Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:33 PM GMT

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PDB ID	:	4P72
Title	:	PheRS in complex with compound 2a
Authors	:	Ferguson, A.D.
Deposited on	:	2014-03-25
Resolution	:	2.62 Å(reported)

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 2.62 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.
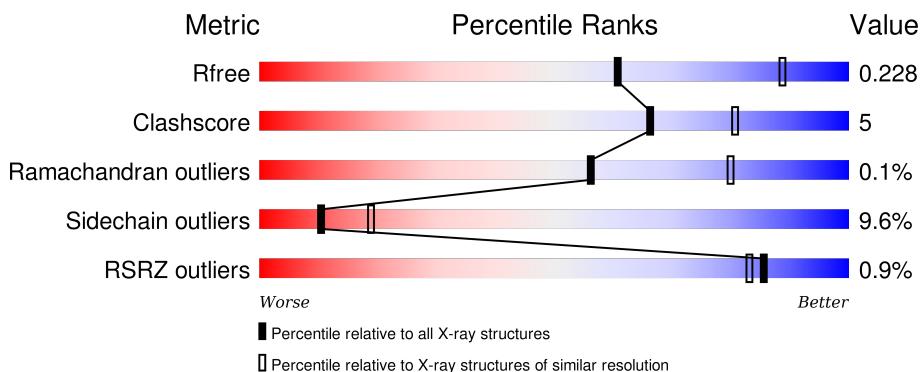
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 >=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 <=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	82% 16% •
1	B	792	83% 15% •
2	C	338	59% 9% • 30%
2	D	338	60% 10% • 28%

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	2NL	C	301	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16183 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	235	Total	C	N	O	S	0	0	0
			1897	1203	335	345	14			
2	D	244	Total	C	N	O	S	0	0	0
			1954	1238	345	356	15			

- Molecule 3 is 2-{3-[(4-chloropyridin-2-yl)amino]phenoxy}-N-methylacetamide (three-letter code: 2NL) (formula: $C_{14}H_{14}ClN_3O_2$).
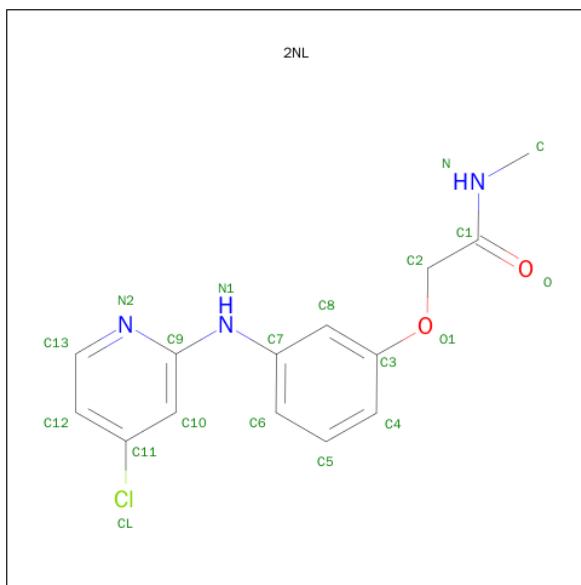
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	Cl	N	O	0	0
			20	14	1	3	2		
3	D	1	Total	C	Cl	N	O	0	0
			20	14	1	3	2		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	43	Total	O	0	0
			43	43		
4	C	6	Total	O	0	0
			6	6		
4	D	4	Total	O	0	0
			4	4		

