



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2018 – 04:30 PM EST

PDB ID : 5VER
Title : MOUSE KYNURENINE AMINOTRANSFERASE III, RE-REFINEMENT OF THE PDB STRUCTURE 3E2Z
Authors : Wlodawer, A.; Dauter, Z.; Minor, W.; Stanfield, R.; Porebski, P.; Jaskolski, M.; Pozharski, E.; Weichenberger, C.X.; Rupp, B.
Deposited on : 2017-04-05
Resolution : 2.81 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030736

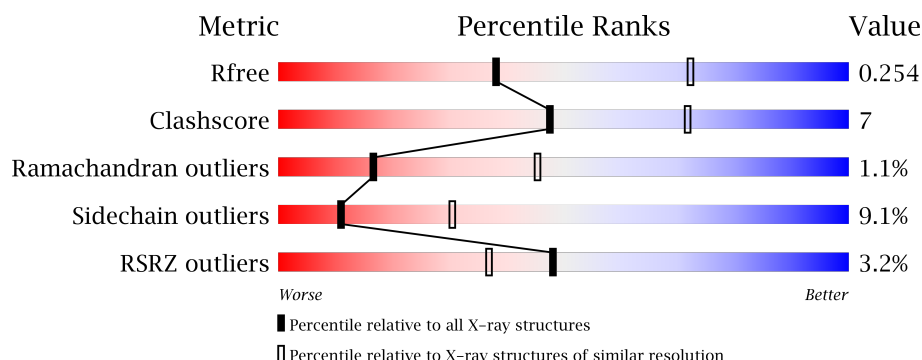
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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}	100719	2917 (2.84-2.80)
Clashscore	112137	3382 (2.84-2.80)
Ramachandran outliers	110173	3324 (2.84-2.80)
Sidechain outliers	110143	3326 (2.84-2.80)
RSRZ outliers	101464	2948 (2.84-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	410	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	B	410	<div> <div>4%</div> <div>80%</div> <div>16%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	A	705	-	-	-	X
8	PEG	B	503	-	-	-	X

2 Entry composition [i](#)

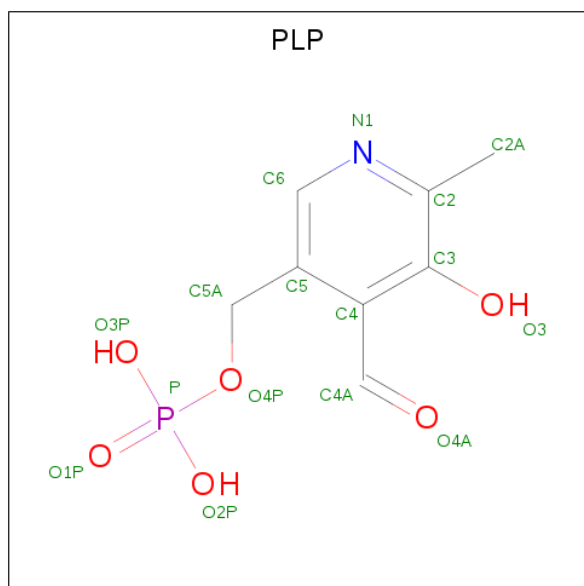
There are 9 unique types of molecules in this entry. The entry contains 6727 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Kynurenine--oxoglutarate transaminase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	1	0
			3260	2107	536	599	18			
1	B	410	Total	C	N	O	S	0	1	0
			3260	2107	536	599	18			

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



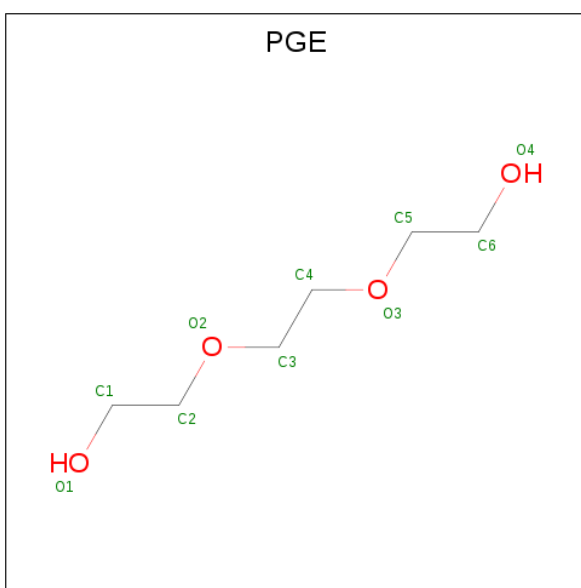
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

