



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 30, 2016 – 07:47 AM EST

PDB ID : 4R2N
Title : Crystal structure of Rv3772 in complex with its substrate
Authors : Nasir, N.; Anant, A.; Vyas, R.; Biswal, B.K.
Deposited on : 2014-08-12
Resolution : 1.98 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

<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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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) : rb-20028320

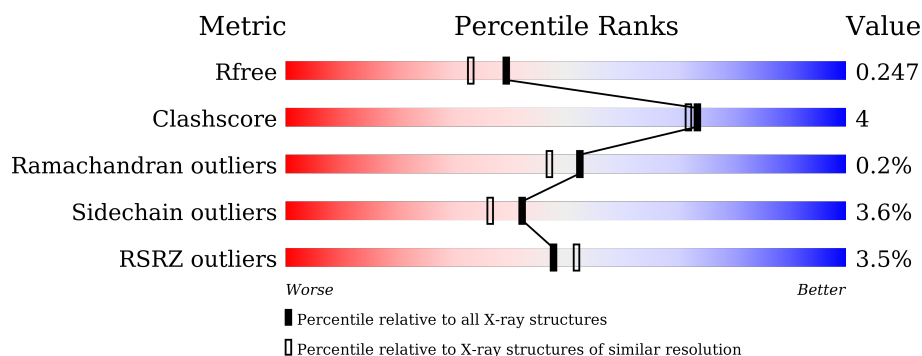
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 $\leq 5\%$. 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	367	<div> <div>4%</div> <div>85% 11% .</div> </div>
1	B	367	<div> <div>2%</div> <div>86% 10% . .</div> </div>
1	C	367	<div> <div>4%</div> <div>86% 10% . .</div> </div>
1	D	367	<div> <div>4%</div> <div>83% 12% . .</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
2	PLP	D	401	-	-	X	-
3	PHE	A	402	-	-	-	X
3	PHE	B	402	-	-	-	X
3	PHE	C	402	-	-	-	X
4	EPE	B	403	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11881 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 Putative phenylalanine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	353	Total	C	N	O	S	0	3	0
			2699	1717	481	495	6			
1	B	353	Total	C	N	O	S	0	3	0
			2703	1718	484	495	6			
1	C	353	Total	C	N	O	S	0	4	0
			2704	1720	482	496	6			
1	D	353	Total	C	N	O	S	0	3	0
			2699	1717	481	495	6			

There are 60 discrepancies between the modelled and reference sequences:

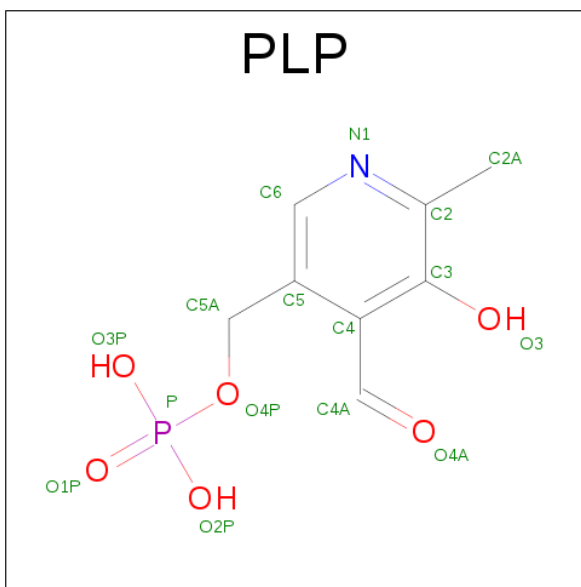
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
A	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
A	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
A	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
A	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
A	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4
A	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
A	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
A	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
A	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
A	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
B	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
B	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
B	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
B	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
B	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4

