



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:38 PM GMT

PDB ID : 1PYS  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

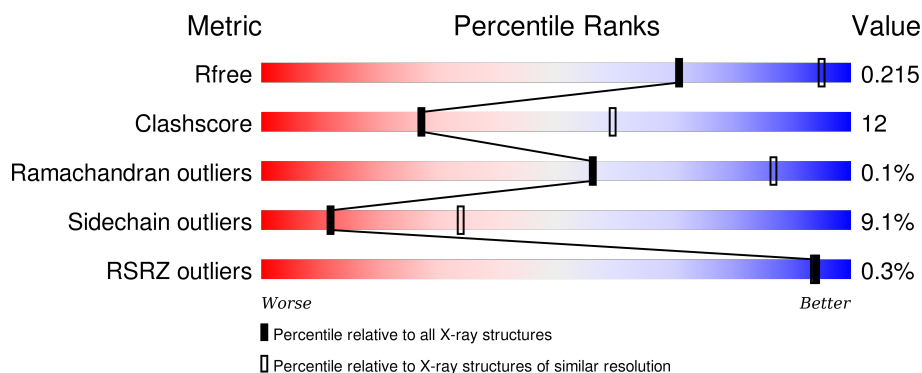
# 1 Overall quality at a glance

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))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	 55% 19% • 24%
2	B	785	 71% 26% •

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	MG	A	351	-	-	-	X

## 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 (three-letter code: MG) (formula: Mg).

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

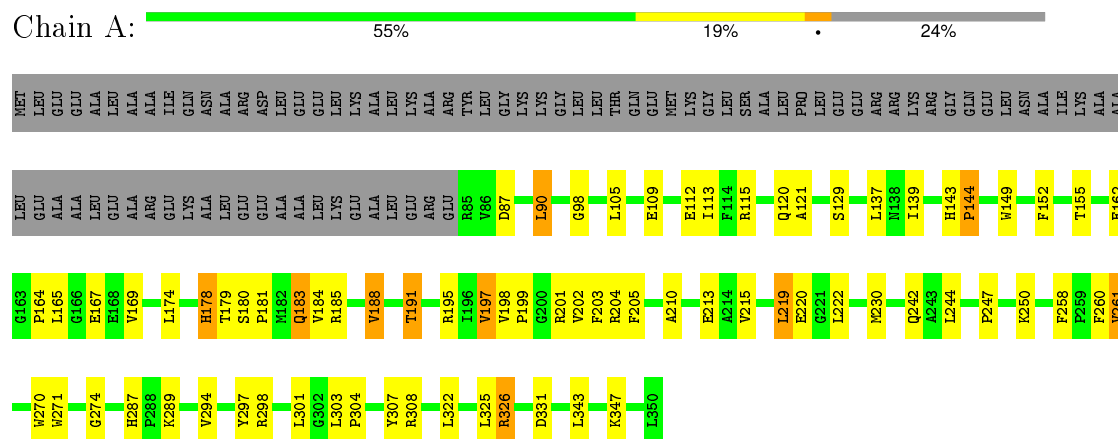
- Molecule 4 is water.

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		

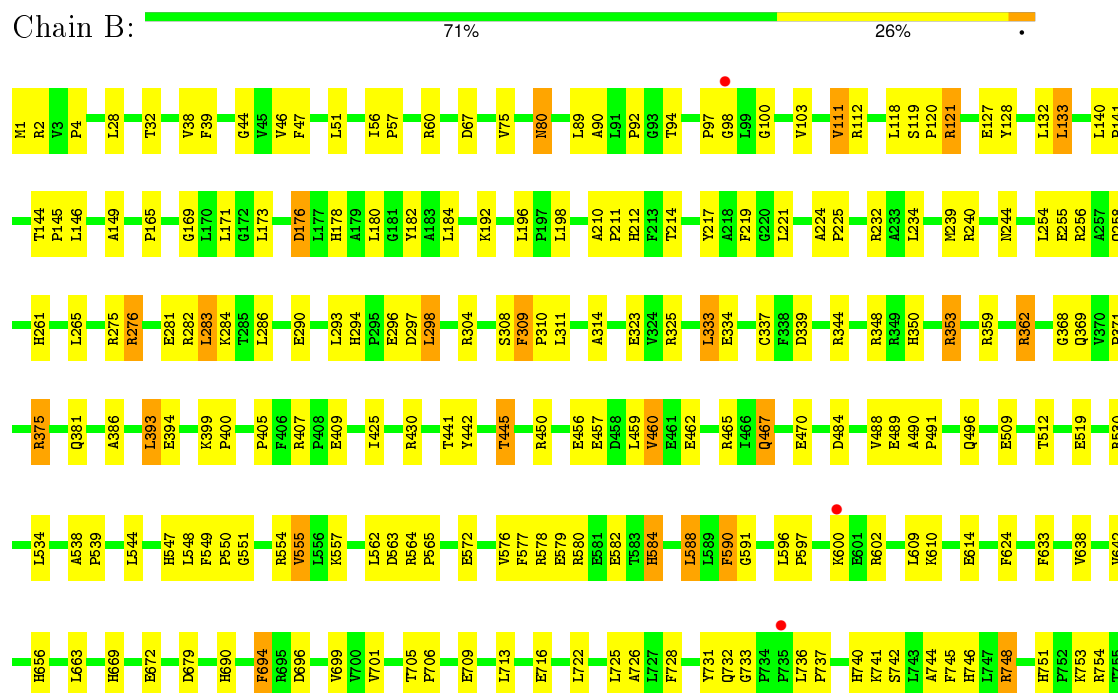
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



