Full wwPDB X-ray Structure Validation Report (i)

Apr 7, 2022 – 10:18 AM EDT

PDB ID	:	5VEP
Title	:	MOUSE KYNURENINE AMINOTRANSFERASE III, RE-REFINEMENT OF THE PDB STRUCTURE 3E2F
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	:	2.59 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 (i) symbol.

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

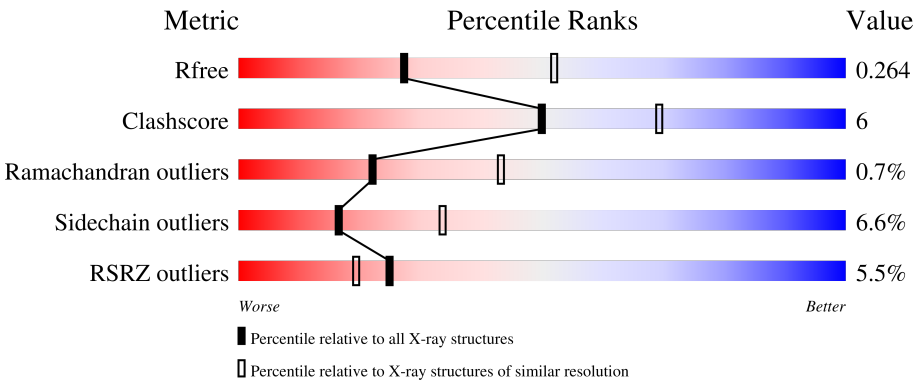
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	4% 84% 16% •
1	B	410	7% 79% 18% •

2 Entry composition (i)

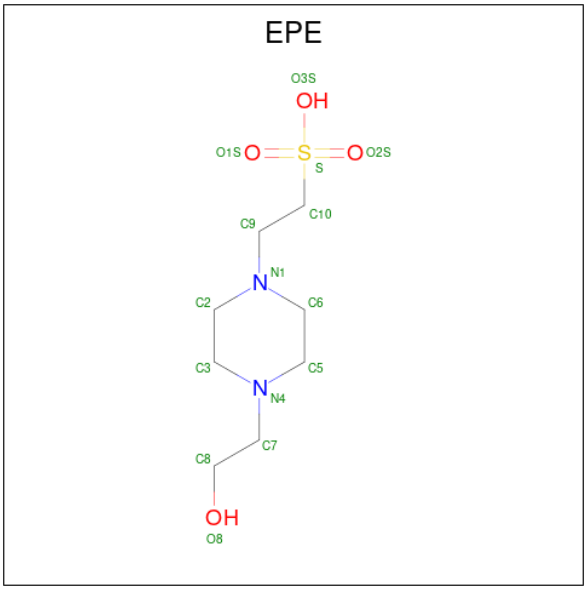
There are 6 unique types of molecules in this entry. The entry contains 6782 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

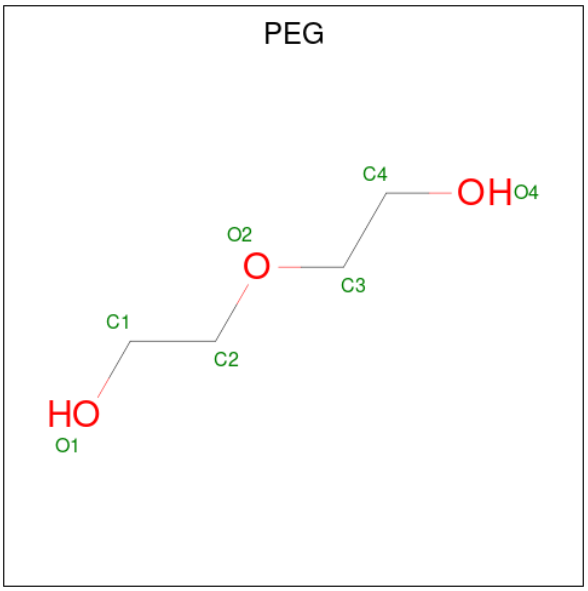
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	410	3268	2108	537	604	1	18	0	0	0
1	B	410	3268	2108	537	604	1	18	0	0	0

