Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 04:37 PM EDT

PDB ID	:	4P71
Title	:	Apo PheRS from P. aeuriginosa
Authors	:	Ferguson, A.D.
Deposited on	:	2014-03-25
Resolution	:	2.79 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:

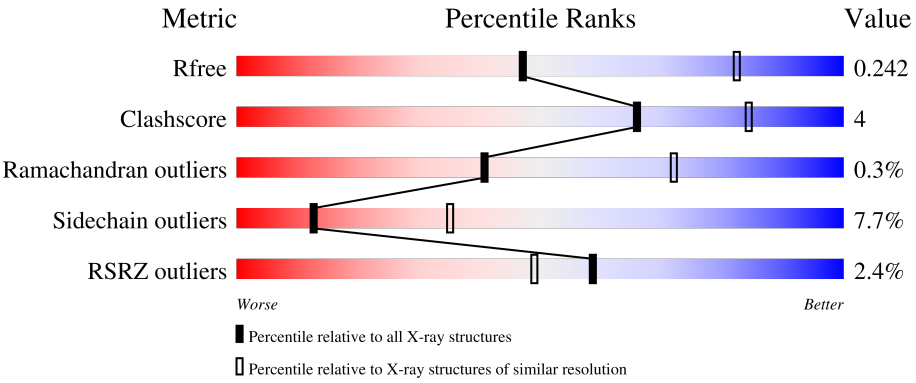
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	792	2% 84% 15%
1	B	792	3% 84% 14%
2	C	338	2% 61% 9% 29%
2	D	338	3% 61% 11% 28%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16150 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 Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			
1	B	791	Total	C	N	O	S	0	0	0
			6103	3854	1087	1141	21			

- Molecule 2 is a protein called Phenylalanine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	239	Total	C	N	O	S	0	0	0
			1923	1218	340	351	14			
2	D	243	Total	C	N	O	S	0	0	0
			1952	1238	344	355	15			

- Molecule 3 is water.

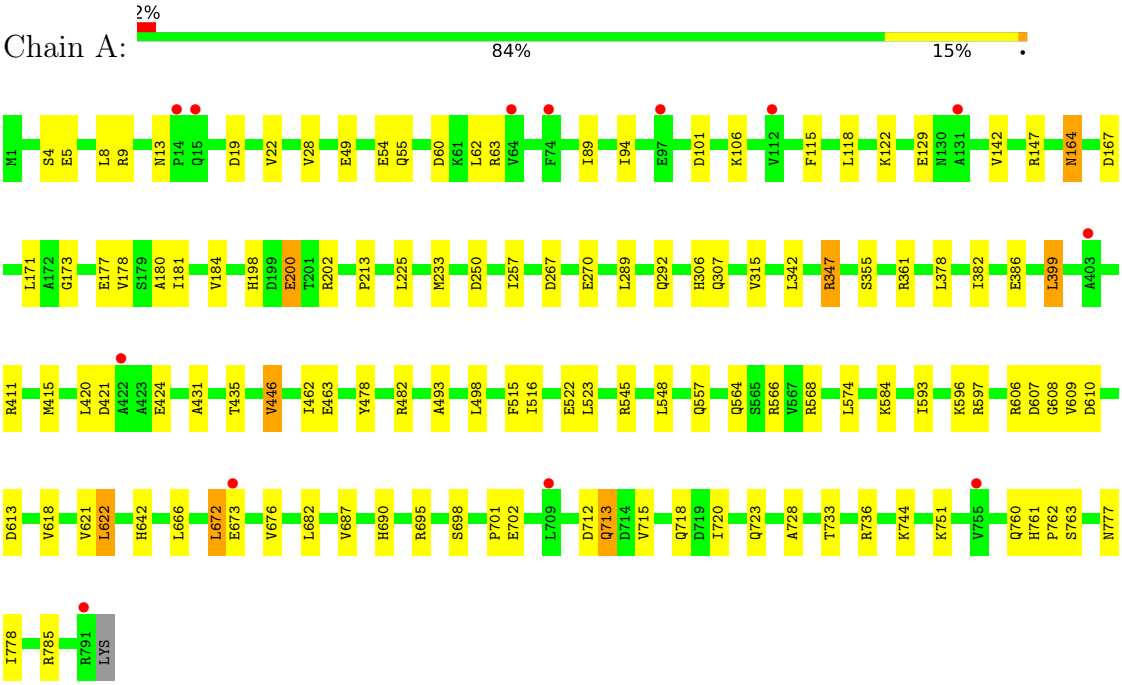
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	37	Total	O	0	0
			37	37		
3	C	5	Total	O	0	0
			5	5		
3	D	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

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.