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: Phenylalanine–tRNA ligase beta subunit
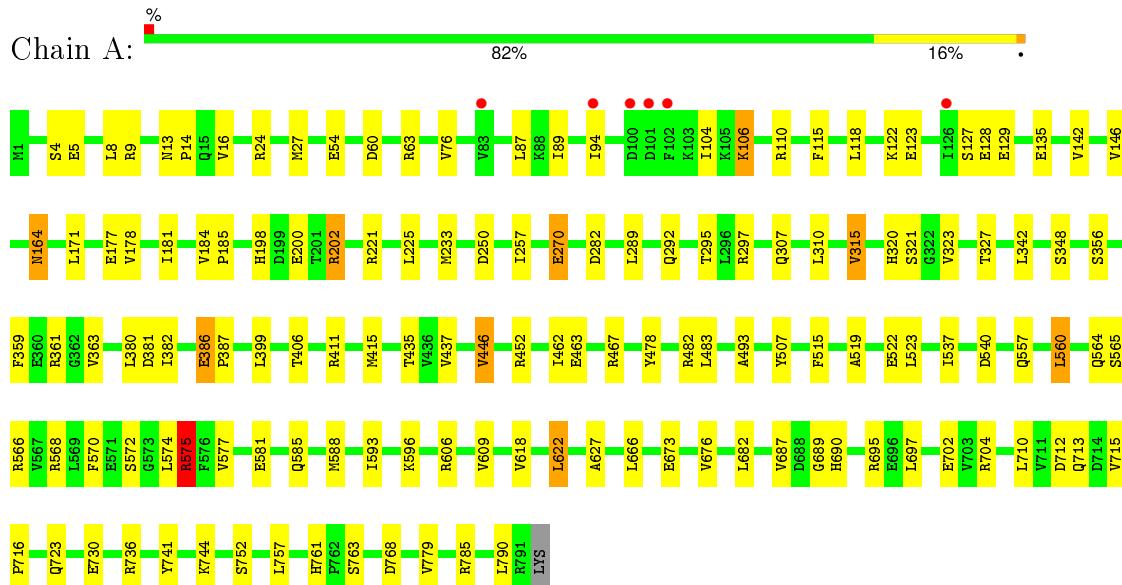
• Molecule 1: Phenylalanine–tRNA ligase beta subunit

• Molecule 2: Phenylalanine–tRNA ligase alpha subunit

Chain C:

59%	9%	•	30%

MET GLU ASN LEU ASP ALA LEU VAL SER GLN ALA LEU GLU ALA VAL ARG HIS THR GLU ASP VAL ALA ASN ALA LEU GLU GLN ILE ARG VAL HIS TYR LEU LEU GLY LYS GLY LEU GLU THR GLN MET LYS THR GLY ASP PRO ALA GLU ARG PRO LYS VAL GLY ALA LEU ILE

ASN VAL ALA LYS GLU LYS VAL GLN ASP VAL LEU ASN ALA ARG LYS THR GLU LEU GLY GLY ALA ALA LEU ALA ARG LEU ALA ALA **E11** **V15** **T16** **Q22** **H28** **P29** **V30** **L64** **H70** **P71** **A72** **N84** **H90** **T91** **S92** **P93** **V94** **Q95** **Q103** **V109** **C117**

D118 **S119** **D120** **L121** **T122** **G132** **R153** **Q159** **L160** **R163** **F171** **D179** **C182** VAL ILE CYS SER GLY ASN GLY CYS ARG VAL CYS LYS GLN THR **G197** **W198** **L199** **M206** **F227** **G228** **R233** **L234** **L252** **R253** **F254** **R259**

• Molecule 2: Phenylalanine–tRNA ligase alpha subunit

%

Chain D:

60%	10%	•	28%

MET GLU ASN LEU ASP ALA LEU VAL SER GLN ALA LEU GLU ALA VAL ARG HIS THR GLU ASP VAL ALA ASN ALA LEU GLU GLN ILE ARG VAL HIS TYR LEU LEU GLY LYS GLY LEU GLU THR GLN MET LYS THR GLY ASP PRO ALA GLU ARG PRO LYS VAL GLY ALA LEU ILE

