



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:15 AM UTC

PDB ID : 5VEP / pdb_00005vep
Title : MOUSE KYNURENINE AMINOTRANSFERASE III, RE-REFINEMENT OF THE PDB STRUCTURE 3E2F
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Deposited on : 2017-04-05
Resolution : 2.59 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

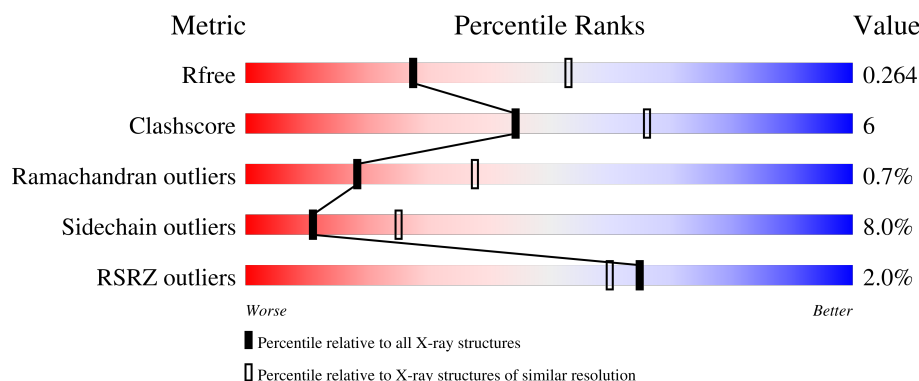
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	82% 16% .
1	B	410	3% 78% 18% .

2 Entry composition [i](#)

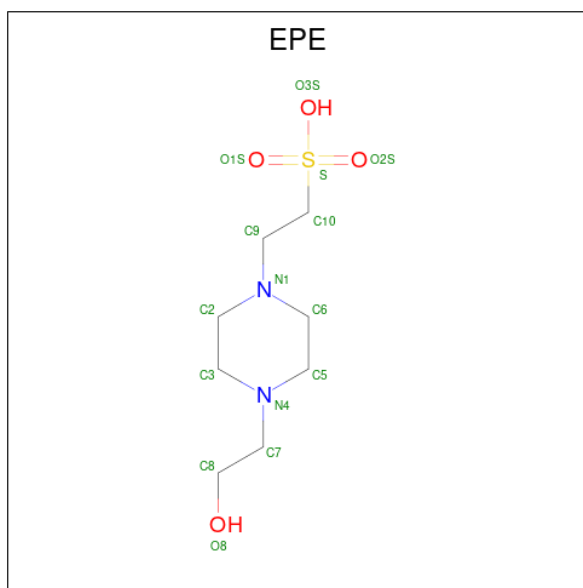
There are 6 unique types of molecules in this entry. The entry contains 6782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

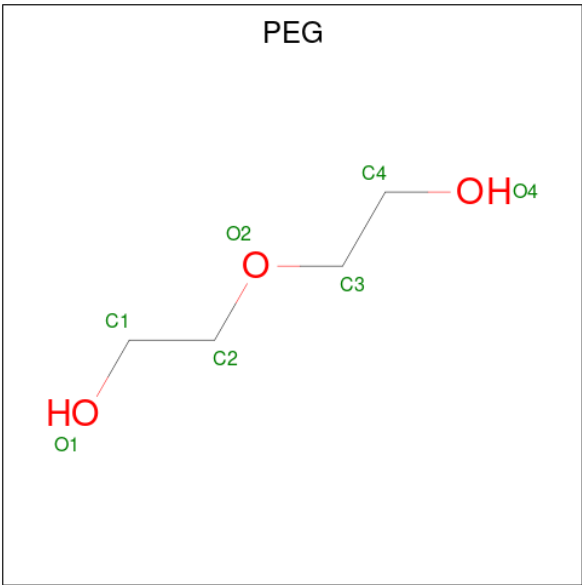
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	P	S	0	0	0
			3268	2108	537	604	1	18			
1	B	410	Total	C	N	O	P	S	0	0	0
			3268	2108	537	604	1	18			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



