



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:33 PM GMT

PDB ID : 4P75  
Title : PheRS in complex with compound 4a  
Authors : Ferguson, A.D.  
Deposited on : 2014-03-25  
Resolution : 2.96 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.

---

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

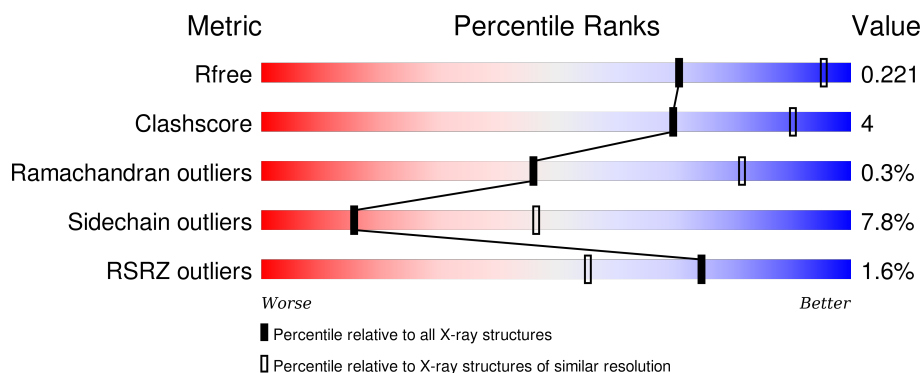
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.96 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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	792	<div> <div>3%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	B	792	<div> <div>%</div> <div>84%</div> <div>14%</div> <div>.</div> </div>
2	C	338	<div> <div>59%</div> <div>10%</div> <div>30%</div> <div>.</div> </div>
2	D	338	<div> <div>59%</div> <div>12%</div> <div>28%</div> <div>.</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16132 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.

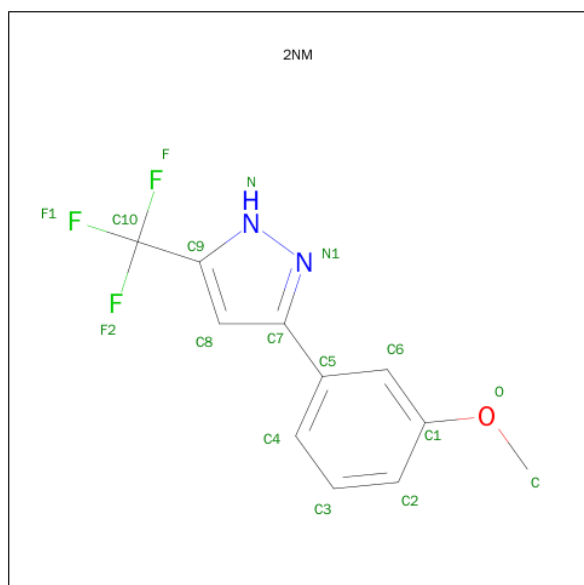
- Molecule 1 is a protein called Phenylalanine–tRNA ligase beta subunit.

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	243	Total	C	N	O	S	0	0	0
			1946	1234	343	354	15			

- Molecule 3 is 3-(3-methoxyphenyl)-5-(trifluoromethyl)-1H-pyrazole (three-letter code: 2NM) (formula: C<sub>11</sub>H<sub>9</sub>F<sub>3</sub>N<sub>2</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	F	N	O	0	0
			17	11	3	2	1		
3	D	1	Total	C	F	N	O	0	0
			17	11	3	2	1		