ASN VAL ALA LYS GLU LYS VAL GLN ASP VAL LEU ASN ALA ARG LYS THR GLU LEU GLU GLY ALA ALA LEU ALA ALA ARG **L8** **V15** **P18** **G19** **R20** **H28** **P29** **V30** **I44** **D57** **L64** **H69** **H70** **P71** **A72** **N84** **H90** **T91** **S92** **P93** **V94** **Q95** **Q103**

V109 **C117** **D118** **S119** **D120** **L121** **T122** **M126** **G132** **K145** **G146** **E150** **R153** **K158** **Q159** **L160** **R163** **S167** **P174** **E177** **V178** **D179** **I184** **N188** GLY CYS ARG VAL CYS LYS GLN THR **G197** **W198** **L199** **F227** **L234** **L252** **Q257** **F258** **R259**

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.30Å 218.83Å 107.63Å 90.00° 101.94° 90.00°	Depositor
Resolution (Å)	75.87 – 2.62 60.93 – 2.62	Depositor EDS
% Data completeness (in resolution range)	99.1 (75.87-2.62) 99.7 (60.93-2.62)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.61Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.184 , 0.221 0.190 , 0.228	Depositor DCC
R_{free} test set	3822 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	48.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 76026 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16183	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 2NL

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	0.51	0/6221	0.75	1/8450 (0.0%)
1	B	0.50	0/6221	0.75	1/8450 (0.0%)
2	C	0.53	0/1946	0.78	1/2628 (0.0%)
2	D	0.55	0/2003	0.76	3/2706 (0.1%)
All	All	0.51	0/16391	0.76	6/22234 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	118	ASP	C-N-CA	8.29	142.44	121.70
1	B	575	ARG	CB-CA-C	-7.50	95.40	110.40
2	D	153	ARG	CD-NE-CZ	6.46	132.65	123.60
1	A	575	ARG	N-CA-CB	5.67	120.80	110.60
2	D	153	ARG	CG-CD-NE	-5.48	100.29	111.80
2	D	103	GLN	CB-CG-CD	5.07	124.78	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	386	GLU	Sidechain

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	64	0
1	B	6103	0	6136	69	0
2	C	1897	0	1821	25	0
2	D	1954	0	1881	28	0
3	C	20	0	14	3	0
3	D	20	0	14	2	0
4	A	33	0	0	0	0
4	B	43	0	0	0	0
4	C	6	0	0	0	0
4	D	4	0	0	0	0
All	All	16183	0	16002	158	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 5.