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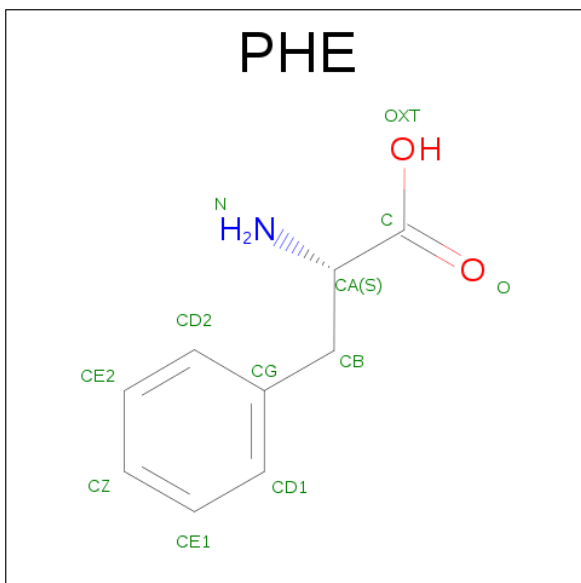
Chain	Residue	Modelled	Actual	Comment	Reference
B	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
B	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
B	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
B	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
B	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
C	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
C	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
C	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
C	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
C	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4
C	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
C	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
C	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
C	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
C	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	0	MET	-	EXPRESSION TAG	UNP I6Y4H4
D	1	VAL	-	EXPRESSION TAG	UNP I6Y4H4
D	354	LYS	-	EXPRESSION TAG	UNP I6Y4H4
D	355	LEU	-	EXPRESSION TAG	UNP I6Y4H4
D	356	ALA	-	EXPRESSION TAG	UNP I6Y4H4
D	357	ALA	-	EXPRESSION TAG	UNP I6Y4H4
D	358	ALA	-	EXPRESSION TAG	UNP I6Y4H4
D	359	LEU	-	EXPRESSION TAG	UNP I6Y4H4
D	360	GLU	-	EXPRESSION TAG	UNP I6Y4H4
D	361	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	362	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	363	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	364	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	365	HIS	-	EXPRESSION TAG	UNP I6Y4H4
D	366	HIS	-	EXPRESSION TAG	UNP I6Y4H4

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



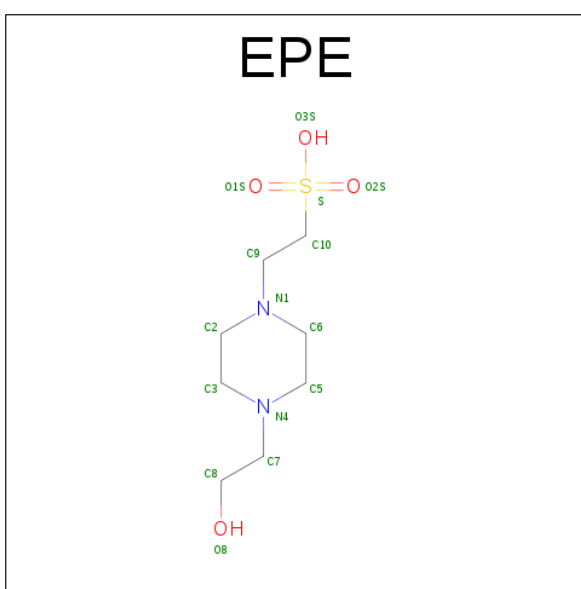
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		

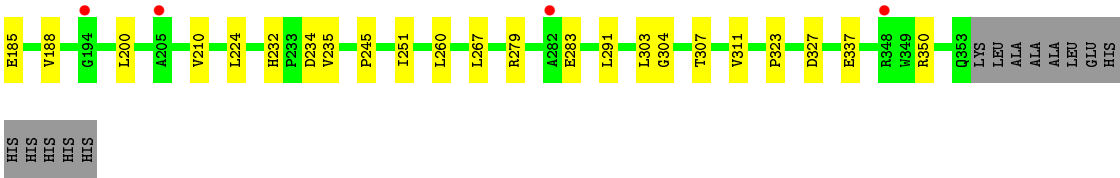
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	246	Total 246	O 246	0	0
5	C	210	Total 210	O 210	0	0
5	D	200	Total 200	O 200	0	0

- Molecule 1: Putative phenylalanine aminotransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.41Å 164.46Å 178.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.21 – 1.98 48.21 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.21-1.98) 99.3 (48.21-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.208 , 0.244 0.214 , 0.247	Depositor DCC
R_{free} test set	5680 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11881	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.72 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.1667e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: EPE, PLP

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	0.34	0/2768	0.55	0/3790
1	B	0.33	0/2772	0.56	0/3794
1	C	0.31	0/2776	0.53	0/3801
1	D	0.33	0/2768	0.55	0/3790
All	All	0.33	0/11084	0.55	0/15175