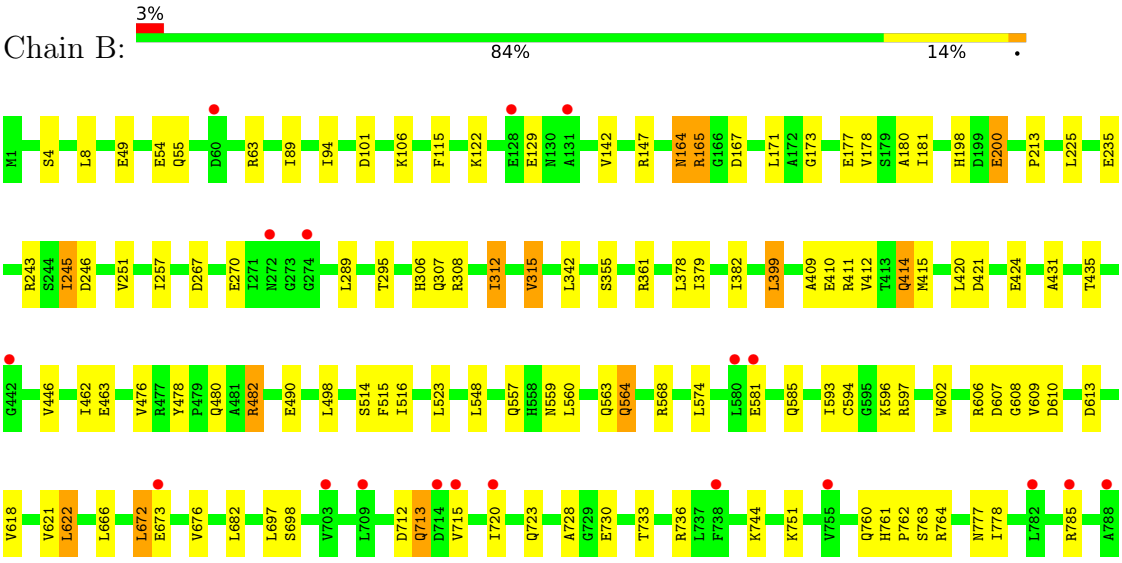
• Molecule 1: Phenylalanine–tRNA ligase beta subunit

Chain A:



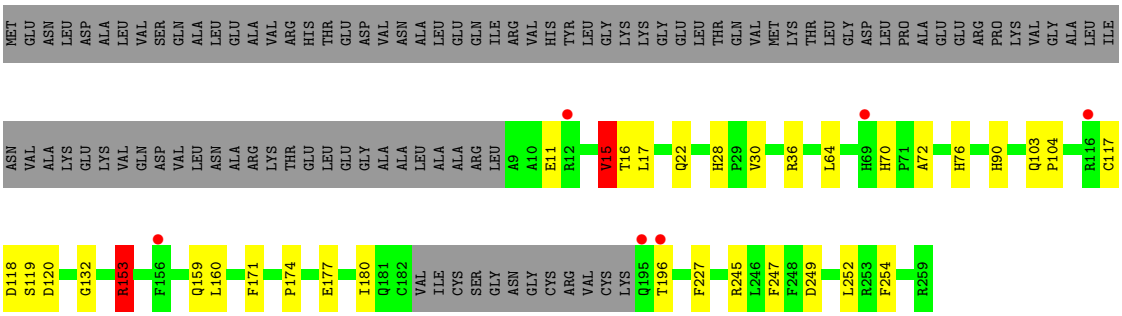
• Molecule 1: Phenylalanine–tRNA ligase beta subunit

Chain B:



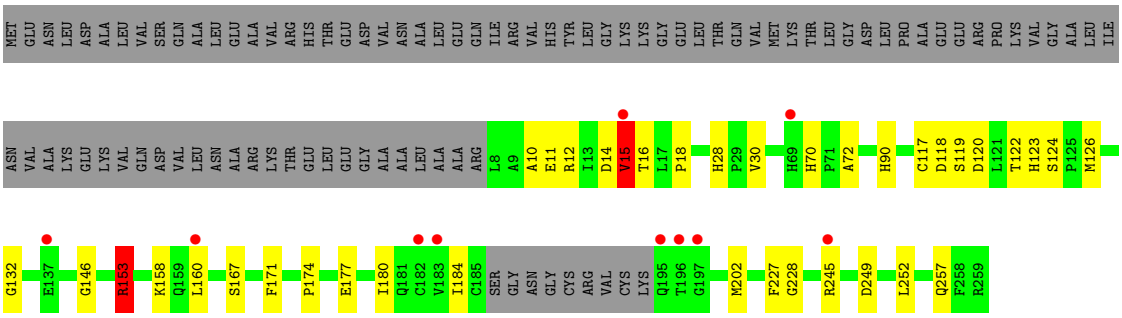
• Molecule 2: Phenylalanine–tRNA ligase alpha subunit

Chain C:



• Molecule 2: Phenylalanine–tRNA ligase alpha subunit

Chain D:



4 Data and refinement statistics (i)

Property	Value
Space group	C 1 2 1
Cell constants a, b, c, α, β, γ	112.78Å 219.08Å 107.13Å 90.00° 101.91° 90.00°
Resolution (Å)	39.00 – 2.79 37.02 – 2.79
% Data completeness (in resolution range)	99.0 (39.00-2.79) 99.0 (37.02-2.79)
R_{merge}	0.07
R_{sym}	(Not available)
$< I/\sigma(I) >$ [1]	1.71 (at 2.81Å)
Refinement program	BUSTER 2.11.5, ROVERSI, SHARFF, SMART, VONRHEIN, MATTH
R, R_{free}	0.191 , 0.227 0.203 , 0.242
R_{free} test set	3162 reflections (5.06%)
Wilson B-factor (Å^2)	51.4
Anisotropy	0.810
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 33.1
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$
Estimated twinning fraction	No twinning to report.
F_o,F_c correlation	0.94
Total number of atoms	16150
Average B, all atoms (Å^2)	64.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.46	0/6221	0.70	0/8450
1	B	0.46	0/6221	0.71	0/8450
2	C	0.49	0/1972	0.70	2/2664 (0.1%)
2	D	0.50	0/2001	0.73	3/2704 (0.1%)
All	All	0.47	0/16415	0.71	5/22268 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	15	VAL	C-N-CA	8.22	142.25	121.70
2	C	15	VAL	C-N-CA	6.43	137.78	121.70
2	D	153	ARG	CD-NE-CZ	5.76	131.67	123.60
2	D	14	ASP	C-N-CA	5.60	135.70	121.70
2	C	153	ARG	CD-NE-CZ	5.12	130.78	123.60

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	6103	0	6136	54	0
1	B	6103	0	6136	58	0
2	C	1923	0	1846	15	0
2	D	1952	0	1882	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	0	0	0
3	B	37	0	0	1	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
All	All	16150	0	16000	128	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 4.