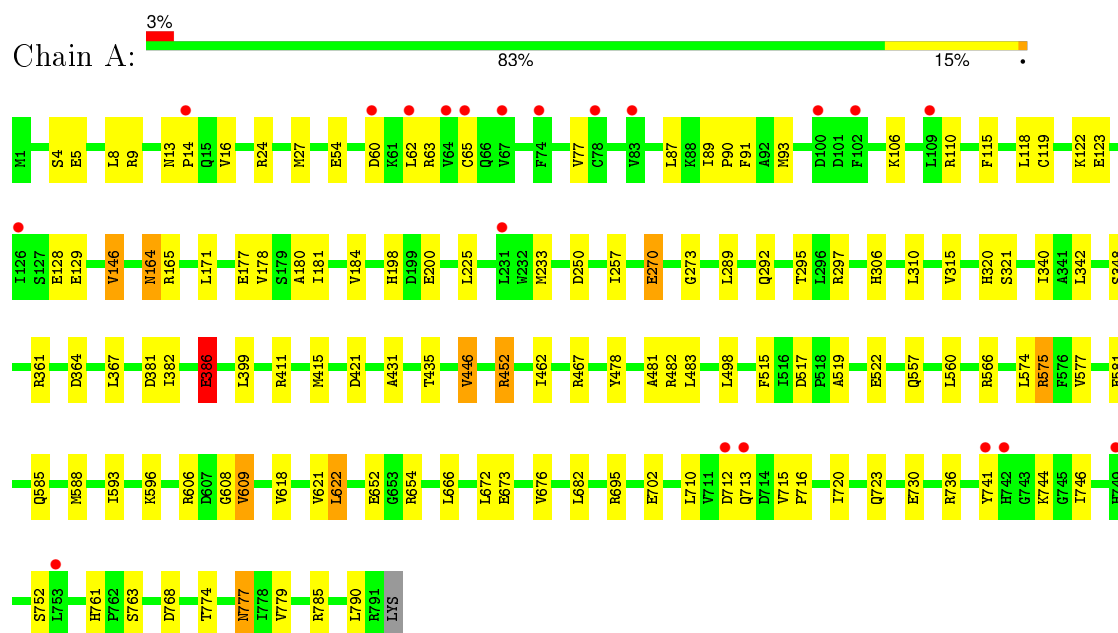
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	24	Total	O	0	0
			24	24		
4	C	6	Total	O	0	0
			6	6		
4	D	3	Total	O	0	0
			3	3		

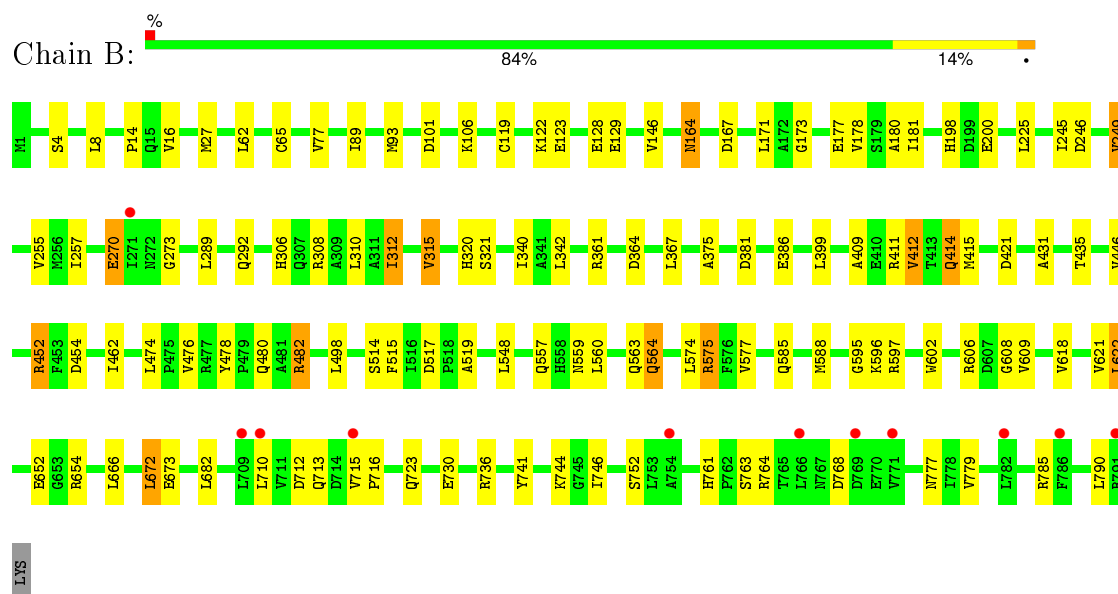
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