All (158) 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:C:228:GLY:HA3	3:C:301:2NL:H1	1.45	0.97
1:A:566:ARG:HH12	2:C:22:GLN:HE22	1.09	0.93
1:B:559:ASN:HD21	2:D:252:LEU:H	1.23	0.85
1:B:312:ILE:HG12	1:B:315:VAL:HG13	1.59	0.84
1:B:761:HIS:HD2	1:B:763:SER:H	1.28	0.81
1:A:761:HIS:HD2	1:A:763:SER:H	1.27	0.81
1:A:566:ARG:HH12	2:C:22:GLN:NE2	1.79	0.80
1:A:198:HIS:HD2	1:A:200:GLU:H	1.26	0.80
1:B:463:GLU:HG2	2:D:174:PRO:HB3	1.64	0.78
1:B:198:HIS:HD2	1:B:200:GLU:H	1.29	0.77
1:B:564:GLN:HG2	2:D:252:LEU:HD12	1.68	0.75
1:A:483:LEU:HB3	2:D:44:ILE:CG1	2.17	0.74
1:A:695:ARG:H	2:D:257:GLN:HE22	1.34	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:VAL:HG11	1:A:790:LEU:HD21	1.71	0.70
1:A:94:ILE:O	1:A:104:ILE:O	2.12	0.68
1:B:564:GLN:HE21	2:D:252:LEU:HB2	1.57	0.68
2:D:28:HIS:HD2	2:D:30:VAL:H	1.42	0.67
1:A:483:LEU:HB3	2:D:44:ILE:HG13	1.76	0.67
1:B:615:LYS:NZ	2:C:16:THR:HG22	2.09	0.67
2:C:70:HIS:HD2	2:C:72:ALA:H	1.41	0.66
1:B:514:SER:H	2:D:126:MET:CE	2.09	0.66
1:B:514:SER:H	2:D:126:MET:HE1	1.61	0.65
2:C:28:HIS:HD2	2:C:30:VAL:H	1.43	0.65
2:D:70:HIS:HD2	2:D:72:ALA:H	1.43	0.65
2:D:167:SER:HB2	2:D:177:GLU:HG3	1.79	0.65
1:B:703:VAL:HG11	1:B:771:VAL:HG21	1.77	0.65
1:A:564:GLN:HE21	2:C:252:LEU:HB2	1.63	0.64
1:A:359:PHE:CE1	1:A:363:VAL:HG21	2.33	0.62
1:A:359:PHE:CD1	1:A:363:VAL:HG21	2.35	0.61
1:B:559:ASN:ND2	2:D:252:LEU:H	1.98	0.60
1:B:615:LYS:HZ1	2:C:16:THR:HG22	1.66	0.59
1:A:779:VAL:CG1	1:A:790:LEU:HD21	2.33	0.58
1:B:557:GLN:HE21	1:B:672:LEU:HD12	1.68	0.57
3:D:301:2NL:N2	3:D:301:2NL:H8	2.19	0.57
1:B:409:ALA:HA	1:B:412:VAL:HG13	1.87	0.56
1:A:200:GLU:OE1	1:A:221:ARG:HD3	2.05	0.56
1:B:310:LEU:HD22	1:B:321:SER:HB3	1.87	0.56
1:A:106:LYS:HE3	1:A:115:PHE:CE1	2.41	0.56
1:B:164:ASN:H	1:B:164:ASN:HD22	1.53	0.56
2:C:233:ARG:HH11	2:C:233:ARG:HG3	1.71	0.55
1:A:323:VAL:HG22	1:A:327:THR:HG21	1.88	0.55
1:B:312:ILE:HG12	1:B:315:VAL:CG1	2.34	0.55
1:B:251:VAL:HG21	1:B:379:ILE:HG13	1.89	0.55
1:B:597:ARG:HA	1:B:609:VAL:CG1	2.36	0.55
1:A:702:GLU:H	1:B:563:GLN:HE22	1.54	0.54
1:A:310:LEU:HD22	1:A:321:SER:HB3	1.88	0.54
1:B:414:GLN:HG3	1:B:415:MET:N	2.22	0.54
2:C:132:GLY:HA3	2:C:227:PHE:CZ	2.42	0.54
1:B:713:GLN:HB2	1:B:742:HIS:HE1	1.73	0.54
1:A:493:ALA:O	1:A:687:VAL:HG12	2.09	0.53
3:C:301:2NL:H8	3:C:301:2NL:N2	2.23	0.53
1:B:581:GLU:H	1:B:581:GLU:CD	2.11	0.53