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2699	0	2726	26	0
1	B	2703	0	2730	22	0
1	C	2704	0	2729	24	0
1	D	2699	0	2723	29	0
2	A	15	0	6	3	0
2	B	15	0	6	0	0
2	C	15	0	6	2	0
2	D	15	0	6	6	0
3	A	12	0	8	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	8	0	0
3	C	12	0	8	0	0
3	D	12	0	8	0	0
4	A	15	0	18	0	0
4	B	15	0	18	0	0
4	C	15	0	18	0	0
4	D	15	0	18	0	0
5	A	252	0	0	1	0
5	B	246	0	0	2	0
5	C	210	0	0	1	0
5	D	200	0	0	0	0
All	All	11881	0	11036	90	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 (90) 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:D:304:GLY:O	1:D:307:THR:HG23	1.78	0.83
1:A:86[A]:VAL:HG11	3:A:402:PHE:CE2	2.15	0.81
1:A:101:ASP:HB3	1:A:148:ARG:HG3	1.72	0.69
1:A:112:LEU:HD21	1:C:245:PRO:HG2	1.75	0.68
1:A:251:ILE:HD12	1:C:224:LEU:HD21	1.76	0.67
1:C:304:GLY:O	1:C:307:THR:HG23	1.94	0.67
1:A:224:LEU:HD21	1:C:251:ILE:HD12	1.76	0.66
1:C:101:ASP:HB3	1:C:148:ARG:HG3	1.77	0.65
1:B:304:GLY:O	1:B:307:THR:HG23	1.97	0.65
1:D:85:SER:OG	2:D:401:PLP:C5A	2.46	0.63
1:D:85:SER:OG	2:D:401:PLP:H5A1	1.99	0.62
1:A:187:TYR:CE1	1:A:217:LYS:HD2	2.35	0.62
1:A:86[A]:VAL:HG11	3:A:402:PHE:HE2	1.62	0.60
1:A:86[A]:VAL:HG13	2:A:401:PLP:C5A	2.31	0.60
1:A:304:GLY:O	1:A:307:THR:HG23	2.02	0.60
1:D:279:ARG:O	1:D:283:GLU:HG2	2.02	0.59
1:D:210[B]:VAL:HG11	1:D:235:VAL:HG11	1.83	0.59
1:C:139:MET:O	1:C:142:THR:HG22	2.03	0.58
1:D:108:ARG:NH1	1:D:327:ASP:OD2	2.37	0.58
1:C:110:PHE:CG	2:C:401:PLP:H2A3	2.40	0.57
1:B:112:LEU:HD21	1:D:245:PRO:HG2	1.87	0.56
1:C:322:ARG:HG2	1:C:324:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:VAL:HA	5:C:622:HOH:O	2.06	0.56
1:A:51:VAL:CG2	1:C:224:LEU:HG	2.36	0.56
1:A:86[A]:VAL:HG13	2:A:401:PLP:H5A1	1.89	0.55
1:A:86[B]:VAL:CG2	1:A:112:LEU:HD22	2.37	0.55
1:B:41[A]:ARG:NH1	1:D:49:ASP:OD1	2.39	0.55
1:D:311:VAL:HG21	1:D:323:PRO:HB3	1.89	0.53
1:D:113:TYR:HB2	1:D:114:PRO:HD3	1.90	0.53
5:A:704:HOH:O	1:C:17:PRO:HB3	2.08	0.53
1:B:311:VAL:HG21	1:B:323:PRO:HB3	1.91	0.53
1:B:187:TYR:CE1	1:B:217:LYS:HD2	2.43	0.52
1:A:86[A]:VAL:HG13	2:A:401:PLP:H5A2	1.91	0.52
1:B:69:HIS:ND1	5:B:618:HOH:O	2.32	0.52
1:D:185:GLU:HB3	1:D:188:VAL:HB	1.92	0.51
1:D:157:ASN:HB3	2:D:401:PLP:H2A1	1.92	0.50
1:B:232:HIS:CD2	1:B:234:ASP:H	2.29	0.50
1:B:125:ILE:HG21	1:B:142:THR:HG23	1.93	0.50
1:D:105:PHE:HB3	1:D:151:PHE:HB2	1.93	0.50
1:C:46:ARG:NH1	1:C:49:ASP:OD2	2.45	0.50
1:B:224:LEU:HD21	1:D:251:ILE:HD12	1.93	0.49
