



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:35 AM GMT

PDB ID : 3PCO  
Title : crystal structure of E. coli phenylalanine-tRNA synthetase complexed with phenylalanine and AMP  
Authors : Mermershtain, I.; Finarov, I.; Klipcan, L.; Kessler, N.; Rozenberg, H.; Safro, M.G.  
Deposited on : 2010-10-21  
Resolution : 3.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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



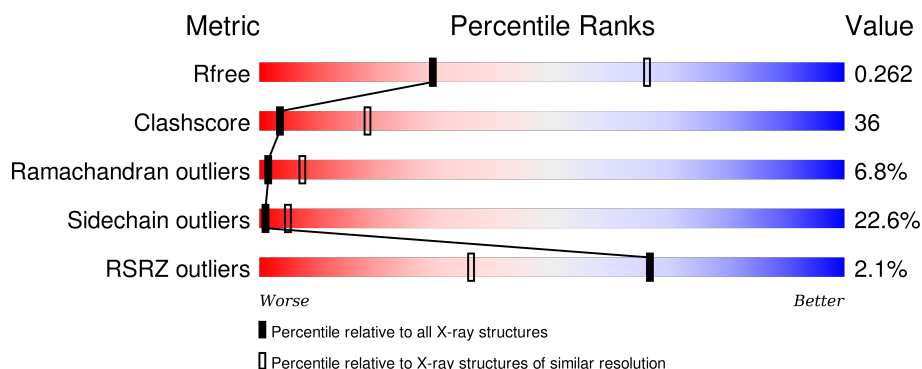
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.02 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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	327	<div> <div>29%</div> <div>32%</div> <div>11%</div> <div>•</div> <div>26%</div> </div>
1	C	327	<div> <div>9%</div> <div>43%</div> <div>40%</div> <div>13%</div> <div>• •</div> </div>
2	B	795	<div> <div>45%</div> <div>40%</div> <div>13%</div> <div>•</div> </div>
2	D	795	<div> <div>46%</div> <div>38%</div> <div>14%</div> <div>•</div> </div>

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PHE	A	980	-	-	-	X
4	AMP	A	992	-	-	X	X
4	AMP	C	999	-	-	X	-



## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16724 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.

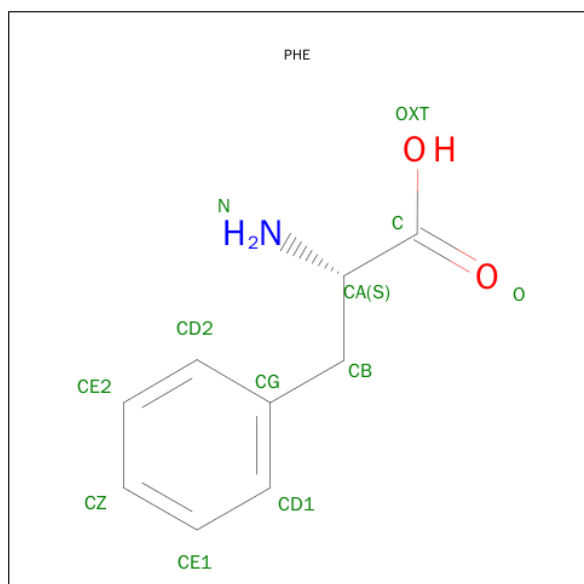
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase, alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1964	1250	347	358	9			
1	C	323	Total	C	N	O	S	0	0	0
			2462	1552	445	456	9			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase, beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	795	Total	C	N	O	S	0	0	0
			6111	3845	1081	1158	27			
2	D	795	Total	C	N	O	S	0	0	0
			6117	3848	1081	1161	27			

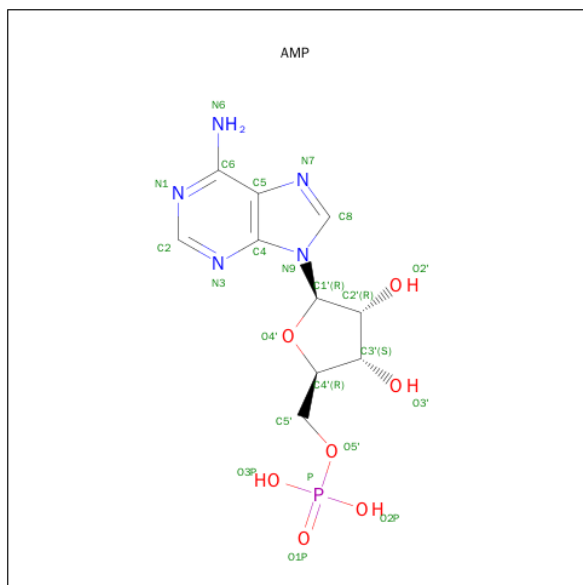
- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	9	1	2		
3	C	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