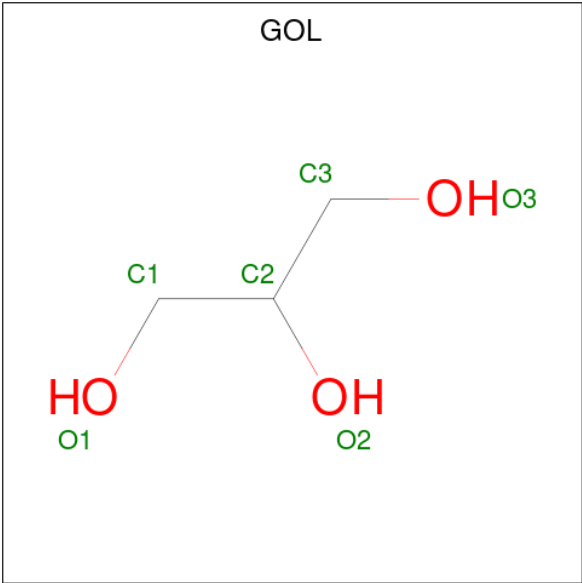
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

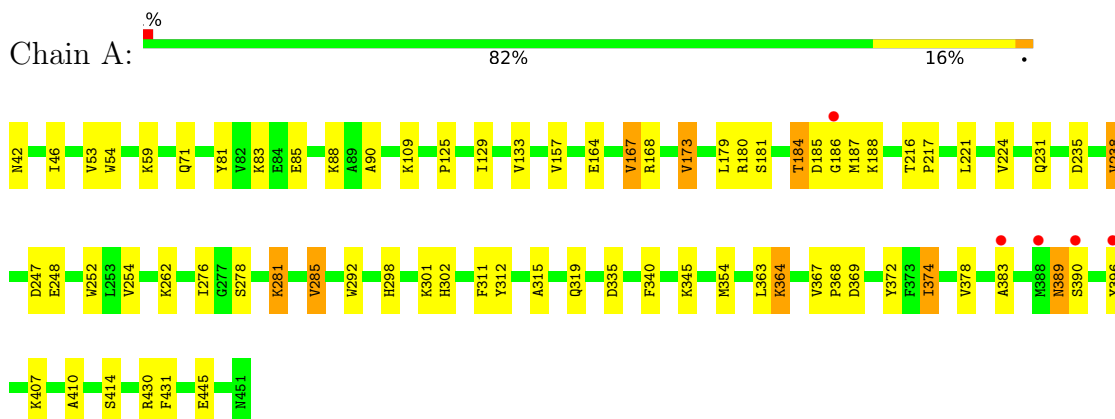
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total	O	0	0
			72	72		
6	B	90	Total	O	0	0
			90	90		

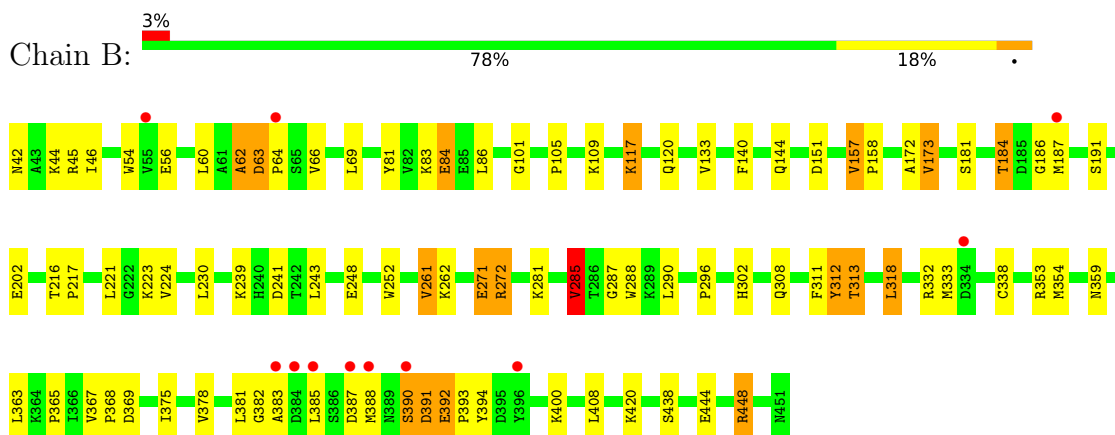
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 ($RSRZ > 2$). 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	91.82Å 91.82Å 233.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.21 – 2.59 29.21 – 2.59	Depositor EDS
% Data completeness (in resolution range)	90.9 (29.21-2.59) 90.9 (29.21-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.264 0.193 , 0.264	Depositor DCC
R_{free} test set	1476 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6782	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: PEG, GOL, CA, LLP, EPE