1:D:85:SER:OG	2:D:401:PLP:H5A2	2.11	0.49
1:B:251:ILE:HD12	1:D:224:LEU:HD21	1.93	0.49
1:A:112:LEU:HD21	1:C:245:PRO:CG	2.43	0.48
1:A:311:VAL:HG22	1:A:321:VAL:HG23	1.95	0.48
1:C:303:LEU:HB2	1:C:307:THR:HG22	1.95	0.48
1:D:44:ILE:HG12	1:D:251:ILE:HG23	1.95	0.48
1:C:311:VAL:HG21	1:C:323:PRO:HB3	1.95	0.47
1:D:153:CYS:SG	2:D:401:PLP:H2A2	2.53	0.47
1:C:113:TYR:HB2	1:C:114:PRO:HD3	1.96	0.47
1:B:232:HIS:HD2	1:B:234:ASP:H	1.62	0.47
1:D:232:HIS:HD2	1:D:234:ASP:H	1.63	0.47
1:A:153:CYS:HB3	1:A:156:ASN:HD22	1.81	0.46
1:B:75:ALA:HB1	1:B:76:PRO:HD2	1.98	0.46
1:B:200:LEU:HA	1:B:203:VAL:HG12	1.97	0.45
1:A:113:TYR:HB2	1:A:114:PRO:HD3	1.99	0.45
1:D:110:PHE:CG	2:D:401:PLP:H2A3	2.52	0.45
1:D:232:HIS:CD2	1:D:234:ASP:H	2.35	0.45
1:D:303:LEU:HB2	1:D:307:THR:HG22	1.99	0.45
1:C:232:HIS:HD2	1:C:234:ASP:H	1.64	0.44
1:C:89:CYS:CB	1:C:116:GLN:HE22	2.30	0.44
1:D:180:LEU:HD11	1:D:210[A]:VAL:HG23	1.99	0.44
1:C:15:TYR:O	1:C:16:VAL:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:TRP:CD2	1:B:108:ARG:HA	2.53	0.44
1:B:112:LEU:HD21	1:D:245:PRO:CD	2.48	0.44
1:B:95:VAL:HG23	1:B:96:THR:HG23	1.99	0.44
1:B:112:LEU:HD21	1:D:245:PRO:CG	2.48	0.43
1:D:101:ASP:HB3	1:D:148:ARG:HG3	2.00	0.43
1:C:185:GLU:HB3	1:C:188:VAL:HB	2.01	0.43
1:D:95:VAL:HG23	1:D:96:THR:HG23	2.00	0.43
1:A:107:TRP:CD2	1:A:108:ARG:HA	2.54	0.42
1:B:318:ARG:HD3	5:B:628:HOH:O	2.20	0.42
1:A:311:VAL:HG21	1:A:323:PRO:HB3	2.01	0.42
1:A:75:ALA:HB1	1:A:76:PRO:HD2	2.00	0.42
1:A:28:ALA:HB2	1:A:320:VAL:HG12	2.01	0.42
1:A:304:GLY:HA2	1:A:326:THR:O	2.18	0.42
1:A:215:PHE:HZ	1:A:260:LEU:HD21	1.85	0.41
1:C:279:ARG:O	1:C:283:GLU:HG2	2.19	0.41
1:C:85:SER:OG	2:C:401:PLP:H5A1	2.21	0.41
1:C:107:TRP:CD2	1:C:108:ARG:HA	2.55	0.41
1:A:8:GLU:N	1:A:8:GLU:OE1	2.49	0.41
1:B:241:LYS:HE2	1:D:14:VAL:HG13	2.02	0.41
1:B:55:PRO:HA	1:B:250:SER:OG	2.21	0.41
1:D:125:ILE:HG21	1:D:142:THR:HG23	2.03	0.41
3:A:402:PHE:CD1	3:A:402:PHE:C	2.95	0.40
1:B:86:VAL:CG2	1:B:112:LEU:HD22	2.51	0.40
1:C:337:GLU:CD	1:C:337:GLU:H	2.25	0.40
1:A:105:PHE:HB3	1:A:151:PHE:HB2	2.04	0.40
1:B:192:ARG:HG3	1:B:274:VAL:HG11	2.03	0.40
1:C:232:HIS:CD2	1:C:234:ASP:H	2.39	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	354/367 (96%)	344 (97%)	10 (3%)	0	100	100
1	B	354/367 (96%)	341 (96%)	11 (3%)	2 (1%)	30	21
1	C	355/367 (97%)	345 (97%)	9 (2%)	1 (0%)	46	39
1	D	354/367 (96%)	343 (97%)	11 (3%)	0	100	100
All	All	1417/1468 (96%)	1373 (97%)	41 (3%)	3 (0%)	52	47