1:A:177:GLU:OE2	1:A:467:ARG:NH1	2.41	0.53
2:D:132:GLY:HA3	2:D:227:PHE:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD21	1:B:178:VAL:HG21	1.90	0.53
1:A:741:TYR:HB3	1:A:752:SER:HB3	1.91	0.52
1:A:482:ARG:HD2	1:B:478:TYR:O	2.09	0.52
1:B:697:LEU:HD11	2:C:254:PHE:HB2	1.92	0.52
1:B:741:TYR:HB3	1:B:752:SER:HB3	1.91	0.52
1:A:164:ASN:H	1:A:164:ASN:HD22	1.56	0.52
2:C:199:LEU:HD23	2:C:233:ARG:HH22	1.74	0.52
1:A:8:LEU:HD21	1:A:178:VAL:HG21	1.91	0.51
1:A:233:MET:CE	1:A:250:ASP:HB3	2.40	0.51
2:D:163:ARG:HB3	2:D:179:ASP:HB2	1.93	0.51
1:B:476:VAL:HG13	2:D:146:GLY:HA2	1.91	0.51
1:A:89:ILE:HD13	1:A:118:LEU:HD22	1.92	0.51
1:A:87:LEU:HD21	1:A:135:GLU:HG2	1.92	0.51
2:C:163:ARG:HB3	2:C:179:ASP:HB2	1.93	0.51
1:A:380:LEU:HD11	1:A:387:PRO:HG3	1.93	0.50
1:B:380:LEU:HD11	1:B:387:PRO:HG3	1.94	0.50
1:A:483:LEU:HB3	2:D:44:ILE:HG12	1.90	0.50
2:C:64:LEU:HD11	2:C:92:SER:HB2	1.94	0.50
1:B:597:ARG:HA	1:B:609:VAL:HG12	1.94	0.50
1:B:716:PRO:HA	2:C:15:VAL:HG21	1.94	0.49
2:C:28:HIS:CD2	2:C:30:VAL:H	2.27	0.49
1:A:478:TYR:O	1:B:482:ARG:HG3	2.12	0.49
2:D:64:LEU:HD11	2:D:92:SER:HB2	1.94	0.49
1:B:38:VAL:HG12	1:B:156:THR:HG23	1.93	0.49
1:B:575:ARG:HG3	1:B:588:MET:SD	2.53	0.49
1:A:575:ARG:HD2	1:A:577:VAL:HG23	1.95	0.48
1:A:716:PRO:HA	2:D:15:VAL:HG21	1.95	0.48
1:B:713:GLN:HB2	1:B:742:HIS:CE1	2.48	0.48
1:A:177:GLU:O	1:A:181:ILE:HG13	2.13	0.48
2:D:28:HIS:CD2	2:D:30:VAL:H	2.27	0.48
1:B:514:SER:N	2:D:126:MET:HE1	2.26	0.48
1:A:415:MET:HG2	1:A:462:ILE:HG21	1.94	0.48
1:B:55:GLN:HE21	1:B:56:HIS:N	2.12	0.48
1:A:537:ILE:HD13	2:C:117:CYS:O	2.14	0.47
1:B:198:HIS:HD2	1:B:200:GLU:N	2.06	0.47
1:A:519:ALA:O	1:A:523:LEU:CD2	2.63	0.47
1:B:575:ARG:HD2	1:B:577:VAL:HG23	1.96	0.47
1:B:618:VAL:HG12	1:B:622:LEU:HD22	1.96	0.47
1:A:452:ARG:HD2	1:A:452:ARG:HA	1.83	0.46
1:A:270:GLU:HG2	1:A:320:HIS:O	2.15	0.46
1:A:297:ARG:NH1	1:A:348:SER:HB2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:MET:SD	2:C:206:MET:HG3	2.55	0.46
2:C:199:LEU:HD23	2:C:233:ARG:NH2	2.30	0.46
1:B:270:GLU:HG2	1:B:320:HIS:O	2.16	0.46
1:A:618:VAL:HG12	1:A:622:LEU:HD22	1.98	0.46
1:B:202:ARG:HD3	1:B:202:ARG:HA	1.77	0.46
1:B:315:VAL:HB	1:B:356:SER:HB3	1.97	0.46
2:D:167:SER:CB	2:D:177:GLU:HG3	2.45	0.46
1:B:575:ARG:HG3	1:B:588:MET:CG	2.47	0.45
1:A:315:VAL:HB	1:A:356:SER:HB3	1.98	0.45