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	0.84	0/3331	1.11	7/4525 (0.2%)
1	B	0.82	0/3331	1.11	7/4525 (0.2%)
All	All	0.83	0/6662	1.11	14/9050 (0.2%)

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	B	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	285	VAL	CB-CA-C	7.57	123.70	111.29
1	A	173	VAL	CB-CA-C	6.21	117.92	110.78
1	B	392	GLU	CA-C-N	6.08	126.04	119.78
1	B	392	GLU	C-N-CA	6.08	126.04	119.78
1	B	187	MET	N-CA-C	5.97	117.59	111.14
1	B	285	VAL	CB-CA-C	5.92	120.99	111.29
1	A	389	ASN	N-CA-C	5.72	117.61	108.41
1	A	167	VAL	N-CA-CB	5.50	118.01	110.54
1	A	46	ILE	N-CA-C	5.47	117.37	112.17
1	A	238	VAL	N-CA-CB	5.37	117.45	110.57
1	B	393	PRO	N-CA-C	5.32	119.67	111.21
1	B	173	VAL	CB-CA-C	5.31	116.96	110.85
1	A	364	LYS	CB-CA-C	5.25	115.17	110.44
1	B	391	ASP	N-CA-C	5.01	118.47	110.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	391	ASP	Peptide

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	3268	0	3235	34	0
1	B	3268	0	3235	52	0
2	A	15	0	18	3	0
2	B	15	0	18	3	0
3	A	7	0	10	0	0
3	B	7	0	10	0	0
4	A	24	0	32	2	0
4	B	12	0	16	1	0
5	A	3	0	0	0	0
5	B	1	0	0	0	0
6	A	72	0	0	0	0
6	B	90	0	0	1	0
All	All	6782	0	6574	79	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 6.