All (128) 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:D:15:VAL:HG22	2:D:16:THR:H	1.25	1.01
2:C:15:VAL:HG12	2:C:16:THR:H	1.40	0.86
1:A:198:HIS:HD2	1:A:200:GLU:H	1.31	0.77
1:B:198:HIS:HD2	1:B:200:GLU:H	1.32	0.76
1:B:559:ASN:HD21	2:D:252:LEU:H	1.31	0.76
1:A:761:HIS:HD2	1:A:763:SER:H	1.34	0.75
1:B:312:ILE:HG12	1:B:315:VAL:HG13	1.69	0.75
1:B:761:HIS:HD2	1:B:763:SER:H	1.34	0.72
1:A:566:ARG:HH12	2:C:22:GLN:HE21	1.39	0.70
1:B:414:GLN:HG3	1:B:415:MET:N	2.08	0.68
2:D:15:VAL:CG2	2:D:16:THR:H	2.00	0.66
1:B:564:GLN:HE21	2:D:252:LEU:HB2	1.62	0.64
1:A:233:MET:CE	1:A:250:ASP:HB3	2.27	0.63
1:A:718:GLN:HB2	2:D:16:THR:HB	1.81	0.62
1:B:564:GLN:HG2	2:D:252:LEU:HD12	1.82	0.61
1:B:596:LYS:HA	1:B:608:GLY:HA2	1.84	0.59
1:B:463:GLU:HG2	2:D:174:PRO:HB3	1.83	0.59
1:A:596:LYS:HA	1:A:608:GLY:HA2	1.85	0.58
2:D:167:SER:HB2	2:D:177:GLU:HG3	1.86	0.58
1:A:493:ALA:O	1:A:687:VAL:HG12	2.05	0.56
1:A:482:ARG:HD3	1:B:478:TYR:O	2.04	0.56
1:B:164:ASN:HD22	1:B:164:ASN:H	1.54	0.56
1:B:559:ASN:ND2	2:D:252:LEU:H	2.01	0.56
1:A:5:GLU:HG2	1:A:9:ARG:HD2	1.88	0.56
2:D:132:GLY:HA3	2:D:227:PHE:CZ	2.41	0.56
1:A:564:GLN:HE21	2:C:252:LEU:HB2	1.71	0.55
1:A:28:VAL:HG21	1:A:181:ILE:CD1	2.36	0.55
1:B:514:SER:H	2:D:126:MET:CE	2.18	0.55
1:A:177:GLU:O	1:A:181:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:HIS:HE2	2:D:12:ARG:HH21	1.54	0.55
2:C:132:GLY:HA3	2:C:227:PHE:CZ	2.41	0.55
1:A:213:PRO:HB2	1:A:399:LEU:HD13	1.88	0.55
1:A:28:VAL:HG21	1:A:181:ILE:HD13	1.88	0.54
1:A:347:ARG:HD3	2:C:76:HIS:CE1	2.43	0.54
1:B:94:ILE:HD11	1:B:115:PHE:HA	1.88	0.54
1:B:213:PRO:HB2	1:B:399:LEU:HD13	1.90	0.54
1:A:13:ASN:O	1:A:184:VAL:HG21	2.08	0.54
2:C:70:HIS:HD2	2:C:72:ALA:H	1.55	0.54
1:A:94:ILE:HD11	1:A:115:PHE:HA	1.89	0.54
2:D:70:HIS:HD2	2:D:72:ALA:H	1.56	0.54
1:B:177:GLU:O	1:B:181:ILE:HG12	2.08	0.53
1:A:164:ASN:H	1:A:164:ASN:HD22	1.56	0.53
1:B:409:ALA:HA	1:B:412:VAL:HG13	1.92	0.52
1:B:49:GLU:HB2	1:B:142:VAL:HG11	1.92	0.52
1:A:8:LEU:HD21	1:A:178:VAL:HG21	1.90	0.51
1:A:233:MET:HE3	1:A:250:ASP:HB3	1.93	0.51
2:C:28:HIS:HD2	2:C:30:VAL:H	1.57	0.51
1:A:180:ALA:HA	1:A:431:ALA:HB1	1.93	0.50
1:A:478:TYR:O	1:B:482:ARG:HG3	2.12	0.50
1:B:557:GLN:HB3	1:B:672:LEU:HD11	1.92	0.50
2:D:28:HIS:HD2	2:D:30:VAL:H	1.57	0.50
1:B:514:SER:H	2:D:126:MET:HE1	1.75	0.50
1:A:593:ILE:HD12	1:A:609:VAL:HG21	1.93	0.50
1:B:8:LEU:HD21	1:B:178:VAL:HG21	1.93	0.49
1:A:701:PRO:HA	1:B:563:GLN:HE22	1.78	0.49
1:B:568:ARG:HA	1:B:593:ILE:HG22	1.95	0.49
1:A:695:ARG:H	2:D:257:GLN:HE22	1.60	0.48
2:D:15:VAL:HG22	2:D:16:THR:N	2.09	0.48
2:C:103:GLN:HG2	2:C:104:PRO:HD2	1.95	0.48
1:B:251:VAL:HG21	1:B:379:ILE:HG13	1.96	0.48
1:B:712:ASP:O	1:B:715:VAL:HG12	2.13	0.48
1:A:49:GLU:HB2	1:A:142:VAL:HG11	1.94	0.48
1:A:702:GLU:H	1:B:563:GLN:HE22	1.60	0.48
1:B:476:VAL:HG13	2:D:146:GLY:HA2	1.95	0.48
1:B:235:GLU:HG3	3:B:831:HOH:O	2.14	0.48
1:B:198:HIS:HD2	1:B:200:GLU:N	2.08	0.48
1:B:761:HIS:CD2	1:B:763:SER:H	2.24	0.48
1:A:712:ASP:O	1:A:715:VAL:HG12	2.13	0.47
1:B:180:ALA:HA	1:B:431:ALA:HB1	1.97	0.47