1:A:5:GLU:HG2	1:A:9:ARG:HD2	1.99	0.45
1:A:435:THR:O	1:A:446:VAL:HA	2.16	0.45
1:A:519:ALA:O	1:A:523:LEU:HD22	2.16	0.45
1:B:435:THR:O	1:B:446:VAL:HA	2.16	0.45
1:A:507:TYR:HB3	1:A:570:PHE:HD2	1.82	0.45
1:A:574:LEU:HD13	1:A:585:GLN:HB3	1.98	0.45
1:B:507:TYR:HB3	1:B:570:PHE:HD2	1.81	0.45
2:D:92:SER:N	2:D:93:PRO:HD2	2.31	0.45
2:C:153:ARG:HG2	2:C:159:GLN:HA	1.99	0.44
1:A:627:ALA:HB2	1:A:689:GLY:HA2	1.99	0.44
3:D:301:2NL:N2	3:D:301:2NL:C6	2.81	0.44
1:A:202:ARG:HD3	1:A:202:ARG:HA	1.75	0.44
1:B:627:ALA:HB2	1:B:689:GLY:HA2	2.00	0.44
1:A:575:ARG:HG2	1:A:588:MET:CG	2.48	0.44
1:A:13:ASN:O	1:A:184:VAL:HG21	2.17	0.44
1:A:566:ARG:HD2	1:A:596:LYS:O	2.18	0.44
1:B:415:MET:HG2	1:B:462:ILE:HG21	2.00	0.44
2:C:92:SER:N	2:C:93:PRO:HD2	2.33	0.43
1:A:9:ARG:NH1	1:A:16:VAL:O	2.49	0.43
1:B:474:LEU:HB2	2:D:145:LYS:HE2	2.01	0.43
1:B:761:HIS:CD2	1:B:763:SER:H	2.20	0.43
1:A:198:HIS:HD2	1:A:200:GLU:N	2.03	0.43
1:B:597:ARG:HA	1:B:609:VAL:HG13	2.00	0.43
1:B:177:GLU:O	1:B:181:ILE:HG12	2.19	0.43
1:A:359:PHE:CD1	1:A:363:VAL:CG2	3.01	0.43
1:B:167:ASP:O	1:B:173:GLY:HA3	2.19	0.42
1:B:87:LEU:HD13	1:B:89:ILE:HD13	2.01	0.42
3:C:301:2NL:N2	3:C:301:2NL:C6	2.82	0.42
1:B:165:ARG:HA	1:B:165:ARG:HD2	1.76	0.42
1:A:568:ARG:HA	1:A:593:ILE:HG22	2.02	0.42
1:B:572:SER:HA	1:B:588:MET:O	2.20	0.42
1:B:14:PRO:HB2	1:B:16:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:VAL:HG13	2:D:146:GLY:CA	2.49	0.41
1:A:575:ARG:HG2	1:A:588:MET:HG3	2.02	0.41
1:B:566:ARG:HD2	1:B:596:LYS:O	2.20	0.41
1:A:557:GLN:HA	1:A:560:LEU:HB2	2.01	0.41
1:B:602:TRP:CD1	2:D:18:PRO:HD2	2.55	0.41
1:B:557:GLN:HA	1:B:560:LEU:HB2	2.03	0.41
2:D:153:ARG:HG3	2:D:158:LYS:O	2.19	0.41
1:A:712:ASP:O	1:A:715:VAL:HG12	2.20	0.41
1:B:478:TYR:HE1	2:D:150:GLU:HG2	1.86	0.41
1:A:572:SER:HA	1:A:588:MET:O	2.20	0.41
1:A:14:PRO:HB2	1:A:16:VAL:HG22	2.02	0.41
1:A:704:ARG:HA	1:A:757:LEU:O	2.21	0.41
1:B:615:LYS:HZ2	2:C:16:THR:HG22	1.83	0.40
2:C:199:LEU:CD2	2:C:233:ARG:HH22	2.34	0.40
1:B:248:VAL:O	1:B:251:VAL:HG22	2.21	0.40
2:C:163:ARG:HB2	2:C:198:TRP:CZ3	2.56	0.40
1:B:715:VAL:HA	1:B:716:PRO:HD3	2.00	0.40
1:B:455:ILE:HD13	1:B:460:ASP:HB3	2.03	0.40
1:B:568:ARG:HA	1:B:593:ILE:HG22	2.02	0.40
1:B:633:PHE:HB3	2:C:16:THR:HG21	2.03	0.40
1:A:184:VAL:CG2	1:A:185:PRO:HD2	2.50	0.40
1:A:593:ILE:HD12	1:A:609:VAL:HG21	2.03	0.40