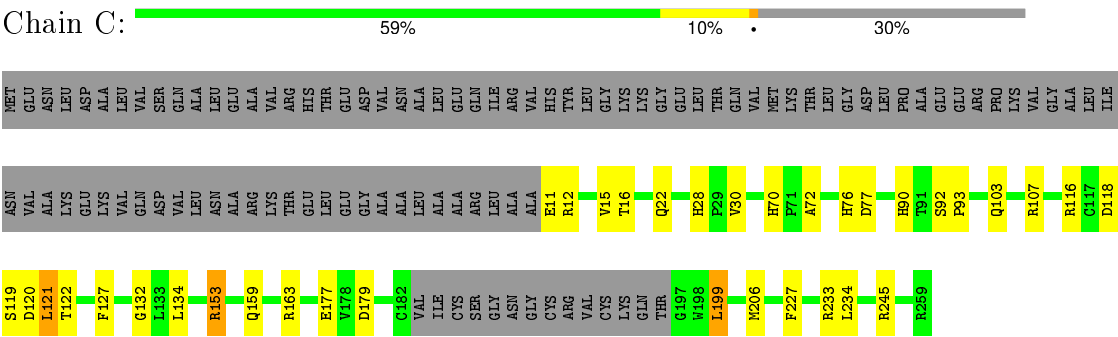
- Molecule 1: Phenylalanine-tRNA ligase beta subunit



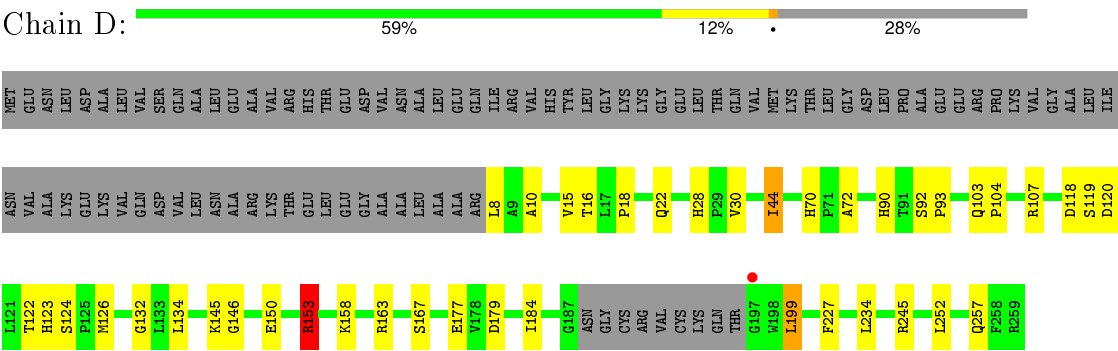
- Molecule 1: Phenylalanine-tRNA ligase beta subunit



● Molecule 2: Phenylalanine–tRNA ligase alpha subunit



● Molecule 2: Phenylalanine–tRNA ligase alpha subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.00Å 219.56Å 107.52Å 90.00° 102.02° 90.00°	Depositor
Resolution (Å)	59.20 – 2.96 55.63 – 2.96	Depositor EDS
% Data completeness (in resolution range)	97.5 (59.20-2.96) 97.8 (55.63-2.96)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.96Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, $R_{free}$	0.184 , 0.213 0.196 , 0.221	Depositor DCC
$R_{free}$ test set	2637 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.4	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 51923 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2NM