1:B:697:LEU:HD11	2:C:254:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ARG:HA	1:B:609:VAL:HG12	1.98	0.46
1:B:728:ALA:HA	1:B:778:ILE:HD11	1.97	0.46
1:A:415:MET:HG2	1:A:462:ILE:HG21	1.96	0.46
2:D:122:THR:HG23	2:D:123:HIS:CE1	2.50	0.46
1:A:728:ALA:HA	1:A:778:ILE:HD11	1.98	0.46
1:A:568:ARG:HA	1:A:593:ILE:HG22	1.97	0.46
1:A:435:THR:O	1:A:446:VAL:HA	2.16	0.46
1:A:557:GLN:HB3	1:A:672:LEU:HD11	1.96	0.46
1:A:89:ILE:HD13	1:A:118:LEU:HD22	1.98	0.45
1:B:198:HIS:CD2	1:B:200:GLU:HB2	2.52	0.45
1:B:435:THR:O	1:B:446:VAL:HA	2.16	0.45
1:B:167:ASP:O	1:B:173:GLY:HA3	2.16	0.45
2:C:153:ARG:HG2	2:C:159:GLN:HA	1.99	0.45
1:B:245:ILE:HG13	1:B:246:ASP:N	2.32	0.45
1:B:559:ASN:HD21	2:D:252:LEU:N	2.07	0.45
1:B:602:TRP:CD1	2:D:18:PRO:HD2	2.51	0.45
1:A:545:ARG:CZ	1:A:548:LEU:HD22	2.47	0.45
1:A:498:LEU:HD22	1:A:621:VAL:HG13	1.99	0.45
2:C:64:LEU:O	2:C:171:PHE:HB3	2.17	0.45
1:A:420:LEU:HD22	1:A:424:GLU:HG2	1.99	0.44
1:B:490:GLU:HG3	2:C:36:ARG:HD2	2.00	0.44
1:B:597:ARG:HA	1:B:609:VAL:CG1	2.47	0.44
1:B:698:SER:HB2	1:B:762:PRO:HA	1.99	0.44
1:A:202:ARG:HD3	1:A:202:ARG:HA	1.84	0.44
1:B:378:LEU:O	1:B:382:ILE:HG12	2.18	0.43
1:B:415:MET:HG2	1:B:462:ILE:HG21	2.00	0.43
1:A:19:ASP:HA	1:A:22:VAL:HG22	1.99	0.43
1:A:698:SER:HB2	1:A:762:PRO:HA	2.00	0.43
1:A:715:VAL:HG13	1:A:720:ILE:HD11	2.00	0.43
1:B:594:CYS:HB3	1:B:676:VAL:HG22	2.00	0.43
1:B:574:LEU:HD13	1:B:585:GLN:HB3	2.01	0.43
2:D:153:ARG:HG3	2:D:158:LYS:O	2.18	0.43
1:A:167:ASP:O	1:A:173:GLY:HA3	2.18	0.43
2:C:15:VAL:HB	2:C:17:LEU:HG	2.00	0.43
1:B:498:LEU:HD22	1:B:621:VAL:HG13	2.00	0.43
1:A:198:HIS:CD2	1:A:200:GLU:HB2	2.53	0.42
1:A:378:LEU:O	1:A:382:ILE:HG12	2.19	0.42
1:B:165:ARG:HA	1:B:165:ARG:HD2	1.89	0.42
1:A:233:MET:HE3	1:A:250:ASP:C	2.40	0.42
1:A:267:ASP:HB3	1:A:270:GLU:HG2	2.00	0.42
1:B:267:ASP:HB3	1:B:270:GLU:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:SER:HA	2:D:245:ARG:HH22	1.83	0.42
1:B:733:THR:HG21	1:B:760:GLN:HB3	2.02	0.42
1:A:463:GLU:HG2	2:C:174:PRO:HB3	2.01	0.42
1:A:713:GLN:HA	1:A:751:LYS:HG2	2.02	0.42
1:A:761:HIS:CD2	1:A:763:SER:H	2.24	0.42
2:C:28:HIS:HE1	2:C:247:PHE:O	2.02	0.42
1:B:514:SER:N	2:D:126:MET:HE1	2.35	0.41
1:A:89:ILE:CD1	1:A:118:LEU:HD22	2.50	0.41
1:B:618:VAL:HG12	1:B:622:LEU:HD22	2.03	0.41
1:A:597:ARG:HD3	1:A:613:ASP:OD2	2.21	0.41
1:B:715:VAL:HG13	1:B:720:ILE:HD11	2.02	0.41
1:A:618:VAL:HG12	1:A:622:LEU:HD22	2.03	0.41
1:A:733:THR:HG21	1:A:760:GLN:HB3	2.02	0.41
1:B:420:LEU:HD22	1:B:424:GLU:HG2	2.02	0.41
1:B:597:ARG:HD3	1:B:613:ASP:OD2	2.20	0.41
1:B:713:GLN:HA	1:B:751:LYS:HG2	2.03	0.41
2:D:202:MET:HB2	2:D:228:GLY:O	2.21	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	789/792 (100%)	768 (97%)	21 (3%)	0	100 100
1	B	789/792 (100%)	766 (97%)	23 (3%)	0	100 100
2	C	235/338 (70%)	224 (95%)	9 (4%)	2 (1%)	17 46
2	D	239/338 (71%)	223 (93%)	12 (5%)	4 (2%)	9 29
All	All	2052/2260 (91%)	1981 (96%)	65 (3%)	6 (0%)	41 72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	15	VAL
2	C	118	ASP
2	D	118	ASP
2	D	10	ALA
2	D	120	ASP
2	C	120	ASP