There are no symmetry-related clashes.

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	789/792 (100%)	770 (98%)	19 (2%)	0	100	100
1	B	789/792 (100%)	772 (98%)	17 (2%)	0	100	100
2	C	231/338 (68%)	220 (95%)	10 (4%)	1 (0%)	39	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	240/338 (71%)	228 (95%)	10 (4%)	2 (1%)	24	44
All	All	2049/2260 (91%)	1990 (97%)	56 (3%)	3 (0%)	56	80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	120	ASP
2	C	122	THR
2	D	122	THR

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%)	583 (90%)	62 (10%)	10	19
1	B	645/646 (100%)	576 (89%)	69 (11%)	8	14
2	C	205/287 (71%)	189 (92%)	16 (8%)	16	29
2	D	211/287 (74%)	194 (92%)	17 (8%)	15	27
All	All	1706/1866 (91%)	1542 (90%)	164 (10%)	10	19

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	24	ARG
1	A	27	MET
1	A	54	GLU
1	A	60	ASP
1	A	63	ARG
1	A	76	VAL
1	A	106	LYS
1	A	110	ARG
1	A	122	LYS
1	A	123	GLU

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Mol	Chain	Res	Type
1	A	127	SER
1	A	128	GLU
1	A	129	GLU
1	A	142	VAL
1	A	146	VAL
1	A	164	ASN
1	A	171	LEU
1	A	202	ARG
1	A	225	LEU
1	A	257	ILE
1	A	270	GLU
1	A	282	ASP
1	A	289	LEU
1	A	292	GLN
1	A	295	THR
1	A	307	GLN
1	A	315	VAL
1	A	342	LEU
1	A	361	ARG
1	A	381	ASP
1	A	382	ILE
1	A	386	GLU
1	A	399	LEU
1	A	406	THR
1	A	411	ARG
1	A	437	VAL
1	A	446	VAL
1	A	463	GLU
1	A	515	PHE
1	A	522	GLU
1	A	540	ASP
1	A	560	LEU
1	A	565	SER
1	A	575	ARG
1	A	581	GLU
1	A	606	ARG
1	A	622	LEU
1	A	666	LEU
1	A	673	GLU
1	A	676	VAL
1	A	682	LEU
1	A	690	HIS

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	710	LEU
1	A	713	GLN
1	A	723	GLN
1	A	730	GLU
1	A	736	ARG
1	A	744	LYS
1	A	768	ASP
1	A	785	ARG
1	B	4	SER
1	B	27	MET
1	B	76	VAL
1	B	89	ILE
1	B	93	MET
1	B	101	ASP
1	B	106	LYS
1	B	122	LYS
1	B	123	GLU
1	B	128	GLU
1	B	129	GLU
1	B	142	VAL
1	B	146	VAL
1	B	164	ASN
1	B	165	ARG
1	B	171	LEU
1	B	202	ARG
1	B	225	LEU
1	B	243	ARG
1	B	245	ILE
1	B	249	VAL
1	B	257	ILE
1	B	270	GLU
1	B	282	ASP
1	B	289	LEU
1	B	292	GLN
1	B	307	GLN
1	B	308	ARG
1	B	312	ILE
1	B	342	LEU
1	B	361	ARG
1	B	381	ASP
1	B	382	ILE