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	0.50	0/6221	0.74	1/8450 (0.0%)
1	B	0.50	0/6221	0.74	0/8450
2	C	0.52	0/1946	0.76	2/2628 (0.1%)
2	D	0.55	0/1995	0.75	1/2695 (0.0%)
All	All	0.51	0/16383	0.74	4/22223 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	ARG	CG-CD-NE	-7.52	96.01	111.80
2	D	153	ARG	CD-NE-CZ	5.69	131.56	123.60
2	C	121	LEU	C-N-CA	5.61	135.72	121.70
2	C	177	GLU	CB-CG-CD	5.17	128.15	114.20

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	58	0
1	B	6103	0	6136	60	0
2	C	1897	0	1821	18	0
2	D	1946	0	1875	35	0
3	C	17	0	9	0	0
3	D	17	0	9	0	0
4	A	16	0	0	0	0
4	B	24	0	0	0	0
4	C	6	0	0	0	0
4	D	3	0	0	0	0
All	All	16132	0	15986	144	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 (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:GLN:HG2	2:D:252:LEU:HD12	1.56	0.86
1:B:559:ASN:HD21	2:D:252:LEU:H	1.25	0.85
1:A:198:HIS:HD2	1:A:200:GLU:H	1.22	0.85
1:B:198:HIS:HD2	1:B:200:GLU:H	1.21	0.84
1:B:716:PRO:HA	2:C:15:VAL:HG21	1.64	0.78
1:B:761:HIS:HD2	1:B:763:SER:H	1.32	0.77
1:A:761:HIS:HD2	1:A:763:SER:H	1.31	0.77
1:A:695:ARG:H	2:D:257:GLN:HE22	1.33	0.76
2:C:199:LEU:HD23	2:C:233:ARG:HH22	1.50	0.75
1:A:566:ARG:HH12	2:C:22:GLN:HE22	1.35	0.74
1:A:716:PRO:HA	2:D:15:VAL:HG21	1.70	0.74
1:B:514:SER:H	2:D:126:MET:HE1	1.55	0.71
1:B:414:GLN:HG3	1:B:415:MET:N	2.07	0.69
1:B:514:SER:H	2:D:126:MET:CE	2.07	0.68
1:B:564:GLN:HE21	2:D:252:LEU:HB2	1.59	0.68
1:B:312:ILE:HG12	1:B:315:VAL:HG13	1.77	0.67
2:D:120:ASP:O	2:D:123:HIS:O	2.12	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:70:HIS:HD2	2:C:72:ALA:H	1.43	0.66
2:D:28:HIS:HD2	2:D:30:VAL:H	1.44	0.66
2:C:15:VAL:HG22	2:C:16:THR:H	1.61	0.65
1:A:566:ARG:HH12	2:C:22:GLN:NE2	1.93	0.65
2:C:28:HIS:HD2	2:C:30:VAL:H	1.44	0.65
2:D:70:HIS:HD2	2:D:72:ALA:H	1.44	0.64
1:A:557:GLN:HE21	1:A:672:LEU:HD13	1.63	0.64
2:D:15:VAL:HG22	2:D:16:THR:H	1.63	0.64
1:A:415:MET:HG2	1:A:462:ILE:HG21	1.80	0.64
1:A:482:ARG:HD2	1:B:478:TYR:O	2.00	0.62
2:D:167:SER:HB2	2:D:177:GLU:HG3	1.82	0.61
1:A:702:GLU:H	1:B:563:GLN:HE22	1.50	0.60
1:B:164:ASN:H	1:B:164:ASN:HD22	1.49	0.60
1:A:310:LEU:HD22	1:A:321:SER:HB3	1.85	0.58
1:B:597:ARG:HA	1:B:609:VAL:CG1	2.33	0.58
1:A:779:VAL:HG11	1:A:790:LEU:HD21	1.85	0.58
1:B:246:ASP:HB2	1:B:249:VAL:HG23	1.84	0.57
1:B:476:VAL:HG13	2:D:146:GLY:HA2	1.86	0.57
2:C:163:ARG:HB3	2:C:179:ASP:HB2	1.85	0.57
1:B:779:VAL:HG11	1:B:790:LEU:HD21	1.86	0.57
1:B:415:MET:HG2	1:B:462:ILE:HG21	1.86	0.56
1:A:761:HIS:CD2	1:A:763:SER:H	2.18	0.56
1:B:310:LEU:HD22	1:B:321:SER:HB3	1.86	0.56
1:A:89:ILE:HD13	1:A:118:LEU:HD22	1.86	0.56