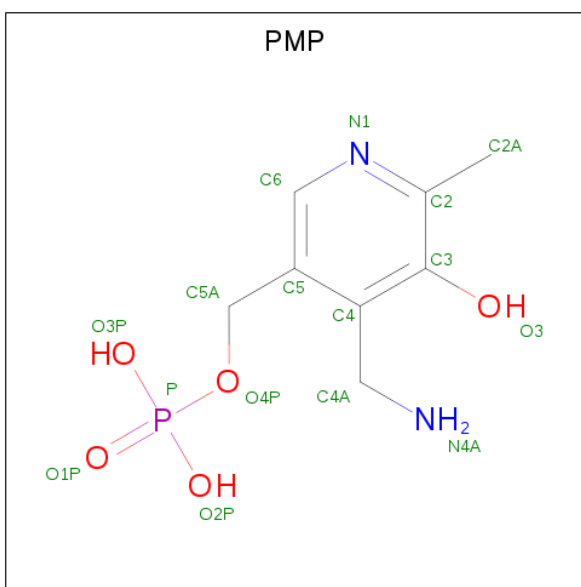


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

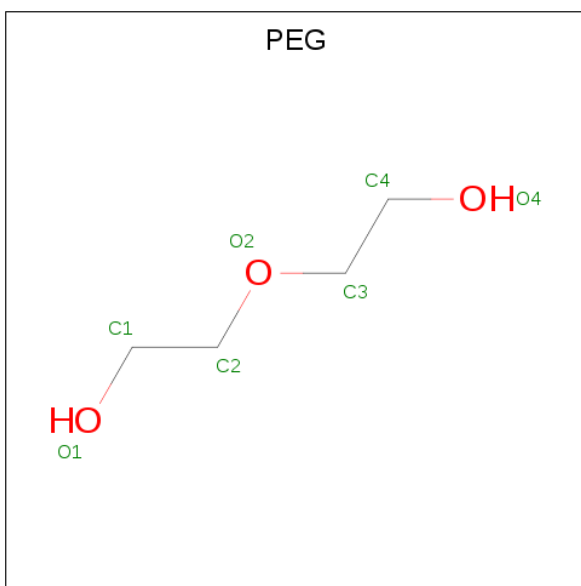
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	A	3	Total	Ca	0	0
			3	3		

- Molecule 7 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: C₈H₁₃N₂O₅P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

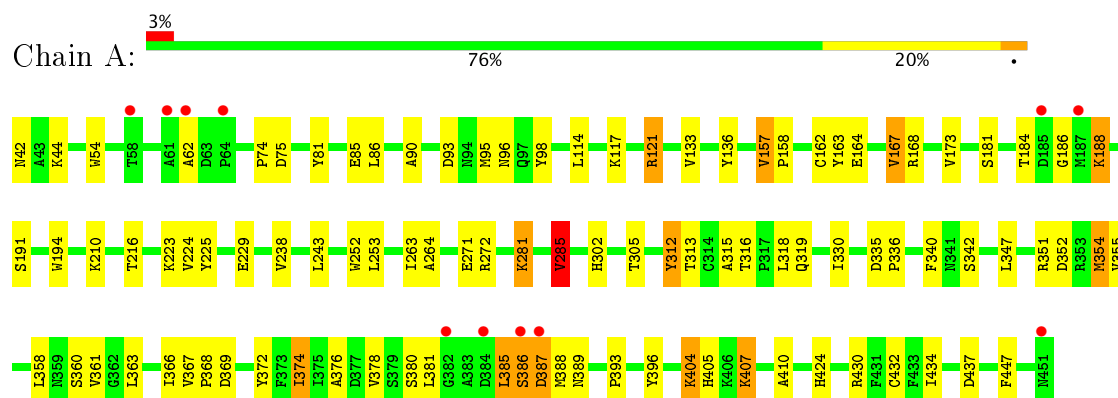
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	55	Total 55	O 55	0	0
9	B	46	Total 46	O 46	0	0