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	16	VAL
1	B	18	GLY
1	B	19	LYS

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	285/293 (97%)	275 (96%)	10 (4%)	43	38
1	B	285/293 (97%)	277 (97%)	8 (3%)	51	48
1	C	286/293 (98%)	278 (97%)	8 (3%)	51	48
1	D	285/293 (97%)	272 (95%)	13 (5%)	33	25
All	All	1141/1172 (97%)	1102 (97%)	39 (3%)	42	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	70	LEU
1	A	130	THR
1	A	142	THR
1	A	200	LEU
1	A	203	VAL
1	A	260	LEU
1	A	267	LEU

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Mol	Chain	Res	Type
1	A	291	LEU
1	A	350	ARG
1	B	70	LEU
1	B	111	GLU
1	B	142	THR
1	B	199	SER
1	B	260	LEU
1	B	267	LEU
1	B	291	LEU
1	B	318	ARG
1	C	45	ASP
1	C	46	ARG
1	C	70	LEU
1	C	142	THR
1	C	170	ARG
1	C	199	SER
1	C	200	LEU
1	C	337	GLU
1	D	12	LEU
1	D	46	ARG
1	D	70	LEU
1	D	108	ARG
1	D	131	ASP
1	D	142	THR
1	D	170	ARG
1	D	200	LEU
1	D	260	LEU
1	D	267	LEU
1	D	291	LEU
1	D	337	GLU
1	D	350	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	61	GLN
1	A	116	GLN
1	A	156	ASN
1	A	232	HIS
1	A	308	GLN
1	B	30	ASN

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Mol	Chain	Res	Type
1	B	116	GLN
1	B	156	ASN
1	B	232	HIS
1	C	30	ASN
1	C	116	GLN
1	C	156	ASN
1	C	232	HIS
1	D	30	ASN
1	D	61	GLN
1	D	116	GLN
1	D	156	ASN
1	D	232	HIS

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](#)

12 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
2	PLP	A	401	3	15,15,16	3.47	3 (20%)	21,22,23	1.54	4 (19%)
3	PHE	A	402	2	9,12,12	0.27	0	10,15,15	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EPE	A	403	-	15,15,15	1.81	1 (6%)	19,20,20	3.08	9 (47%)
2	PLP	B	401	3	15,15,16	3.26	3 (20%)	21,22,23	1.26	1 (4%)
3	PHE	B	402	2	9,12,12	0.26	0	10,15,15	0.20	0
4	EPE	B	403	-	15,15,15	1.71	1 (6%)	19,20,20	3.37	11 (57%)
2	PLP	C	401	1	15,15,16	3.54	3 (20%)	21,22,23	1.42	3 (14%)
3	PHE	C	402	-	9,12,12	0.28	0	10,15,15	0.14	0
4	EPE	C	403	-	15,15,15	1.87	1 (6%)	19,20,20	3.43	11 (57%)
2	PLP	D	401	1	15,15,16	3.75	3 (20%)	21,22,23	1.66	6 (28%)
3	PHE	D	402	-	9,12,12	0.24	0	10,15,15	0.17	0
4	EPE	D	403	-	15,15,15	1.81	1 (6%)	19,20,20	3.51	9 (47%)