All (79) 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:184:THR:HG23	1:B:186:GLY:H	1.45	0.81
1:B:62:ALA:O	1:B:64:PRO:HD3	1.93	0.68
1:A:224:VAL:HG23	1:A:369:ASP:HB2	1.75	0.68
1:B:448:ARG:HH11	1:B:448:ARG:HG3	1.59	0.67
1:A:42:ASN:HB3	1:B:302:HIS:CE1	2.31	0.66
1:B:312:TYR:CD2	1:B:313:THR:HG22	2.33	0.64
1:B:448:ARG:HH11	1:B:448:ARG:CG	2.11	0.64
1:B:311:PHE:HB2	6:B:662:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:VAL:HG21	1:B:133:VAL:HG21	1.82	0.60
1:A:184:THR:CG2	1:A:186:GLY:H	2.17	0.58
1:B:202:GLU:OE2	1:B:239:LYS:NZ	2.36	0.57
1:B:117:LYS:HE3	1:B:333:MET:CE	2.34	0.57
1:B:312:TYR:HD2	1:B:313:THR:HG22	1.70	0.57
1:B:101:GLY:HA2	1:B:313:THR:HB	1.86	0.56
1:B:69:LEU:HD13	1:B:354:MET:HE1	1.88	0.55
1:A:184:THR:HG23	1:A:186:GLY:H	1.73	0.54
1:A:311:PHE:CD1	1:B:311:PHE:CZ	2.96	0.54
1:B:252:TRP:CZ3	4:B:504:GOL:H2	2.43	0.53
1:B:332:ARG:O	1:B:338:CYS:HB2	2.09	0.52
1:A:54:TRP:CE2	2:A:501:EPE:H61	2.44	0.52
1:A:54:TRP:CH2	2:A:501:EPE:H101	2.45	0.52
1:A:311:PHE:HD1	1:B:311:PHE:CZ	2.27	0.52
1:B:448:ARG:HG3	1:B:448:ARG:NH1	2.25	0.52
1:A:164:GLU:OE2	1:A:168:ARG:NH1	2.43	0.50
1:A:315:ALA:HA	1:B:287:GLY:O	2.11	0.50
1:B:191:SER:OG	1:B:368:PRO:HA	2.11	0.50
1:B:230:LEU:HD12	1:B:261:VAL:HG22	1.94	0.50
1:B:216:THR:HA	1:B:217:PRO:C	2.36	0.50
1:A:363:LEU:HD22	1:A:378:VAL:HG12	1.94	0.49
1:B:63:ASP:HB2	1:B:66:VAL:H	1.78	0.49
1:A:185:ASP:OD1	1:A:187:MET:N	2.45	0.49
1:A:216:THR:HA	1:A:217:PRO:C	2.38	0.49
1:B:363:LEU:HD22	1:B:378:VAL:HG12	1.95	0.49
1:A:302:HIS:CE1	1:B:42:ASN:HB3	2.49	0.48
1:B:117:LYS:HE3	1:B:333:MET:HE1	1.96	0.48
1:A:90:ALA:O	1:B:83:LYS:HG2	2.14	0.47
1:B:45:ARG:HG3	1:B:46:ILE:HG23	1.95	0.47
1:B:117:LYS:HE3	1:B:333:MET:HE3	1.96	0.47
1:B:363:LEU:O	1:B:365:PRO:HD3	2.15	0.47
1:A:396:TYR:HE1	1:A:414:SER:OG	1.98	0.47
1:B:60:LEU:HD21	1:B:400:LYS:HG2	1.96	0.47
1:A:125:PRO:HA	1:A:129:ILE:HD12	1.97	0.46
1:B:448:ARG:HH11	1:B:448:ARG:CB	2.29	0.46
1:B:353:ARG:HH11	1:B:444:GLU:HG3	1.80	0.46
1:B:54:TRP:CE2	2:B:501:EPE:H61	2.51	0.46
1:B:151:ASP:O	1:B:172:ALA:HB1	2.15	0.46
1:B:81:TYR:HA	1:B:84:GLU:HB2	1.98	0.45
1:B:290:LEU:HD11	1:B:318:LEU:HB3	1.99	0.45
1:B:184:THR:HG23	1:B:186:GLY:N	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:GLU:OE1	1:A:262:LYS:HG2	2.15	0.45
1:A:231:GLN:NE2	1:A:235:ASP:OD1	2.48	0.45
1:B:157:VAL:HA	1:B:158:PRO:C	2.41	0.45
1:B:54:TRP:CD2	2:B:501:EPE:H61	2.53	0.44
1:B:120:GLN:HA	1:B:120:GLN:OE1	2.18	0.44
1:A:81:TYR:O	1:A:85:GLU:HG2	2.18	0.44
1:A:298:HIS:HA	1:A:301:LYS:HE2	2.00	0.44
1:A:247:ASP:OD2	1:A:281:LLP:N1	2.52	0.43
1:A:368:PRO:HD3	1:A:374:ILE:HD12	2.01	0.43
1:A:410:ALA:HB1	1:A:430:ARG:O	2.19	0.43
1:A:354:MET:HE1	1:A:431:PHE:HB3	2.01	0.43
1:B:140:PHE:CZ	1:B:144:GLN:HG3	2.54	0.43
1:A:181:SER:O	4:A:503:GOL:O3	2.35	0.42
1:B:248:GLU:OE1	1:B:262:LYS:HG2	2.19	0.42
1:B:86:LEU:HD22	1:B:288:TRP:CZ2	2.54	0.42
1:A:54:TRP:CD2	2:A:501:EPE:H61	2.55	0.42
1:A:164:GLU:O	1:A:168:ARG:HG3	2.20	0.42
1:B:224:VAL:HG23	1:B:369:ASP:HB2	2.02	0.42
1:A:276:ILE:HA	1:A:292:TRP:O	2.19	0.41
1:B:383:ALA:HB1	1:B:394:TYR:OH	2.20	0.41
1:A:231:GLN:HE22	4:A:504:GOL:H12	1.85	0.41
1:B:241:ASP:OD1	1:B:272:ARG:NH2	2.52	0.41
1:B:221:LEU:HA	1:B:375:ILE:HD12	2.02	0.41
1:B:285:VAL:HG13	1:B:285:VAL:O	2.20	0.41
1:A:252:TRP:CE3	1:A:340:PHE:HB3	2.56	0.41
1:B:69:LEU:HD12	1:B:408:LEU:HD11	2.02	0.41
1:A:312:TYR:CE1	2:B:501:EPE:H71	2.55	0.40
1:B:271:GLU:HA	1:B:296:PRO:HG3	2.03	0.40
1:A:315:ALA:O	1:A:319:GLN:HG3	2.21	0.40
1:B:191:SER:HB3	1:B:223:LYS:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	407/410 (99%)	385 (95%)	20 (5%)	2 (0%)	24	46
1	B	407/410 (99%)	387 (95%)	16 (4%)	4 (1%)	12	28
All	All	814/820 (99%)	772 (95%)	36 (4%)	6 (1%)	18	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	390	SER
1	A	383	ALA
1	B	62	ALA
1	B	382	GLY
1	A	390	SER
1	B	312	TYR