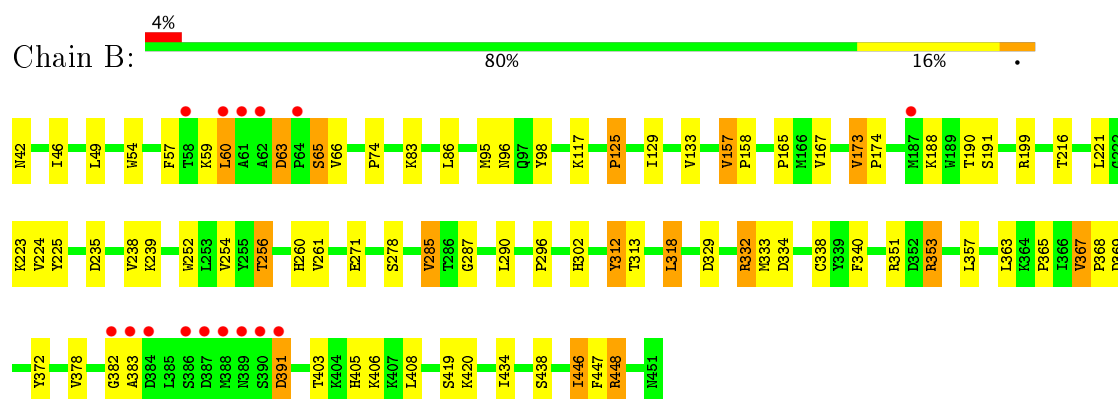
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: Kynurenine--oxoglutarate transaminase 3



- Molecule 1: Kynurenine--oxoglutarate transaminase 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.49 Å 91.49 Å 233.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 2.81 29.64 – 2.81	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.64-2.81) 95.6 (29.64-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 2.80 Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.162 , 0.252 0.165 , 0.254	Depositor DCC
R_{free} test set	1226 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.7	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	6727	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, GOL, PGE, PMP, PLP, CA, PEG

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	0.70	0/3353	0.91	5/4555 (0.1%)
1	B	0.69	0/3353	0.86	2/4555 (0.0%)
All	All	0.70	0/6706	0.89	7/9110 (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	B	0	2
All	All	0	3

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	281	LYS	CB-CA-C	5.87	122.15	110.40
1	A	285	VAL	CB-CA-C	5.56	121.97	111.40
1	A	75	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	63	ASP	CB-CG-OD1	5.29	123.07	118.30
1	B	95	MET	CG-SD-CE	5.25	108.60	100.20
1	A	281	LYS	CD-CE-NZ	5.16	123.57	111.70
1	A	354	MET	CG-SD-CE	5.00	108.21	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	387	ASP	Peptide
1	B	391	ASP	Peptide
1	B	57	PHE	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	3260	0	3236	54	0
1	B	3260	0	3236	50	0
2	A	15	0	6	0	0
3	A	15	0	18	3	0
3	B	15	0	18	2	0
4	A	10	0	14	1	0
5	A	12	0	16	0	0
5	B	12	0	16	2	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
7	B	16	0	10	0	0
8	B	7	0	10	0	0
9	A	55	0	0	0	0
9	B	46	0	0	0	0
All	All	6727	0	6580	92	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 7.