L756	R757		E760	V761	E762	E763	A764	V765	S766	R767	V768		L772		R775	G776	F777	G778	L779		P785
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.00Å 176.00Å 141.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.0 (10.00-2.90) 93.1 (19.99-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	5159 reflections (10.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 80.7	EDS
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 52260 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.59	1/2191 (0.0%)	0.78	0/2971
2	B	0.54	0/6280	0.77	3/8536 (0.0%)
All	All	0.55	1/8471 (0.0%)	0.77	3/11507 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	GLU	CG-CD	5.66	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	VAL	N-CA-C	7.67	131.72	111.00
2	B	133	LEU	CA-CB-CG	6.02	129.15	115.30
2	B	588	LEU	CA-CB-CG	5.78	128.59	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	2123	427	2075	44	0
2	B	6127	1294	6180	157	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	80	160	0	3	0
4	B	252	504	0	17	2
All	All	8583	2385	8255	197	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 12.

All (197) 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
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:HG2	2:B:362:ARG:HH11	1.55	0.71
1:A:155:THR:HB	2:B:534:LEU:HD21	1.70	0.71
2:B:602:ARG:HG3	2:B:602:ARG:HH11	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:281:GLU:HG2	2:B:310:PRO:HG2	1.78	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: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:HG3	2:B:121:ARG:HH11	1.64	0.61
2:B:80:ASN:N	2:B:80:ASN:HD22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	2:B:694:PHE:HD1	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:713:LEU:HD11	2:B:775:ARG:HG3	1.86	0.56
2:B:368:GLY:O	2:B:371:PRO:HD2	2.04	0.56
2:B:694:PHE:CD1	2:B:694:PHE:N	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:751:HIS:HB2	2:B:756:LEU:CD2	2.37	0.55
2:B:192:LYS:H	2:B:381:GLN:HE22	1.55	0.55
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:772:LEU:HD23	2:B:779:LEU:HD11	1.88	0.54
2:B:255:GLU:HB2	4:B:915:HOH:O	2.06	0.54
1:A:250:LYS:HG3	1:A:270:TRP:HB3	1.89	0.54
2:B:90:ALA:HB2	2:B:118:LEU:HD11	1.90	0.54
2:B:467:GLN:HE21	2:B:467:GLN:HA	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: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
2:B:602:ARG:NH1	2:B:602:ARG:HG3	2.23	0.51
2:B:496:GLN:HG2	4:B:961:HOH:O	2.09	0.51
1:A:210:ALA:HA	1:A:331:ASP:OD1	2.10	0.51
2:B:512:THR:HB	2:B:572:GLU:OE2	2.10	0.51
1:A:271:TRP:CE3	1:A:274:GLY:HA3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:362:ARG:NH1	2:B:362:ARG:HG2	2.22	0.51
2:B:344:ARG:O	2:B:348:ARG:HD3	2.11	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:580:ARG:HH11	2:B:580:ARG:HG2	1.76	0.50
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.93	0.50
2:B:564:ARG:N	2:B:564:ARG:HD2	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:353:ARG:C	2:B:353:ARG:HD3	2.33	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
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:120:PRO:HG2	2:B:128:TYR:HD2	1.77	0.48
2:B:97:PRO:HG2	2:B:98:GLY:H	1.77	0.48
2:B:582:GLU:OE2	2:B:584:HIS:HE1	1.97	0.48
2:B:28:LEU:HD13	2:B:176:ASP:HB3	1.96	0.48
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.47	0.48
2:B:368:GLY:C	2:B:371:PRO:HD2	2.34	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:578:ARG:O	2:B:578:ARG:HG3	2.14	0.47
2:B:224:ALA:HB1	2:B:225:PRO:CD	2.45	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
2:B:701:VAL:HG22	2:B:777:PHE:CE1	2.50	0.47
1:A:307:TYR:CD1	1:A:307:TYR:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:SER:N	1:A:181:PRO:HD2	2.30	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
1:A:109:GLU:O	1:A:113:ILE:HG13	2.15	0.46
2:B:706:PRO:HG2	2:B:709:GLU:HB2	1.98	0.46
2:B:762:GLU:O	2:B:765:VAL:HG22	2.16	0.46
1:A:204:ARG:NH1	1:A:204:ARG:HG3	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:669:HIS:CD2	4:B:991:HOH:O	2.68	0.45
2:B:2:ARG:O	2:B:4:PRO:HD3	2.17	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
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
2:B:214:THR:HG22	2:B:394:GLU:HG3	1.99	0.44
1:A:297:TYR:O	1:A:301:LEU:HD13	2.18	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
2:B:239:MET:CE	2:B:254:LEU:HD11	2.48	0.44
2:B:624:PHE:HE1	2:B:642:VAL:HG13	1.83	0.43
2:B:580:ARG:HG2	2:B:580:ARG:NH1	2.33	0.43
1:A:294:VAL:O	1:A:298:ARG:HG3	2.17	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:779:LEU:HA	2:B:779:LEU:HD12	1.87	0.43
1:A:287:HIS:CE1	1:A:289:LYS:HG3	2.53	0.43
1:A:203:PHE:CD1	1:A:203:PHE:N	2.87	0.43
2:B:772:LEU:O	2:B:777:PHE:HB2	2.18	0.43
2:B:196:LEU:HD21	2:B:219:PHE:HZ	1.84	0.43
1:A:162:GLU:O	1:A:185:ARG:NH2	2.51	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:44:GLY:HA3	2:B:94:THR:OG1	2.18	0.43
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
1:A:90:LEU:HA	1:A:90:LEU:HD12	1.88	0.42
2:B:725:LEU:C	2:B:725:LEU:HD23	2.40	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:217:TYR:CE2	2:B:219:PHE:CD1	3.07	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:119:SER:O	2:B:120:PRO:C	2.59	0.41
2:B:722:LEU:HD21	2:B:725:LEU:HB2	2.03	0.41
2:B:450:ARG:HA	2:B:450:ARG:HD2	1.79	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
2:B:234:LEU:HA	2:B:234:LEU:HD23	1.85	0.41
1:A:98:GLY:O	1:A:347:LYS:HE2	2.20	0.41
2:B:46:VAL:CA	4:B:826:HOH:O	2.62	0.41
2:B:333:LEU:HA	2:B:333:LEU:HD23	1.89	0.41
1:A:143:HIS:HA	1:A:144:PRO:HD3	1.96	0.41
2:B:399:LYS:HA	2:B:400:PRO:HD3	1.91	0.41
1:A:178:HIS:HA	1:A:202:VAL:HG11	2.03	0.41
2:B:275:ARG:HG3	2:B:276:ARG:O	2.19	0.41
2:B:368:GLY:HA3	4:B:797:HOH:O	2.21	0.41
1:A:260:PHE:CD1	1:A:260:PHE:N	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:LEU:HD23	2:B:265:LEU:HA	1.95	0.40
2:B:732:GLN:HB3	2:B:741:LYS:HA	2.03	0.40
2:B:633:PHE:O	2:B:656:HIS:HB2	2.21	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%)	56	87
All	All	1047/1135 (92%)	1001 (96%)	45 (4%)	1 (0%)	56	87