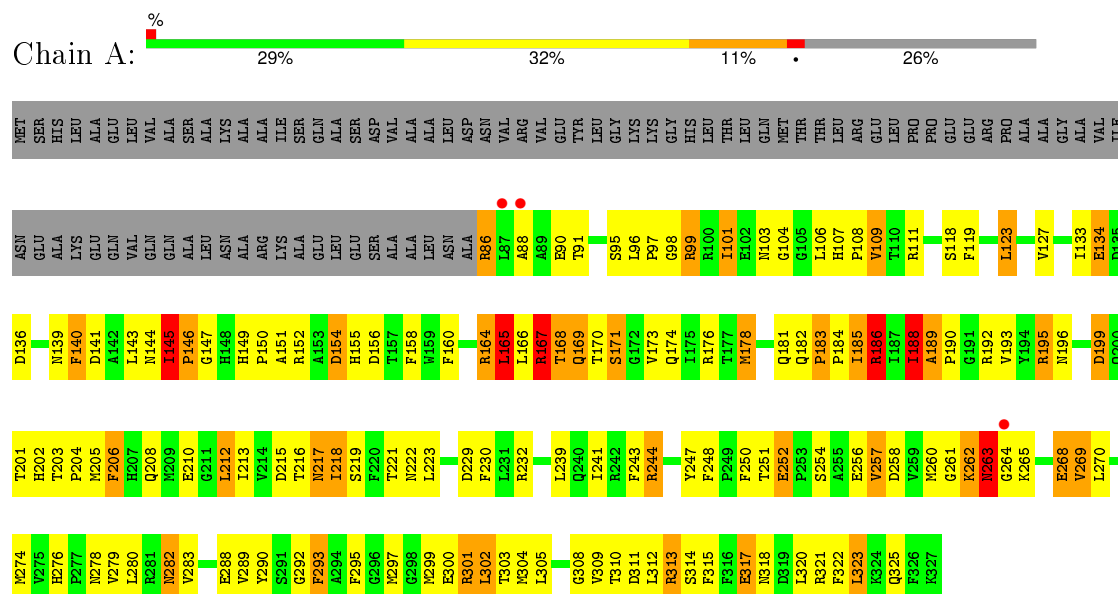
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
4	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		