2:D:163:ARG:HB3	2:D:179:ASP:HB2	1.87	0.56
1:B:597:ARG:HA	1:B:609:VAL:HG13	1.88	0.55
1:A:483:LEU:HB3	2:D:44:ILE:CG1	2.36	0.55
1:A:106:LYS:HE3	1:A:115:PHE:CE1	2.41	0.55
1:A:164:ASN:H	1:A:164:ASN:HD22	1.52	0.55
2:C:116:ARG:HE	2:C:127:PHE:HZ	1.54	0.55
1:B:514:SER:N	2:D:126:MET:HE1	2.20	0.55
1:B:8:LEU:HD21	1:B:178:VAL:HG21	1.88	0.54
1:B:409:ALA:O	1:B:412:VAL:HG13	2.07	0.54
1:B:761:HIS:CD2	1:B:763:SER:H	2.18	0.54
2:D:28:HIS:CD2	2:D:30:VAL:H	2.25	0.54
2:C:132:GLY:HA3	2:C:227:PHE:CZ	2.43	0.54
1:A:8:LEU:HD21	1:A:178:VAL:HG21	1.90	0.53
2:D:132:GLY:HA3	2:D:227:PHE:CZ	2.44	0.53
1:A:5:GLU:HG2	1:A:9:ARG:HD2	1.91	0.53
1:A:478:TYR:O	1:B:482:ARG:HG3	2.09	0.53
1:B:602:TRP:CD1	2:D:18:PRO:HD2	2.45	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:HG2	1:A:320:HIS:O	2.09	0.52
1:B:270:GLU:HG2	1:B:320:HIS:O	2.10	0.52
1:B:575:ARG:HG2	1:B:588:MET:CG	2.40	0.52
1:B:435:THR:O	1:B:446:VAL:HA	2.10	0.51
1:A:233:MET:CE	1:A:250:ASP:HB3	2.41	0.51
2:D:8:LEU:HG	2:D:10:ALA:H	1.76	0.50
1:A:435:THR:O	1:A:446:VAL:HA	2.11	0.50
1:A:498:LEU:HD22	1:A:621:VAL:HG13	1.93	0.50
2:C:28:HIS:CD2	2:C:30:VAL:H	2.26	0.50
1:A:91:PHE:CE2	1:A:93:MET:HG2	2.47	0.50
1:A:575:ARG:HG2	1:A:588:MET:CG	2.42	0.50
1:B:517:ASP:OD2	1:B:519:ALA:HB3	2.11	0.49
1:B:559:ASN:ND2	2:D:252:LEU:H	2.01	0.49
1:B:574:LEU:HD13	1:B:585:GLN:HB3	1.94	0.49
1:B:575:ARG:HG2	1:B:588:MET:HG3	1.94	0.49
1:A:774:THR:HA	1:A:777:ASN:HD22	1.78	0.49
1:B:498:LEU:HD22	1:B:621:VAL:HG13	1.95	0.48
1:B:596:LYS:HA	1:B:608:GLY:HA2	1.94	0.48
2:C:76:HIS:HD2	2:C:77:ASP:OD1	1.96	0.48
1:A:483:LEU:HB3	2:D:44:ILE:HG13	1.96	0.48
1:B:409:ALA:HA	1:B:412:VAL:HG13	1.96	0.47
2:D:153:ARG:HG3	2:D:158:LYS:O	2.13	0.47
1:A:483:LEU:HB3	2:D:44:ILE:HG12	1.96	0.47
1:B:198:HIS:CD2	1:B:200:GLU:H	2.14	0.47
1:B:62:LEU:HD22	1:B:77:VAL:HG12	1.95	0.47
1:B:476:VAL:HG13	2:D:146:GLY:CA	2.45	0.47
2:D:179:ASP:HA	2:D:199:LEU:O	2.15	0.47
1:A:596:LYS:HA	1:A:608:GLY:HA2	1.95	0.47
1:A:517:ASP:OD2	1:A:519:ALA:HB3	2.14	0.47
1:A:177:GLU:OE2	1:A:467:ARG:NH1	2.48	0.47
1:A:198:HIS:HD2	1:A:200:GLU:N	2.01	0.47
1:A:575:ARG:HD2	1:A:577:VAL:HG23	1.97	0.46
1:A:575:ARG:HG2	1:A:588:MET:HG3	1.98	0.46
2:D:124:SER:HA	2:D:245:ARG:HH22	1.80	0.46
1:A:62:LEU:HD22	1:A:77:VAL:HG12	1.96	0.46
1:B:652:GLU:HB2	1:B:654:ARG:HH21	1.79	0.46
2:C:153:ARG:HG2	2:C:159:GLN:HA	1.98	0.46
1:B:198:HIS:HD2	1:B:200:GLU:N	2.01	0.46
1:A:273:GLY:O	1:A:306:HIS:CE1	2.69	0.46
1:B:474:LEU:HB2	2:D:145:LYS:HE2	1.98	0.46
1:B:741:TYR:HB3	1:B:752:SER:HB3	1.97	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:ARG:HD2	1:B:577:VAL:HG23	1.99	0.45