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%)	192 (90%)	22 (10%)	9	26
2	B	630/630 (100%)	575 (91%)	55 (9%)	13	36
All	All	844/907 (93%)	767 (91%)	77 (9%)	12	34

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

Mol	Chain	Res	Type
1	A	90	LEU
1	A	105	LEU
1	A	129	SER
1	A	144	PRO
1	A	169	VAL
1	A	174	LEU
1	A	178	HIS
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	213	GLU
1	A	219	LEU
1	A	230	MET
1	A	244	LEU
1	A	261	VAL
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	121	ARG
2	B	127	GLU
2	B	133	LEU
2	B	171	LEU
2	B	173	LEU

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Mol	Chain	Res	Type
2	B	176	ASP
2	B	180	LEU
2	B	184	LEU
2	B	256	ARG
2	B	276	ARG
2	B	283	LEU
2	B	298	LEU
2	B	308	SER
2	B	309	PHE
2	B	333	LEU
2	B	334	GLU
2	B	337	CYS
2	B	339	ASP
2	B	353	ARG
2	B	362	ARG
2	B	375	ARG
2	B	393	LEU
2	B	409	GLU
2	B	441	THR
2	B	445	THR
2	B	459	LEU
2	B	460	VAL
2	B	467	GLN
2	B	470	GLU
2	B	488	VAL
2	B	519	GLU
2	B	530	ARG
2	B	548	LEU
2	B	555	VAL
2	B	562	LEU
2	B	576	VAL
2	B	584	HIS
2	B	588	LEU
2	B	590	PHE
2	B	600	LYS
2	B	609	LEU
2	B	638	VAL
2	B	679	ASP
2	B	694	PHE
2	B	716	GLU
2	B	748	ARG
2	B	763	GLU

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Mol	Chain	Res	Type
2	B	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	183	GLN
1	A	218	GLN
2	B	80	ASN
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	467	GLN
2	B	584	HIS
2	B	669	HIS
2	B	690	HIS
2	B	746	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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, 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	265/350 (75%)	-0.88	0	100   100	2, 15, 57, 78	0
2	B	779/785 (99%)	-0.76	3 (0%)	93   92	3, 22, 68, 102	0
All	All	1044/1135 (91%)	-0.79	3 (0%)	94   94	2, 20, 66, 102	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	98	GLY	2.6
2	B	600	LYS	2.4
2	B	735	PRO	2.3

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	A	351	1/1	0.99	0.20	2.85	27,27,27,27	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.