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	645/646 (100%)	593 (92%)	52 (8%)	11 33
1	B	645/646 (100%)	587 (91%)	58 (9%)	9 28
2	C	207/287 (72%)	195 (94%)	12 (6%)	20 50
2	D	211/287 (74%)	201 (95%)	10 (5%)	26 59
All	All	1708/1866 (92%)	1576 (92%)	132 (8%)	13 35

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	54	GLU
1	A	55	GLN
1	A	60	ASP
1	A	62	LEU
1	A	63	ARG
1	A	101	ASP
1	A	106	LYS
1	A	122	LYS
1	A	129	GLU
1	A	147	ARG
1	A	164	ASN
1	A	171	LEU
1	A	200	GLU
1	A	225	LEU
1	A	257	ILE

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Mol	Chain	Res	Type
1	A	289	LEU
1	A	292	GLN
1	A	306	HIS
1	A	307	GLN
1	A	315	VAL
1	A	342	LEU
1	A	347	ARG
1	A	355	SER
1	A	361	ARG
1	A	386	GLU
1	A	399	LEU
1	A	411	ARG
1	A	421	ASP
1	A	446	VAL
1	A	515	PHE
1	A	516	ILE
1	A	522	GLU
1	A	523	LEU
1	A	574	LEU
1	A	584	LYS
1	A	606	ARG
1	A	607	ASP
1	A	610	ASP
1	A	622	LEU
1	A	666	LEU
1	A	672	LEU
1	A	673	GLU
1	A	676	VAL
1	A	682	LEU
1	A	690	HIS
1	A	713	GLN
1	A	723	GLN
1	A	736	ARG
1	A	744	LYS
1	A	777	ASN
1	A	785	ARG
1	B	4	SER
1	B	54	GLU
1	B	55	GLN
1	B	63	ARG
1	B	89	ILE
1	B	101	ASP

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Mol	Chain	Res	Type
1	B	106	LYS
1	B	122	LYS
1	B	129	GLU
1	B	147	ARG
1	B	164	ASN
1	B	165	ARG
1	B	171	LEU
1	B	200	GLU
1	B	225	LEU
1	B	243	ARG
1	B	245	ILE
1	B	257	ILE
1	B	289	LEU
1	B	295	THR
1	B	306	HIS
1	B	307	GLN
1	B	308	ARG
1	B	312	ILE
1	B	315	VAL
1	B	342	LEU
1	B	355	SER
1	B	361	ARG
1	B	399	LEU
1	B	410	GLU
1	B	411	ARG
1	B	414	GLN
1	B	421	ASP
1	B	480	GLN
1	B	482	ARG
1	B	515	PHE
1	B	516	ILE
1	B	523	LEU
1	B	548	LEU
1	B	560	LEU
1	B	564	GLN
1	B	581	GLU
1	B	606	ARG
1	B	607	ASP
1	B	610	ASP
1	B	622	LEU
1	B	666	LEU
1	B	672	LEU