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Mol	Chain	Res	Type
1	B	386	GLU
1	B	399	LEU
1	B	406	THR
1	B	411	ARG
1	B	412	VAL
1	B	414	GLN
1	B	421	ASP
1	B	437	VAL
1	B	452	ARG
1	B	463	GLU
1	B	480	GLN
1	B	482	ARG
1	B	515	PHE
1	B	548	LEU
1	B	560	LEU
1	B	564	GLN
1	B	565	SER
1	B	575	ARG
1	B	581	GLU
1	B	606	ARG
1	B	622	LEU
1	B	645	GLN
1	B	666	LEU
1	B	672	LEU
1	B	673	GLU
1	B	682	LEU
1	B	710	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	768	ASP
1	B	777	ASN
1	B	785	ARG
2	C	11	GLU
2	C	15	VAL
2	C	84	ASN
2	C	90	HIS
2	C	92	SER
2	C	95	GLN

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Mol	Chain	Res	Type
2	C	103	GLN
2	C	109	VAL
2	C	117	CYS
2	C	118	ASP
2	C	121	LEU
2	C	153	ARG
2	C	160	LEU
2	C	171	PHE
2	C	199	LEU
2	C	234	LEU
2	D	8	LEU
2	D	15	VAL
2	D	20	ARG
2	D	44	ILE
2	D	57	ASP
2	D	84	ASN
2	D	90	HIS
2	D	92	SER
2	D	95	GLN
2	D	109	VAL
2	D	117	CYS
2	D	122	THR
2	D	153	ARG
2	D	160	LEU
2	D	184	ILE
2	D	199	LEU
2	D	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	75	GLN
1	A	144	GLN
1	A	164	ASN
1	A	198	HIS
1	A	564	GLN
1	A	713	GLN
1	A	723	GLN
1	A	742	HIS
1	A	761	HIS
1	B	55	GLN

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Mol	Chain	Res	Type
1	B	144	GLN
1	B	164	ASN
1	B	198	HIS
1	B	261	GLN
1	B	559	ASN
1	B	563	GLN
1	B	564	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	95	GLN
2	D	28	HIS
2	D	70	HIS
2	D	95	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

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value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
3	2NL	C	301	-	21,21,21	0.31	0	24,27,27	0.71	0
3	2NL	D	301	-	21,21,21	0.31	0	24,27,27	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	2NL	C	301	-	-	0/11/11/11	0/2/2/2
3	2NL	D	301	-	-	0/11/11/11	0/2/2/2

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.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	2NL	3	0
3	D	301	2NL	2	0

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 (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	791/792 (99%)	-0.06	6 (0%)	87 85	33, 51, 84, 107	0
1	B	791/792 (99%)	-0.11	9 (1%)	82 79	29, 49, 82, 107	0
2	C	235/338 (69%)	-0.16	1 (0%)	93 91	38, 49, 78, 112	0
2	D	244/338 (72%)	-0.05	2 (0%)	87 85	35, 50, 88, 114	0
All	All	2061/2260 (91%)	-0.09	18 (0%)	85 83	29, 50, 83, 114	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	709	LEU	3.7
1	A	102	PHE	3.6
1	A	101	ASP	2.8
1	B	782	LEU	2.8
1	B	746	ILE	2.4
1	A	94	ILE	2.4
1	B	754	ALA	2.3
1	B	401	LYS	2.3
1	B	673	GLU	2.3
1	B	790	LEU	2.2
2	D	118	ASP	2.2
1	B	738	PHE	2.2
2	C	120	ASP	2.2
2	D	69	HIS	2.1
1	A	83	VAL	2.1
1	B	402	VAL	2.1
1	A	100	ASP	2.1
1	A	126	ILE	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	2NL	C	301	20/20	0.93	0.21	2.04	32,42,57,75	0
3	2NL	D	301	20/20	0.91	0.20	1.31	39,46,62,77	0

6.5 Other polymers (i)

There are no such residues in this entry.