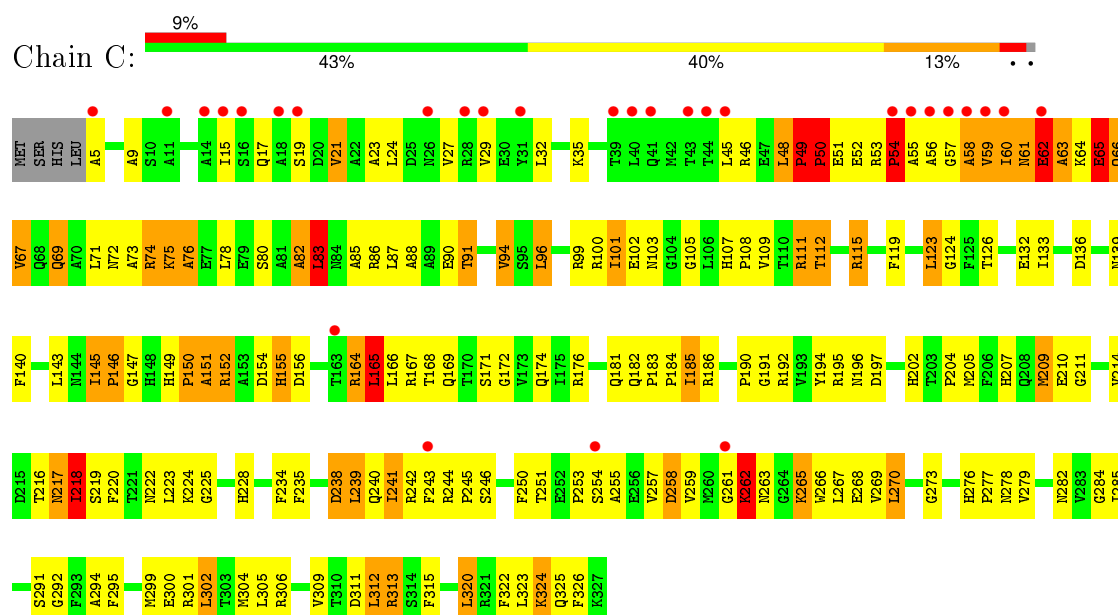
### 3 Residue-property plots

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, alpha subunit

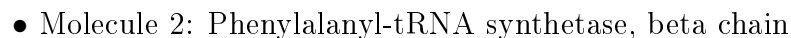


- Molecule 1: Phenylalanyl-tRNA synthetase, alpha subunit





Chain B:  45% 40% 13% 2%





E770	E771	I774	V778	A779	K780	A784	L785	K786	E787	Q790	A791	S792	L793	K794	E795	L689	A690	D691	R692	R698	E699	I700	S701	R702	F703	F704	A705	E639	A640	N641	F642	A643	L644	H645	S649	Y653	L654	K655	I723	L724	K729	V730	G731	V732	N733	Q734	V735	N739	L740	F741	R745	Q746	K747	K754	I758	S759	L760	L761	L762	Q763	D764	T765	S766	T767	T768	L769	S623	Y624	L625	D626	L627	T628	Q629	K630	L631	E632	E633	V634	E635	E639	A640	N641	F642	A643	L644	H645	S649	Y653	L654	K655	I723	L724	K729	V730	G731	V732	N733	Q734	V735	N739	L740	F741	R745	Q746	K747	K754	I758	S759	L760	L761	L762	Q763	D764	T765	S766	T767	T768	L769	L552	L553	A554	T555	V556	N559	Q560	N561	R562	Q563	Q564	N565	R566	V567	R568	I569	F570	E571	L574	R575	F576	V577	Q581	A582	P583	L584	G585	I586	R587	L590	N591	L592	A593	G594	V595	I596	C597	R600	E603	H604	N605	N606	K609	E610	T611	Y615	D616	L617	K618	L621	E622	V479	Q480	L483	I484	M485	Q486	T487	E490	L493	V498	K499	D504	K505	G506	F507	Q508	E509	V510	I511	T512	Y513	S514	F515	V516	D517	P518	K519	V520	Q521	Q522	N523	I524	V528	L531	L532	L533	P534	S535	P536	I537	S538	S542	A543	N544	R545	L546	S547	L548	W549	G551	I392	D393	I394	T395	N396	L400	P401	R402	K403	L408	S411	K412	L416	D423	V426	T427	D428	I429	L430	R431	R432	V437	T438	E439	G440	R441	D442	E443	N444	Q445	P449	S450	N451	R452	N455	E458	E459	D460	L461	V462	E463	G470	Y471	D472	N473	I474	P475	D476	I302	I303	I304	A305	D306	N307	I311	A312	I316	F317	G318	G319	E320	R321	S322	D326	E327	T328	Q329	N330	C335	A336	F337	F338	L341	S342	Q345	R346	A347	R348	S357	R358	R359	Y360	E361	R362	Q369	R370	E374	R375	T377	R378	L379	L380	I381	A388	R215	T216	L217	K222	G223	T224	K227	A228	P229	T230	T234	L238	R239	R240	C241	G242	I243	S245	I246	D247	L248	T253	N254	V255	V256	L257	L258	E259	Q262	P263	N264	R269	D270	R271	I272	E273	I276	V277	V278	R279	N280	L281	K282	V288	L289	L290	D291	E294
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.55Å 178.94Å 254.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.71 – 3.02 38.71 – 3.02	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.71-3.02) 98.4 (38.71-3.02)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.67 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.232 , 0.300 0.265 , 0.262	Depositor DCC
$R_{free}$ test set	2979 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	75.4	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 58.8	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 58878 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	16724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% 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: AMP

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	0.76	0/2016	0.98	5/2730 (0.2%)
1	C	0.65	0/2516	0.88	8/3412 (0.2%)
2	B	0.69	2/6212 (0.0%)	0.90	10/8432 (0.1%)
2	D	0.63	0/6218	0.84	4/8440 (0.0%)
All	All	0.67	2/16962 (0.0%)	0.89	27/23014 (0.1%)

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
1	C	0	3
2	B	0	9
2	D	0	6
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	463	GLU	CB-CG	5.87	1.63	1.52
2	B	540	GLU	CG-CD	5.10	1.59	1.51

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	563	GLN	N-CA-C	-5.99	94.82	111.00
1	C	54	PRO	N-CA-CB	5.99	110.48	103.30
1	C	49	PRO	N-CA-CB	5.96	110.46	103.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	50	PRO	N-CA-CB	5.82	110.29	103.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	PRO	Peptide
2	B	42	PHE	Peptide
2	B	55	GLN	Peptide
2	B	61	LYS	Peptide
2	B	62	LEU	Peptide

## 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	1964	0	1900	213	0
1	C	2462	0	2307	217	0
2	B	6111	0	6166	419	0
2	D	6117	0	6169	430	0
3	A	12	0	8	2	0
3	C	12	0	8	1	0
4	A	23	0	12	9	0
4	C	23	0	12	9	0
All	All	16724	0	16582	1211	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 36.