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Mol	Chain	Res	Type
1	B	673	GLU
1	B	682	LEU
1	B	713	GLN
1	B	723	GLN
1	B	730	GLU
1	B	736	ARG
1	B	744	LYS
1	B	764	ARG
1	B	777	ASN
1	B	785	ARG
2	C	11	GLU
2	C	15	VAL
2	C	90	HIS
2	C	117	CYS
2	C	119	SER
2	C	153	ARG
2	C	160	LEU
2	C	177	GLU
2	C	180	ILE
2	C	196	THR
2	C	245	ARG
2	C	249	ASP
2	D	11	GLU
2	D	90	HIS
2	D	117	CYS
2	D	119	SER
2	D	153	ARG
2	D	160	LEU
2	D	171	PHE
2	D	180	ILE
2	D	184	ILE
2	D	249	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	164	ASN
1	A	198	HIS
1	A	564	GLN
1	A	723	GLN
1	A	742	HIS

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Mol	Chain	Res	Type
1	A	761	HIS
1	B	164	ASN
1	B	198	HIS
1	B	508	GLN
1	B	557	GLN
1	B	558	HIS
1	B	559	ASN
1	B	563	GLN
1	B	564	GLN
1	B	645	GLN
1	B	723	GLN
1	B	742	HIS
1	B	761	HIS
2	C	22	GLN
2	C	28	HIS
2	C	70	HIS
2	C	129	GLN
2	D	28	HIS
2	D	70	HIS
2	D	129	GLN
2	D	181	GLN
2	D	257	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 monosaccharides 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

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^{th} 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	791/792 (99%)	0.01	13 (1%)	72	66	38, 61, 92, 119	0
1	B	791/792 (99%)	-0.04	21 (2%)	54	44	41, 61, 94, 119	0
2	C	239/338 (70%)	0.14	6 (2%)	57	47	45, 61, 89, 109	0
2	D	243/338 (71%)	0.20	10 (4%)	37	27	41, 60, 97, 134	0
All	All	2064/2260 (91%)	0.03	50 (2%)	59	49	38, 61, 94, 134	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	183	VAL	8.3
2	D	197	GLY	5.0
1	B	709	LEU	4.7
2	C	196	THR	4.7
2	D	195	GLN	4.5
2	C	116	ARG	3.6
2	D	196	THR	3.6
2	D	182	CYS	3.4
1	A	709	LEU	3.2
1	B	782	LEU	3.2
2	C	12	ARG	3.2
2	C	195	GLN	3.1
1	A	64	VAL	3.1
1	B	791	ARG	2.9
2	C	69	HIS	2.8
2	D	137	GLU	2.8
1	A	14	PRO	2.7
1	A	403	ALA	2.7
1	B	755	VAL	2.7
1	B	785	ARG	2.7
1	A	791	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	581	GLU	2.6
1	A	422	ALA	2.5
1	B	673	GLU	2.5
1	B	703	VAL	2.4
1	A	112	VAL	2.4
1	B	788	ALA	2.4
1	A	673	GLU	2.3
2	D	245	ARG	2.3
1	B	442	GLY	2.3
1	A	97	GLU	2.3
1	A	755	VAL	2.3
2	D	15	VAL	2.3
1	B	720	ILE	2.3
2	D	69	HIS	2.2
2	C	156	PHE	2.2
1	B	580	LEU	2.2
1	B	790	LEU	2.2
1	A	74	PHE	2.2
1	A	15	GLN	2.1
1	B	738	PHE	2.1
1	A	131	ALA	2.1
1	B	131	ALA	2.1
1	B	715	VAL	2.1
1	B	714	ASP	2.1
1	B	60	ASP	2.0
2	D	160	LEU	2.0
1	B	128	GLU	2.0
1	B	272	ASN	2.0
1	B	274	GLY	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 monosaccharides 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.