All (92) 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:A:184:THR:HG22	1:A:186:GLY:H	1.29	0.95
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.42	0.84
1:A:352:ASP:O	1:A:355:VAL:HG12	1.83	0.79
1:A:351:ARG:HD2	1:A:368:PRO:HD2	1.67	0.75
1:A:404:LYS:HD2	1:A:405:HIS:CD2	2.25	0.72
1:B:448:ARG:HH11	1:B:448:ARG:HG3	1.58	0.67
1:A:133:VAL:HG21	1:B:133:VAL:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HG23	1:A:158:PRO:HA	1.78	0.66
1:B:448:ARG:HH11	1:B:448:ARG:CG	2.09	0.65
1:A:302:HIS:CE1	1:B:42:ASN:HB2	2.31	0.64
1:A:184:THR:HG23	1:A:188:LYS:O	2.01	0.60
1:B:190:THR:HG22	1:B:367:VAL:HG13	1.84	0.58
1:A:90:ALA:O	1:B:83:LYS:HG2	2.03	0.57
1:A:404:LYS:HD2	1:A:405:HIS:HD2	1.68	0.57
1:B:235:ASP:OD1	5:B:504:GOL:H31	2.05	0.57
1:B:125:PRO:HA	1:B:129:ILE:HD12	1.86	0.56
1:A:361:VAL:HG12	1:A:361:VAL:O	2.05	0.56
1:A:216:THR:HB	1:A:225:TYR:CD1	2.41	0.55
1:B:332:ARG:O	1:B:338:CYS:HB2	2.06	0.55
1:A:252:TRP:CE3	1:A:340:PHE:HB3	2.42	0.54
1:B:191:SER:HB3	1:B:223:LYS:HA	1.90	0.53
1:A:191:SER:OG	1:A:368:PRO:HA	2.08	0.53
1:A:363:LEU:HD22	1:A:378:VAL:HG12	1.90	0.52
1:A:74:PRO:HB3	1:A:434:ILE:HG12	1.92	0.51
3:A:702:EPE:H61	1:B:98:TYR:CE2	2.45	0.51
1:A:385:LEU:O	1:A:386:SER:HB2	2.10	0.51
1:B:60:LEU:HB3	1:B:403:THR:HG21	1.94	0.50
1:A:424:HIS:HB3	4:A:703:PGE:H22	1.94	0.50
1:A:368:PRO:HD3	1:A:374:ILE:HD12	1.94	0.49
1:A:285:VAL:CG2	1:B:96:ASN:HB3	2.43	0.49
1:B:290:LEU:HD11	1:B:318:LEU:HB3	1.94	0.49
1:A:285:VAL:HG23	1:B:96:ASN:HB3	1.94	0.49
1:B:224:VAL:HG23	1:B:369:ASP:HB2	1.94	0.49
1:A:42:ASN:HB3	1:B:302:HIS:CD2	2.47	0.49
1:A:54:TRP:CZ2	3:A:702:EPE:H102	2.48	0.49
1:B:363:LEU:O	1:B:365:PRO:HD3	2.12	0.49
1:A:121:ARG:CG	1:A:121:ARG:HH11	2.22	0.49
1:B:63:ASP:OD1	1:B:65:SER:HB3	2.14	0.48
1:B:271:GLU:HA	1:B:296:PRO:HG3	1.96	0.48
1:A:315:ALA:HA	1:B:287:GLY:O	2.14	0.47
1:B:334:ASP:N	1:B:334:ASP:OD1	2.44	0.47
1:B:448:ARG:HH11	1:B:448:ARG:HB2	1.77	0.47
1:A:194:TRP:HE1	1:A:366:ILE:HD13	1.80	0.47
1:B:448:ARG:CB	1:B:448:ARG:HH11	2.28	0.47
1:B:157:VAL:HA	1:B:158:PRO:C	2.34	0.47
1:A:315:ALA:O	1:A:319:GLN:HG3	2.15	0.47
1:B:173:VAL:HA	1:B:174:PRO:HD2	1.81	0.47
