%)	757 (90%)	87 (10%)	7	23

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	LEU
1	A	95	LEU
1	A	105	LEU
1	A	115	ARG
1	A	129	SER

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Mol	Chain	Res	Type
1	A	144	PRO
1	A	169	VAL
1	A	178	HIS
1	A	179	THR
1	A	183	GLN
1	A	188	VAL
1	A	191	THR
1	A	197	VAL
1	A	198	VAL
1	A	201	ARG
1	A	207	GLN
1	A	219	LEU
1	A	230	MET
1	A	244	LEU
1	A	261	VAL
1	A	288	PRO
1	A	308	ARG
1	A	322	LEU
1	A	325	LEU
1	A	326	ARG
2	B	1	MET
2	B	32	THR
2	B	60	ARG
2	B	80	ASN
2	B	89	LEU
2	B	111	VAL
2	B	112	ARG
2	B	127	GLU
2	B	133	LEU
2	B	171	LEU
2	B	173	LEU
2	B	180	LEU
2	B	184	LEU
2	B	198	LEU
2	B	256	ARG
2	B	282	ARG
2	B	283	LEU
2	B	298	LEU
2	B	308	SER
2	B	323	GLU
2	B	333	LEU
2	B	334	GLU

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Mol	Chain	Res	Type
2	B	339	ASP
2	B	375	ARG
2	B	393	LEU
2	B	409	GLU
2	B	441	THR
2	B	445	THR
2	B	454	ARG
2	B	459	LEU
2	B	460	VAL
2	B	467	GLN
2	B	470	GLU
2	B	488	VAL
2	B	512	THR
2	B	519	GLU
2	B	526	LEU
2	B	532	LEU
2	B	548	LEU
2	B	555	VAL
2	B	562	LEU
2	B	576	VAL
2	B	578	ARG
2	B	588	LEU
2	B	590	PHE
2	B	600	LYS
2	B	609	LEU
2	B	638	VAL
2	B	661	GLN
2	B	670	LEU
2	B	679	ASP
2	B	694	PHE
2	B	695	ARG
2	B	700	VAL
2	B	701	VAL
2	B	716	GLU
2	B	748	ARG
2	B	763	GLU
2	B	767	ARG
2	B	772	LEU
2	B	775	ARG
2	B	779	LEU

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	120	GLN
1	A	142	HIS
1	A	183	GLN
1	A	190	HIS
1	A	218	GLN
2	B	54	HIS
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	212	HIS
2	B	231	GLN
2	B	258	GLN
2	B	261	HIS
2	B	381	GLN
2	B	424	GLN
2	B	467	GLN
2	B	485	ASN
2	B	584	HIS
2	B	661	GLN
2	B	669	HIS
2	B	690	HIS
2	B	746	HIS

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	265/350 (75%)	-0.64	1 (0%) 88 85	2, 12, 46, 70	0
2	B	779/785 (99%)	-0.47	11 (1%) 73 65	3, 18, 57, 93	0
All	All	1044/1135 (91%)	-0.51	12 (1%) 78 71	2, 17, 55, 93	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	767	ARG	6.2
2	B	773	ARG	4.1
2	B	774	ALA	2.9
1	A	273	GLU	2.8
2	B	661	GLN	2.7
2	B	735	PRO	2.4
2	B	736	LEU	2.2
2	B	757	ARG	2.1
2	B	100	GLY	2.1
2	B	779	LEU	2.1
2	B	101	GLN	2.0
2	B	737	PRO	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 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
3	MG	A	351	1/1	0.98	0.10	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.