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	357/357 (100%)	330 (92%)	27 (8%)	12	27
1	B	357/357 (100%)	327 (92%)	30 (8%)	10	23
All	All	714/714 (100%)	657 (92%)	57 (8%)	11	25

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	A	59	LYS
1	A	71	GLN
1	A	83	LYS
1	A	88	LYS
1	A	109	LYS
1	A	157	VAL

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Mol	Chain	Res	Type
1	A	167	VAL
1	A	173	VAL
1	A	179	LEU
1	A	180	ARG
1	A	184	THR
1	A	188	LYS
1	A	221	LEU
1	A	238	VAL
1	A	254	VAL
1	A	278	SER
1	A	285	VAL
1	A	335	ASP
1	A	345	LYS
1	A	364	LYS
1	A	367	VAL
1	A	372	TYR
1	A	374	ILE
1	A	389	ASN
1	A	407	LYS
1	A	445	GLU
1	B	44	LYS
1	B	56	GLU
1	B	63	ASP
1	B	84	GLU
1	B	105	PRO
1	B	109	LYS
1	B	117	LYS
1	B	157	VAL
1	B	173	VAL
1	B	181	SER
1	B	184	THR
1	B	243	LEU
1	B	261	VAL
1	B	271	GLU
1	B	272	ARG
1	B	285	VAL
1	B	308	GLN
1	B	313	THR
1	B	318	LEU
1	B	359	ASN
1	B	367	VAL
1	B	381	LEU

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Mol	Chain	Res	Type
1	B	385	LEU
1	B	387	ASP
1	B	388	MET
1	B	390	SER
1	B	392	GLU
1	B	420	LYS
1	B	438	SER
1	B	448	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	258	HIS
1	A	341	ASN
1	A	451	ASN
1	B	42	ASN
1	B	94	ASN
1	B	144	GLN
1	B	231	GLN
1	B	405	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	281	1	23,24,25	2.32	5 (21%)	25,32,34	1.65	5 (20%)
1	LLP	B	281	1	23,24,25	2.69	5 (21%)	25,32,34	1.55	4 (16%)