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
2	PLP	A	401	3	-	0/6/6/8	0/1/1/1
3	PHE	A	402	2	-	0/4/8/8	0/1/1/1
4	EPE	A	403	-	-	0/9/19/19	0/1/1/1
2	PLP	B	401	3	-	0/6/6/8	0/1/1/1
3	PHE	B	402	2	-	0/4/8/8	0/1/1/1
4	EPE	B	403	-	-	0/9/19/19	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
3	PHE	C	402	-	-	0/4/8/8	0/1/1/1
4	EPE	C	403	-	-	0/9/19/19	0/1/1/1
2	PLP	D	401	1	-	0/6/6/8	0/1/1/1
3	PHE	D	402	-	-	0/4/8/8	0/1/1/1
4	EPE	D	403	-	-	0/9/19/19	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	403	EPE	C10-S	-6.96	1.67	1.77
4	D	403	EPE	C10-S	-6.77	1.67	1.77
4	A	403	EPE	C10-S	-6.77	1.67	1.77
4	B	403	EPE	C10-S	-6.34	1.68	1.77
2	A	401	PLP	C3-C4	3.55	1.48	1.40
2	C	401	PLP	C3-C4	3.60	1.48	1.40
2	B	401	PLP	C3-C4	3.65	1.48	1.40
2	D	401	PLP	C3-C4	3.86	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C5-C4	6.54	1.48	1.40
2	C	401	PLP	C5-C4	6.84	1.48	1.40
2	B	401	PLP	C5-C4	7.16	1.49	1.40
2	D	401	PLP	C5-C4	7.49	1.49	1.40
2	B	401	PLP	C3-C2	9.45	1.47	1.40
2	A	401	PLP	C3-C2	10.87	1.48	1.40
2	C	401	PLP	C3-C2	10.91	1.48	1.40
2	D	401	PLP	C3-C2	11.56	1.49	1.40

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PLP	C3-C4-C5	-3.13	115.02	118.68
4	A	403	EPE	C6-C5-N4	-3.13	104.56	110.65
4	C	403	EPE	C6-C5-N4	-3.10	104.61	110.65
4	C	403	EPE	C5-C6-N1	-2.63	105.52	110.65
2	D	401	PLP	P-O4P-C5A	-2.54	114.90	120.79
2	C	401	PLP	O4P-P-O1P	-2.51	100.77	107.08
2	D	401	PLP	C5A-C5-C6	-2.28	115.06	119.33
4	C	403	EPE	O2S-S-O1S	-2.24	107.64	113.96
4	D	403	EPE	O2S-S-O1S	-2.21	107.72	113.96
2	C	401	PLP	C3-C4-C5	-2.07	116.26	118.68
4	B	403	EPE	O2S-S-O1S	-2.03	108.22	113.96
4	B	403	EPE	C5-C6-N1	-2.02	106.72	110.65
4	B	403	EPE	O3S-S-C10	2.06	109.27	104.99
2	D	401	PLP	C5A-C5-C4	2.10	124.45	121.63
2	B	401	PLP	C6-N1-C2	2.17	123.61	119.26
4	B	403	EPE	C7-N4-C5	2.19	116.01	111.25
2	D	401	PLP	C4A-C4-C5	2.21	123.18	120.90
2	C	401	PLP	C6-C5-C4	2.23	120.02	118.12
4	B	403	EPE	O1S-S-C10	2.31	108.50	106.87
2	A	401	PLP	C6-N1-C2	2.34	123.97	119.26
4	B	403	EPE	C9-N1-C6	2.39	116.46	111.25
2	A	401	PLP	C6-C5-C4	2.60	120.33	118.12
2	A	401	PLP	O3P-P-O2P	2.65	117.16	107.44
4	C	403	EPE	C9-N1-C6	2.68	117.09	111.25
2	D	401	PLP	C6-C5-C4	2.75	120.46	118.12
4	A	403	EPE	C9-N1-C6	2.98	117.74	111.25
4	D	403	EPE	C9-N1-C6	3.11	118.02	111.25
4	A	403	EPE	C7-N4-C5	3.27	118.37	111.25
2	A	401	PLP	O3-C3-C2	3.30	122.36	117.53
4	A	403	EPE	O3S-S-C10	3.54	112.34	104.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	EPE	C7-N4-C5	3.57	119.02	111.25
4	D	403	EPE	C7-N4-C5	3.68	119.26	111.25
4	D	403	EPE	C7-N4-C3	4.36	120.74	111.25
4	D	403	EPE	O1S-S-C10	4.37	109.96	106.87
4	C	403	EPE	C7-N4-C3	4.41	120.85	111.25
4	B	403	EPE	C6-N1-C2	4.55	119.05	108.87
4	B	403	EPE	C5-N4-C3	4.58	119.11	108.87
4	D	403	EPE	C6-N1-C2	4.74	119.48	108.87