1:B:285:VAL:O	1:B:285:VAL:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:LYS:O	1:B:446:ILE:HG21	2.14	0.47
1:A:95:MET:O	1:A:316:THR:HB	2.16	0.46
1:B:60:LEU:CD2	1:B:63:ASP:HB2	2.46	0.46
1:B:448:ARG:HG3	1:B:448:ARG:NH1	2.24	0.46
1:A:114:LEU:HB2	1:A:330:ILE:HD11	1.97	0.46
1:B:238:VAL:HG21	5:B:504:GOL:H11	1.97	0.46
1:A:42:ASN:HB3	1:B:302:HIS:NE2	2.30	0.46
1:A:163:TYR:O	1:A:167:VAL:HG13	2.16	0.46
1:B:329:ASP:OD1	1:B:332:ARG:NH1	2.48	0.46
1:A:302:HIS:ND1	1:B:42:ASN:HB2	2.30	0.46
1:A:358:LEU:HD13	1:A:376:ALA:HB2	1.98	0.45
1:A:98:TYR:CD2	3:B:502:EPE:H61	2.52	0.45
1:B:216:THR:HB	1:B:225:TYR:CD1	2.52	0.45
1:A:253:LEU:HD22	1:A:347:LEU:HD12	1.99	0.45
1:B:351:ARG:HD2	1:B:368:PRO:HD2	1.99	0.44
1:A:361:VAL:HG21	1:A:447:PHE:HD1	1.82	0.44
1:A:96:ASN:HB3	1:B:285:VAL:HG22	2.00	0.43
1:B:285:VAL:CG1	1:B:285:VAL:O	2.67	0.43
1:A:184:THR:HG22	1:A:186:GLY:N	2.12	0.43
1:A:121:ARG:NH1	1:A:121:ARG:HG2	2.20	0.43
1:A:318:LEU:HD11	1:B:318:LEU:HD22	2.01	0.43
1:A:393:PRO:HD2	1:A:396:TYR:CD1	2.54	0.43
1:A:432:CYS:SG	1:A:434:ILE:HG22	2.57	0.43
1:B:54:TRP:CZ2	3:B:502:EPE:H102	2.54	0.43
1:A:223:LYS:HZ1	1:A:229:GLU:CD	2.22	0.43
3:A:702:EPE:H61	1:B:98:TYR:CD2	2.54	0.42
1:B:353:ARG:O	1:B:357:LEU:HG	2.19	0.42
1:B:357:LEU:HB3	1:B:447:PHE:CD2	2.54	0.42
1:B:49:LEU:HD22	1:B:165:PRO:HB3	2.02	0.42
1:A:404:LYS:O	1:A:407:LYS:NZ	2.53	0.41
1:B:117:LYS:HD3	1:B:333:MET:CE	2.50	0.41
1:B:332:ARG:HH11	1:B:338:CYS:HA	1.84	0.41
1:A:164:GLU:OE2	1:A:168:ARG:NH1	2.51	0.41
1:A:224:VAL:HG23	1:A:369:ASP:HB2	2.02	0.41
1:B:74:PRO:HB3	1:B:434:ILE:HG12	2.02	0.41
1:A:380:SER:O	1:A:381:LEU:HD12	2.21	0.41
1:B:252:TRP:CE3	1:B:340:PHE:HB3	2.56	0.41
1:A:410:ALA:HB1	1:A:430:ARG:O	2.21	0.41
1:A:305:THR:HB	1:B:46:ILE:HD12	2.03	0.41
1:A:263:ILE:HG23	1:A:264:ALA:N	2.36	0.40
1:A:335:ASP:HA	1:A:336:PRO:HD2	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HA	1:A:158:PRO:C	2.42	0.40
1:A:81:TYR:O	1:A:85:GLU:HG2	2.21	0.40
1:B:254:VAL:HG21	1:B:260:HIS:HB2	2.04	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	409/410 (100%)	380 (93%)	25 (6%)	4 (1%)	18	48
1	B	409/410 (100%)	380 (93%)	24 (6%)	5 (1%)	15	42
All	All	818/820 (100%)	760 (93%)	49 (6%)	9 (1%)	17	45