1:A:14:PRO:HB2	1:A:16:VAL:HG22	1.98	0.45
1:A:364:ASP:HB3	1:A:367:LEU:HB2	1.98	0.45
1:A:741:TYR:HB3	1:A:752:SER:HB3	1.98	0.45
2:D:107:ARG:HG2	2:D:134:LEU:HD12	1.98	0.45
1:A:13:ASN:O	1:A:184:VAL:HG21	2.16	0.45
1:B:273:GLY:O	1:B:306:HIS:CE1	2.70	0.44
1:B:595:GLY:O	1:B:609:VAL:HG22	2.18	0.44
1:B:564:GLN:NE2	2:D:252:LEU:HB2	2.30	0.44
2:C:107:ARG:HG2	2:C:134:LEU:HD12	1.99	0.44
2:C:179:ASP:HA	2:C:199:LEU:O	2.17	0.44
2:D:92:SER:N	2:D:93:PRO:HD2	2.32	0.44
1:A:165:ARG:HH12	1:A:467:ARG:NH1	2.16	0.44
1:A:618:VAL:HG12	1:A:622:LEU:HD22	1.99	0.43
1:A:574:LEU:HD13	1:A:585:GLN:HB3	1.99	0.43
1:A:652:GLU:HB2	1:A:654:ARG:HH21	1.82	0.43
1:B:557:GLN:HE21	1:B:672:LEU:HD12	1.83	0.43
1:A:415:MET:SD	2:C:206:MET:HG3	2.58	0.43
1:A:177:GLU:O	1:A:181:ILE:HG13	2.18	0.43
1:B:312:ILE:HG12	1:B:315:VAL:CG1	2.48	0.43
1:B:597:ARG:HA	1:B:609:VAL:HG12	2.00	0.43
1:B:14:PRO:HB2	1:B:16:VAL:HG22	2.01	0.43
1:B:167:ASP:O	1:B:173:GLY:HA3	2.19	0.43
1:B:177:GLU:O	1:B:181:ILE:HG12	2.19	0.43
1:B:452:ARG:HG3	1:B:454:ASP:OD1	2.19	0.42
1:A:695:ARG:N	2:D:257:GLN:HE22	2.10	0.42
1:A:90:PRO:HB3	1:A:146:VAL:HG21	2.01	0.42
1:B:180:ALA:HA	1:B:431:ALA:HB1	2.00	0.42
2:D:167:SER:CB	2:D:177:GLU:HG3	2.50	0.42
2:D:103:GLN:HG3	2:D:104:PRO:HD2	2.00	0.42
1:A:180:ALA:HA	1:A:431:ALA:HB1	2.02	0.42
1:B:618:VAL:HG12	1:B:622:LEU:HD22	2.01	0.42
2:C:92:SER:N	2:C:93:PRO:HD2	2.34	0.42
1:A:715:VAL:HG13	1:A:720:ILE:HD11	2.02	0.41
1:A:481:ALA:HB2	2:C:107:ARG:NH2	2.36	0.41
1:B:712:ASP:O	1:B:715:VAL:HG12	2.21	0.41
1:A:593:ILE:HD12	1:A:609:VAL:HG21	2.03	0.41
1:B:364:ASP:HB3	1:B:367:LEU:HB2	2.03	0.41
1:B:255:VAL:HG21	1:B:375:ALA:HB2	2.02	0.41
1:A:297:ARG:HH12	1:A:348:SER:CB	2.33	0.40
1:A:297:ARG:NH1	1:A:348:SER:HB2	2.35	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:TYR:HE1	2:D:150:GLU:HG2	1.86	0.40
1:A:712:ASP:O	1:A:715:VAL:HG12	2.22	0.40
1:A:87:LEU:HA	1:A:87:LEU:HD12	1.93	0.40
1:A:386:GLU:H	1:A:386:GLU:HG2	1.75	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%)	770 (98%)	19 (2%)	0	100	100
1	B	789/792 (100%)	770 (98%)	19 (2%)	0	100	100
2	C	231/338 (68%)	218 (94%)	9 (4%)	4 (2%)	11	43
2	D	239/338 (71%)	224 (94%)	13 (5%)	2 (1%)	24	64
All	All	2048/2260 (91%)	1982 (97%)	60 (3%)	6 (0%)	46	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	120	ASP
2	C	121	LEU
2	C	122	THR
2	D	118	ASP
2	D	122	THR
2	C	118	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%)	589 (91%)	56 (9%)	13	40
1	B	645/646 (100%)	585 (91%)	60 (9%)	11	37
2	C	205/287 (71%)	196 (96%)	9 (4%)	35	72
2	D	210/287 (73%)	202 (96%)	8 (4%)	40	76
All	All	1705/1866 (91%)	1572 (92%)	133 (8%)	16	46