The worst 5 of 1211 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:55:GLN:HB2	2:D:56:HIS:CA	1.37	1.46
1:C:58:ALA:C	1:C:60:ILE:HB	1.48	1.34

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:ALA:HB1	1:C:60:ILE:CG2	1.58	1.33
2:D:631:LEU:HD12	2:D:632:ASN:N	1.47	1.27
2:D:55:GLN:HB2	2:D:56:HIS:C	1.56	1.24

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	240/327 (73%)	197 (82%)	31 (13%)	12 (5%)	3	15
1	C	321/327 (98%)	231 (72%)	57 (18%)	33 (10%)	1	3
2	B	793/795 (100%)	631 (80%)	120 (15%)	42 (5%)	2	14
2	D	793/795 (100%)	628 (79%)	106 (13%)	59 (7%)	1	6
All	All	2147/2244 (96%)	1687 (79%)	314 (15%)	146 (7%)	1	7

5 of 146 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	PRO
1	A	167	ARG
1	A	184	PRO
1	A	189	ALA
1	A	217	ASN

### 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	212/276 (77%)	164 (77%)	48 (23%)	1	5
1	C	240/276 (87%)	202 (84%)	38 (16%)	3	14
2	B	656/663 (99%)	496 (76%)	160 (24%)	1	4
2	D	657/663 (99%)	504 (77%)	153 (23%)	1	4
All	All	1765/1878 (94%)	1366 (77%)	399 (23%)	1	5

5 of 399 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	662	VAL
1	C	123	LEU
2	D	631	LEU
2	B	685	GLU
2	B	768	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	560	GLN
1	C	69	GLN
2	D	525	HIS
2	B	581	GLN
2	B	734	GLN

### 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

4 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	PHE	A	980	-	9,12,12	0.35	0	9,15,15	0.28	0
4	AMP	A	992	-	20,25,25	1.40	3 (15%)	22,38,38	2.63	5 (22%)
3	PHE	C	990	-	9,12,12	0.48	0	9,15,15	0.25	0
4	AMP	C	999	-	20,25,25	1.48	3 (15%)	22,38,38	2.34	2 (9%)

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	PHE	A	980	-	-	0/4/8/8	0/1/1/1
4	AMP	A	992	-	-	0/6/26/26	0/3/3/3
3	PHE	C	990	-	-	0/4/8/8	0/1/1/1
4	AMP	C	999	-	-	0/6/26/26	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	992	AMP	C5-N7	-2.09	1.32	1.39
4	C	999	AMP	P-O3P	2.09	1.62	1.54
4	A	992	AMP	P-O3P	2.21	1.62	1.54
4	C	999	AMP	P-O1P	3.81	1.63	1.51
4	A	992	AMP	P-O1P	3.90	1.64	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	992	AMP	N3-C2-N1	-10.13	121.14	128.89
4	C	999	AMP	N3-C2-N1	-9.76	121.42	128.89
4	A	992	AMP	C4'-O4'-C1'	-3.26	106.14	109.72

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	992	AMP	O3P-P-O5'	-2.28	100.01	106.56
4	A	992	AMP	C2'-C1'-N9	2.16	117.59	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	980	PHE	2	0
4	A	992	AMP	9	0
3	C	990	PHE	1	0
4	C	999	AMP	9	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, 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	242/327 (74%)	-0.17	3 (1%) 81 55	50, 63, 87, 145	0
1	C	323/327 (98%)	0.39	29 (8%) 12 4	36, 89, 164, 169	8 (2%)
2	B	795/795 (100%)	-0.19	3 (0%) 93 79	51, 89, 128, 148	0
2	D	795/795 (100%)	-0.01	10 (1%) 79 52	58, 97, 132, 148	0
All	All	2155/2244 (96%)	-0.04	45 (2%) 67 36	36, 90, 138, 169	8 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	19	SER	6.0
1	C	5	ALA	4.8
1	C	18	ALA	4.8
1	C	59	VAL	4.5
1	C	29	VAL	4.3

### 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	PHE	A	980	12/12	0.89	0.38	2.44	73,80,87,87	0
4	AMP	A	992	23/23	0.91	0.37	2.37	96,99,101,101	0
4	AMP	C	999	23/23	0.80	0.34	1.12	137,145,147,147	0
3	PHE	C	990	12/12	0.93	0.30	0.20	95,98,99,99	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.