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	SER
1	A	93	ASP
1	B	312	TYR
1	A	312	TYR
1	B	383	ALA
1	A	62	ALA
1	B	59	LYS
1	B	256	THR
1	B	382	GLY

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	359/358 (100%)	326 (91%)	33 (9%)	11	30
1	B	359/358 (100%)	327 (91%)	32 (9%)	11	31
All	All	718/716 (100%)	653 (91%)	65 (9%)	11	30

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	LYS
1	A	86	LEU
1	A	117	LYS
1	A	121	ARG
1	A	136	TYR
1	A	157	VAL
1	A	162	CYS
1	A	167	VAL
1	A	173	VAL
1	A	181	SER
1	A	188	LYS
1	A	210	LYS
1	A	238	VAL
1	A	243	LEU
1	A	271	GLU
1	A	272	ARG
1	A	281	LYS
1	A	285	VAL
1	A	312	TYR
1	A	313	THR
1	A	342	SER
1	A	354	MET
1	A	360	SER
1	A	367	VAL
1	A	372	TYR
1	A	374	ILE
1	A	385	LEU
1	A	387	ASP
1	A	388	MET
1	A	389	ASN
1	A	404	LYS
1	A	407	LYS
1	A	437	ASP

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	65	SER
1	B	66	VAL
1	B	86	LEU
1	B	125	PRO
1	B	157	VAL
1	B	167	VAL
1	B	173	VAL
1	B	188	LYS
1	B	199	ARG
1	B	221	LEU
1	B	239	LYS
1	B	256	THR
1	B	261	VAL
1	B	278	SER
1	B	285	VAL
1	B	312	TYR
1	B	313	THR
1	B	318	LEU
1	B	332	ARG
1	B	353	ARG
1	B	367	VAL
1	B	372	TYR
1	B	378	VAL
1	B	391	ASP
1	B	405	HIS
1	B	408	LEU
1	B	419	SER
1	B	420	LYS
1	B	438	SER
1	B	446	ILE
1	B	448	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	HIS

5.3.3 RNA ⓘ

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](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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	701	1	15,15,16	4.61	3 (20%)	20,22,23	1.70	5 (25%)
3	EPE	A	702	-	15,15,15	2.07	2 (13%)	18,20,20	2.48	5 (27%)
4	PGE	A	703	-	9,9,9	0.77	0	8,8,8	0.71	0
5	GOL	A	704	-	5,5,5	0.39	0	5,5,5	0.59	0
5	GOL	A	705	-	5,5,5	0.52	0	5,5,5	0.68	0
7	PMP	B	501	-	16,16,16	4.25	3 (18%)	20,23,23	1.52	5 (25%)
3	EPE	B	502	-	15,15,15	2.12	1 (6%)	18,20,20	1.64	5 (27%)
8	PEG	B	503	-	6,6,6	0.72	0	5,5,5	0.32	0
5	GOL	B	504	-	5,5,5	0.39	0	5,5,5	0.72	0
5	GOL	B	505	-	5,5,5	0.30	0	5,5,5	1.28	1 (20%)