4	A	403	EPE	C5-N4-C3	4.79	119.60	108.87
4	A	403	EPE	C7-N4-C3	4.94	122.00	111.25
4	C	403	EPE	C6-N1-C2	4.95	119.96	108.87
4	A	403	EPE	C9-N1-C2	4.96	122.04	111.25
4	D	403	EPE	C5-N4-C3	4.97	119.99	108.87
4	C	403	EPE	C5-N4-C3	5.02	120.11	108.87
4	A	403	EPE	C6-N1-C2	5.04	120.16	108.87
4	D	403	EPE	C9-N1-C2	5.16	122.48	111.25
4	A	403	EPE	O2S-S-C10	5.23	110.56	106.87
4	C	403	EPE	O1S-S-C10	5.33	110.64	106.87
4	C	403	EPE	C9-N1-C2	5.36	122.92	111.25
4	B	403	EPE	C9-N1-C2	6.08	124.49	111.25
4	B	403	EPE	C7-N4-C3	6.26	124.87	111.25
4	C	403	EPE	O2S-S-C10	6.91	111.75	106.87
4	B	403	EPE	O2S-S-C10	7.70	112.31	106.87
4	D	403	EPE	O2S-S-C10	8.81	113.09	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	3	0
3	A	402	PHE	3	0
2	C	401	PLP	2	0
2	D	401	PLP	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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, 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	353/367 (96%)	0.36	13 (3%) 45 49	16, 23, 37, 62	0
1	B	353/367 (96%)	0.33	8 (2%) 64 67	17, 23, 38, 69	0
1	C	353/367 (96%)	0.34	13 (3%) 45 49	18, 26, 39, 64	0
1	D	353/367 (96%)	0.43	15 (4%) 40 44	19, 26, 40, 75	0
All	All	1412/1468 (96%)	0.37	49 (3%) 48 52	16, 25, 39, 75	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	18	GLY	5.8
1	B	14	VAL	5.4
1	B	18	GLY	5.1
1	A	13	PRO	4.8
1	D	20	THR	4.5
1	C	137	TYR	4.4
1	D	15	TYR	4.2
1	D	17	PRO	3.8
1	D	14	VAL	3.8
1	B	13	PRO	3.6
1	C	16	VAL	3.6
1	C	17	PRO	3.5
1	D	19	LYS	3.4
1	D	137	TYR	3.4
1	A	1	VAL	3.4
1	C	18	GLY	3.3
1	A	17	PRO	3.1
1	A	20	THR	3.1
1	C	19	LYS	3.0
1	D	1	VAL	3.0
1	A	19	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	20	THR	2.9
1	C	288	GLY	2.9
1	A	18	GLY	2.8
1	B	15	TYR	2.6
1	B	1	VAL	2.6
1	A	14	VAL	2.5
1	A	352	ASP	2.5
1	B	17	PRO	2.4
1	C	15	TYR	2.4
1	D	348	ARG	2.3
1	D	130[A]	THR	2.3
1	A	350	ARG	2.3
1	A	351	SER	2.3
1	A	137	TYR	2.3
1	D	16	VAL	2.3
1	C	167	ALA	2.3
1	C	305	SER	2.2
1	C	9	LEU	2.2
1	D	145	ASP	2.2
1	C	351	SER	2.2
1	C	166	ASP	2.1
1	A	16	VAL	2.1
1	B	352	ASP	2.1
1	D	194	GLY	2.1
1	D	282	ALA	2.1
1	C	350	ARG	2.1
1	D	205	ALA	2.1
1	A	11	GLY	2.1

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	PHE	C	402	12/12	0.52	0.44	12.39	55,59,62,63	0
3	PHE	A	402	12/12	0.77	0.25	4.93	38,39,41,42	1
3	PHE	B	402	12/12	0.79	0.24	3.06	33,38,39,40	1
4	EPE	B	403	15/15	0.93	0.15	2.08	33,35,36,37	0
4	EPE	C	403	15/15	0.95	0.21	1.82	35,39,44,44	0
4	EPE	A	403	15/15	0.93	0.14	1.51	30,37,40,41	0
3	PHE	D	402	12/12	0.50	0.32	1.18	58,60,63,66	0
2	PLP	D	401	15/16	0.96	0.14	1.15	22,31,35,36	0
2	PLP	C	401	15/16	0.95	0.14	1.11	23,30,32,33	0
2	PLP	A	401	15/16	0.96	0.13	0.24	22,26,30,31	0
2	PLP	B	401	15/16	0.97	0.13	0.08	20,24,27,31	0
4	EPE	D	403	15/15	0.94	0.14	-0.20	36,43,50,51	0

6.5 Other polymers

There are no such residues in this entry.