All (133) 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	65	CYS
1	A	110	ARG
1	A	119	CYS
1	A	122	LYS
1	A	123	GLU
1	A	128	GLU
1	A	129	GLU
1	A	146	VAL
1	A	164	ASN
1	A	171	LEU
1	A	225	LEU
1	A	257	ILE
1	A	270	GLU
1	A	289	LEU
1	A	292	GLN
1	A	295	THR
1	A	315	VAL
1	A	340	ILE
1	A	342	LEU
1	A	361	ARG
1	A	381	ASP
1	A	382	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	386	GLU
1	A	399	LEU
1	A	411	ARG
1	A	421	ASP
1	A	446	VAL
1	A	452	ARG
1	A	515	PHE
1	A	522	GLU
1	A	560	LEU
1	A	575	ARG
1	A	581	GLU
1	A	606	ARG
1	A	609	VAL
1	A	622	LEU
1	A	666	LEU
1	A	673	GLU
1	A	676	VAL
1	A	682	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	746	ILE
1	A	768	ASP
1	A	777	ASN
1	A	785	ARG
1	B	4	SER
1	B	27	MET
1	B	65	CYS
1	B	89	ILE
1	B	93	MET
1	B	101	ASP
1	B	106	LYS
1	B	119	CYS
1	B	122	LYS
1	B	123	GLU
1	B	128	GLU
1	B	129	GLU
1	B	146	VAL
1	B	164	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	171	LEU
1	B	225	LEU
1	B	245	ILE
1	B	249	VAL
1	B	257	ILE
1	B	270	GLU
1	B	289	LEU
1	B	292	GLN
1	B	308	ARG
1	B	312	ILE
1	B	315	VAL
1	B	340	ILE
1	B	342	LEU
1	B	361	ARG
1	B	381	ASP
1	B	386	GLU
1	B	399	LEU
1	B	411	ARG
1	B	412	VAL
1	B	414	GLN
1	B	421	ASP
1	B	452	ARG
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	575	ARG
1	B	606	ARG
1	B	622	LEU
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	746	ILE