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	701	1	-	0/6/6/8	0/1/1/1
3	EPE	A	702	-	-	0/9/19/19	0/1/1/1
4	PGE	A	703	-	-	0/7/7/7	0/0/0/0
5	GOL	A	704	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	705	-	-	0/4/4/4	0/0/0/0
7	PMP	B	501	-	-	0/8/8/8	0/1/1/1
3	EPE	B	502	-	-	0/9/19/19	0/1/1/1
8	PEG	B	503	-	-	0/4/4/4	0/0/0/0
5	GOL	B	504	-	-	0/4/4/4	0/0/0/0
5	GOL	B	505	-	-	0/4/4/4	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	EPE	C10-S	-7.71	1.65	1.77
3	A	702	EPE	C10-S	-7.42	1.66	1.77
3	A	702	EPE	O1S-S	2.19	1.51	1.45
2	A	701	PLP	C3-C4	4.41	1.49	1.40
7	B	501	PMP	C3-C4	5.40	1.48	1.40
7	B	501	PMP	C5-C4	6.99	1.50	1.40
2	A	701	PLP	C5-C4	9.85	1.51	1.40
2	A	701	PLP	C3-C2	13.87	1.50	1.40
7	B	501	PMP	C3-C2	14.35	1.50	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	PLP	O3P-P-O4P	-3.30	97.95	106.73
3	A	702	EPE	C2-C3-N4	-3.06	104.43	110.63
7	B	501	PMP	C3-C4-C5	-3.04	115.71	118.71
3	B	502	EPE	C9-N1-C6	-2.64	104.48	111.26
2	A	701	PLP	C3-C4-C5	-2.63	115.64	118.63
3	A	702	EPE	C9-N1-C6	-2.60	104.59	111.26
7	B	501	PMP	O2P-P-O4P	-2.39	100.37	106.73
5	B	505	GOL	O1-C1-C2	-2.39	98.05	110.07
3	B	502	EPE	C6-C5-N4	-2.02	106.54	110.63
3	B	502	EPE	O2S-S-C10	2.14	108.63	106.79
7	B	501	PMP	C6-C5-C4	2.27	119.81	118.13
7	B	501	PMP	C6-N1-C2	2.38	123.85	119.26
7	B	501	PMP	O3P-P-O2P	2.57	117.99	107.61
2	A	701	PLP	C6-C5-C4	2.67	120.41	118.18
2	A	701	PLP	C6-N1-C2	2.90	124.84	119.26
2	A	701	PLP	C4A-C4-C5	2.98	123.86	120.86
3	B	502	EPE	C6-N1-C2	2.98	115.61	108.87
3	A	702	EPE	O1S-S-C10	3.45	109.75	106.79
3	B	502	EPE	O3S-S-C10	3.61	110.49	106.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	EPE	C6-N1-C2	4.73	119.59	108.87
3	A	702	EPE	O2S-S-C10	5.96	111.91	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	702	EPE	3	0
4	A	703	PGE	1	0
3	B	502	EPE	2	0
5	B	504	GOL	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

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	410/410 (100%)	-0.48	11 (2%) 55 44	13, 25, 61, 111	0
1	B	410/410 (100%)	-0.40	15 (3%) 42 31	14, 27, 70, 109	0
All	All	820/820 (100%)	-0.44	26 (3%) 48 37	13, 26, 62, 111	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	386	SER	5.0
1	B	58	THR	4.8
1	B	384	ASP	4.4
1	A	382	GLY	4.2
1	B	382	GLY	4.2
1	B	187	MET	3.5
1	B	62	ALA	3.4
1	A	451	ASN	3.4
1	B	387	ASP	3.3
1	B	391	ASP	3.2
1	B	60	LEU	3.0
1	A	384	ASP	3.0
1	B	61	ALA	2.9
1	B	389	ASN	2.9
1	B	390	SER	2.6
1	B	64	PRO	2.4
1	B	383	ALA	2.4
1	A	62	ALA	2.4
1	A	386	SER	2.4
1	A	61	ALA	2.4
1	A	58	THR	2.4
1	A	187	MET	2.3
1	A	185	ASP	2.3
1	B	388	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	64	PRO	2.0
1	A	387	ASP	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
5	GOL	A	705	6/6	0.92	0.22	2.96	34,47,57,63	0
8	PEG	B	503	7/7	0.92	0.16	2.43	31,33,40,46	0
4	PGE	A	703	10/10	0.92	0.16	1.46	29,38,45,47	0
5	GOL	B	504	6/6	0.89	0.21	1.18	41,42,46,54	0
5	GOL	A	704	6/6	0.95	0.15	0.89	21,23,31,37	0
7	PMP	B	501	16/16	0.98	0.18	0.52	21,32,39,43	0
2	PLP	A	701	15/16	0.98	0.17	-0.10	14,24,32,34	0
3	EPE	A	702	15/15	0.98	0.13	-0.29	18,30,46,46	0
3	EPE	B	502	15/15	0.97	0.13	-0.41	29,40,51,55	0
6	CA	B	506	1/1	0.99	0.04	-2.63	32,32,32,32	0
6	CA	A	707	1/1	0.99	0.03	-3.51	33,33,33,33	0
5	GOL	B	505	6/6	0.95	0.16	-	28,31,33,45	0
6	CA	A	708	1/1	0.96	0.08	-	48,48,48,48	0
6	CA	A	706	1/1	0.98	0.03	-	32,32,32,32	1

6.5 Other polymers [i](#)

There are no such residues in this entry.