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
1	LLP	A	281	1	-	9/16/17/19	0/1/1/1
1	LLP	B	281	1	-	8/16/17/19	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	LLP	C3-C2	7.78	1.49	1.41
1	A	281	LLP	C3-C2	6.20	1.47	1.41
1	B	281	LLP	C4'-NZ	6.04	1.47	1.27
1	B	281	LLP	C4-C5	5.53	1.49	1.42
1	A	281	LLP	C4'-NZ	5.21	1.44	1.27
1	A	281	LLP	C4-C5	4.73	1.48	1.42
1	B	281	LLP	C4-C3	4.65	1.48	1.41
1	A	281	LLP	C4-C3	4.47	1.48	1.41
1	B	281	LLP	C4-C4'	2.70	1.52	1.46
1	A	281	LLP	C4-C4'	2.00	1.50	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	281	LLP	C4-C4'-NZ	-4.97	101.09	124.04
1	B	281	LLP	C4-C3-C2	-4.64	117.53	120.14
1	B	281	LLP	C4-C4'-NZ	-3.40	108.34	124.04
1	A	281	LLP	C6-N1-C2	2.82	124.32	119.20
1	B	281	LLP	C6-N1-C2	2.62	123.95	119.20
1	A	281	LLP	C3-C2-N1	-2.41	117.93	120.96
1	A	281	LLP	CE-NZ-C4'	2.35	126.24	118.72
1	A	281	LLP	C4-C3-C2	-2.09	118.97	120.14
1	B	281	LLP	O3-C3-C2	2.06	121.85	117.58

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	281	LLP	C5'-OP4-P-OP2
1	A	281	LLP	C5'-OP4-P-OP3
1	B	281	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	B	281	LLP	C5'-OP4-P-OP2
1	B	281	LLP	C5'-OP4-P-OP3
1	A	281	LLP	C4-C4'-NZ-CE
1	A	281	LLP	C3-C4-C4'-NZ
1	B	281	LLP	CG-CD-CE-NZ
1	A	281	LLP	C5'-OP4-P-OP1
1	B	281	LLP	C5'-OP4-P-OP1
1	B	281	LLP	C3-C4-C4'-NZ
1	A	281	LLP	C5-C4-C4'-NZ
1	A	281	LLP	CD-CE-NZ-C4'
1	A	281	LLP	N-CA-CB-CG
1	B	281	LLP	CD-CE-NZ-C4'
1	B	281	LLP	C5-C4-C4'-NZ
1	A	281	LLP	CG-CD-CE-NZ

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	281	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	GOL	B	504	-	5,5,5	0.35	0	5,5,5	0.73	0
4	GOL	A	506	-	5,5,5	0.43	0	5,5,5	0.46	0
4	GOL	A	504	-	5,5,5	0.29	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EPE	B	501	-	15,15,15	1.82	1 (6%)	19,20,20	1.53	4 (21%)
3	PEG	B	502	-	6,6,6	0.61	0	5,5,5	0.63	0
3	PEG	A	502	-	6,6,6	0.79	0	5,5,5	0.73	0
4	GOL	A	503	-	5,5,5	0.15	0	5,5,5	0.63	0
4	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.64	0
4	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.29	0
2	EPE	A	501	-	15,15,15	2.13	1 (6%)	19,20,20	1.69	5 (26%)

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
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	A	506	-	-	4/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
2	EPE	B	501	-	-	5/9/19/19	0/1/1/1
3	PEG	B	502	-	-	2/4/4/4	-
3	PEG	A	502	-	-	4/4/4/4	-
4	GOL	A	503	-	-	3/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	B	503	-	-	4/4/4/4	-
2	EPE	A	501	-	-	4/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EPE	C10-S	-7.65	1.66	1.77
2	B	501	EPE	C10-S	-6.30	1.68	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	EPE	C2-C3-N4	3.84	118.40	110.65
2	B	501	EPE	O2S-S-C10	3.67	112.27	106.73
2	A	501	EPE	C6-N1-C2	3.24	115.82	108.84
2	A	501	EPE	O1S-S-C10	2.73	110.85	106.73
2	A	501	EPE	C5-N4-C3	2.56	114.36	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	EPE	O2S-S-O1S	-2.43	105.92	113.82
2	A	501	EPE	C3-C2-N1	2.39	115.47	110.65
2	B	501	EPE	O1S-S-C10	2.34	110.27	106.73
2	B	501	EPE	C9-N1-C6	-2.23	105.30	111.24