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	764	ARG
1	B	768	ASP
1	B	777	ASN
1	B	785	ARG
2	C	11	GLU
2	C	12	ARG
2	C	90	HIS
2	C	103	GLN
2	C	119	SER
2	C	153	ARG
2	C	199	LEU
2	C	234	LEU
2	C	245	ARG
2	D	22	GLN
2	D	44	ILE
2	D	90	HIS
2	D	119	SER
2	D	153	ARG
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 (25) 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	261	GLN
1	A	761	HIS
1	A	777	ASN
1	B	144	GLN
1	B	164	ASN
1	B	198	HIS
1	B	261	GLN
1	B	306	HIS
1	B	559	ASN
1	B	563	GLN
1	B	564	GLN
1	B	645	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	761	HIS
2	C	22	GLN
2	C	28	HIS
2	C	70	HIS
2	C	76	HIS
2	D	28	HIS
2	D	70	HIS
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 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	2NM	C	301	-	17,18,18	0.59	0	24,26,26	0.82	1 (4%)
3	2NM	D	301	-	17,18,18	0.60	0	24,26,26	0.78	1 (4%)

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	2NM	C	301	-	-	0/12/12/12	0/2/2/2
3	2NM	D	301	-	-	0/12/12/12	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	301	2NM	C8-C7-N1	-2.62	105.75	110.05
3	C	301	2NM	C8-C7-N1	-2.43	106.05	110.05

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 [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<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	791/792 (99%)	0.07	20 (2%) 61 39	33, 58, 91, 115	0
1	B	791/792 (99%)	0.02	11 (1%) 78 59	33, 56, 98, 119	0
2	C	235/338 (69%)	-0.02	0 100 100	42, 56, 85, 103	0
2	D	243/338 (71%)	0.03	1 (0%) 93 83	36, 55, 90, 118	0
All	All	2060/2260 (91%)	0.04	32 (1%) 74 55	33, 56, 92, 119	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	791	ARG	3.9
1	B	782	LEU	3.9
1	A	109	LEU	3.3
1	B	709	LEU	3.2
1	A	742	HIS	3.1
1	A	102	PHE	2.8
1	B	766	LEU	2.8
1	A	126	ILE	2.8
1	A	64	VAL	2.8
2	D	197	GLY	2.7
1	A	749	HIS	2.7
1	A	74	PHE	2.7
1	A	83	VAL	2.6
1	A	100	ASP	2.6
1	B	771	VAL	2.5
1	A	712	ASP	2.5
1	A	78	CYS	2.5
1	A	713	GLN	2.4
1	A	741	TYR	2.4
1	A	65	CYS	2.3
1	B	754	ALA	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	715	VAL	2.2
1	A	62	LEU	2.2
1	A	14	PRO	2.2
1	B	710	LEU	2.2
1	A	753	LEU	2.2
1	A	60	ASP	2.1
1	B	271	ILE	2.1
1	B	769	ASP	2.1
1	A	231	LEU	2.1
1	B	786	PHE	2.0
1	A	67	VAL	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, 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(Å <sup>2</sup> )	Q<0.9
3	2NM	D	301	17/17	0.96	0.23	0.78	40,45,58,63	0
3	2NM	C	301	17/17	0.96	0.23	0.75	40,46,59,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.