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	EPE	C10-C9-N1-C2
2	B	501	EPE	C10-C9-N1-C6
2	B	501	EPE	C9-C10-S-O1S
2	B	501	EPE	C9-C10-S-O2S
2	B	501	EPE	C9-C10-S-O3S
4	A	503	GOL	O1-C1-C2-C3
4	A	505	GOL	C1-C2-C3-O3
4	A	506	GOL	O1-C1-C2-C3
4	B	503	GOL	C1-C2-C3-O3
4	B	504	GOL	C1-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	A	506	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
3	B	502	PEG	O2-C3-C4-O4
4	A	503	GOL	O1-C1-C2-O2
4	A	506	GOL	O1-C1-C2-O2
4	A	506	GOL	O2-C2-C3-O3
4	B	504	GOL	O2-C2-C3-O3
4	B	503	GOL	O1-C1-C2-O2
4	B	503	GOL	O2-C2-C3-O3
2	A	501	EPE	C10-C9-N1-C2
2	A	501	EPE	C10-C9-N1-C6
4	A	503	GOL	C1-C2-C3-O3
3	A	502	PEG	O1-C1-C2-O2
3	B	502	PEG	C1-C2-O2-C3
2	A	501	EPE	C8-C7-N4-C3
3	A	502	PEG	C4-C3-O2-C2
3	A	502	PEG	C1-C2-O2-C3
3	A	502	PEG	O2-C3-C4-O4
2	A	501	EPE	C8-C7-N4-C5

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	504	GOL	1	0
4	A	504	GOL	1	0
2	B	501	EPE	3	0
4	A	503	GOL	1	0
2	A	501	EPE	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	409/410 (99%)	-0.29	5 (1%) 76 73	23, 32, 61, 84	0
1	B	409/410 (99%)	-0.16	11 (2%) 56 50	25, 35, 73, 94	0
All	All	818/820 (99%)	-0.23	16 (1%) 65 60	23, 33, 64, 94	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	VAL	3.8
1	B	387	ASP	3.2
1	B	390	SER	3.2
1	B	384	ASP	3.1
1	B	64	PRO	3.1
1	A	383	ALA	3.0
1	A	390	SER	2.5
1	B	396	TYR	2.4
1	B	383	ALA	2.3
1	B	385	LEU	2.3
1	B	334	ASP	2.3
1	A	388	MET	2.2
1	B	187	MET	2.2
1	B	388	MET	2.1
1	A	396	TYR	2.1
1	A	186	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	281	24/25	0.97	0.06	25,26,27,27	0
1	LLP	B	281	24/25	0.97	0.06	28,29,29,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	PEG	B	502	7/7	0.85	0.13	42,43,43,43	0
4	GOL	B	504	6/6	0.87	0.11	37,38,39,39	0
4	GOL	A	505	6/6	0.88	0.11	50,51,51,51	0
4	GOL	B	503	6/6	0.89	0.11	48,50,51,51	0
3	PEG	A	502	7/7	0.89	0.12	37,38,38,38	0
4	GOL	A	506	6/6	0.90	0.12	44,45,45,45	0
2	EPE	B	501	15/15	0.91	0.12	53,55,59,59	0
4	GOL	A	504	6/6	0.93	0.08	43,43,44,44	0
4	GOL	A	503	6/6	0.94	0.09	44,44,45,45	0
5	CA	A	507	1/1	0.94	0.12	45,45,45,45	1
2	EPE	A	501	15/15	0.95	0.09	50,52,53,54	0
5	CA	A	509	1/1	0.95	0.05	51,51,51,51	0
5	CA	A	508	1/1	0.97	0.07	45,45,45,45	0
5	CA	B	505	1/1	0.98	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.