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



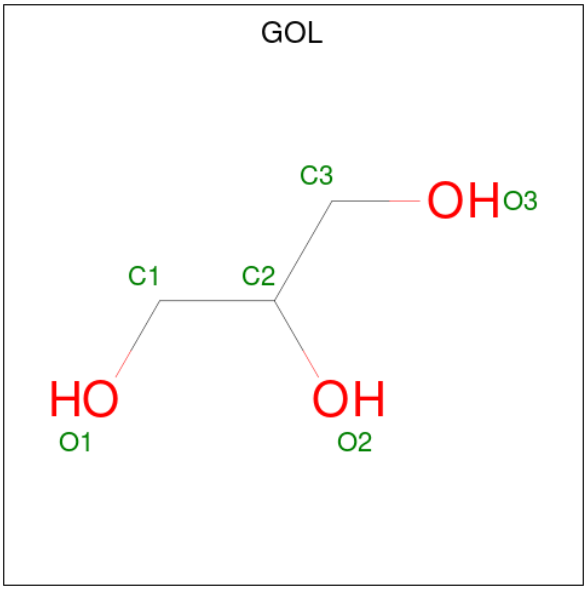
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	15	8	2	4	1	0	0
2	B	1	15	8	2	4	1	0	0

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is water.

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

3 Residue-property plots (i)

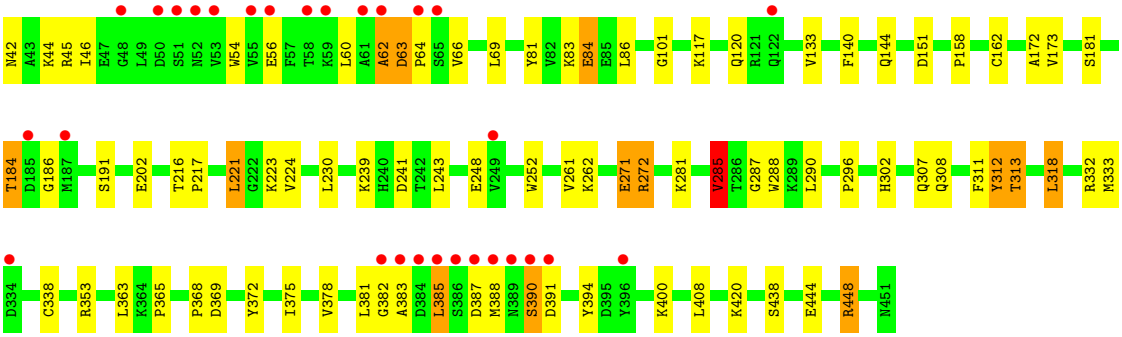
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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

Chain A:

• Molecule 1: Kynurenine--oxoglutarate transaminase 3

Chain B:



4 Data and refinement statistics (i)

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) 91.0 (29.21-2.59)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.38 , 40.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, CA, LLP, PEG, GOL

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	0.68	0/3331	0.84	2/4525 (0.0%)
1	B	0.66	0/3331	0.84	3/4525 (0.1%)
All	All	0.67	0/6662	0.84	5/9050 (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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	385	LEU	CA-CB-CG	6.57	130.41	115.30
1	A	285	VAL	CB-CA-C	6.48	123.70	111.40
1	B	221	LEU	CB-CG-CD2	-5.78	101.18	111.00
1	A	60	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	285	VAL	CB-CA-C	5.05	120.99	111.40

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 (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	3268	0	3235	33	0
1	B	3268	0	3235	50	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	76	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 (76) 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
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:A:184:THR:HG23	1:A:186:GLY:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:117:LYS:HE3	1:B:333:MET:HE1	1.92	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: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: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: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: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
1:A:248:GLU:OE1	1:A:262:LYS:HG2	2.15	0.45
1:B:216:THR:HA	1:B:217:PRO:C	2.36	0.45
1:A:231:GLN:NE2	1:A:235:ASP:OD1	2.48	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:216:THR:HA	1:A:217:PRO:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:117:LYS:HE3	1:B:333:MET:HE3	2.01	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 (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	407/410 (99%)	385 (95%)	20 (5%)	2 (0%)	29	52
1	B	407/410 (99%)	387 (95%)	16 (4%)	4 (1%)	15	32
All	All	814/820 (99%)	772 (95%)	36 (4%)	6 (1%)	22	43

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 (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	357/357 (100%)	336 (94%)	21 (6%)	19	39
1	B	357/357 (100%)	331 (93%)	26 (7%)	14	28
All	All	714/714 (100%)	667 (93%)	47 (7%)	16	33

All (47) 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	109	LYS
1	A	113	CYS
1	A	157	VAL
1	A	173	VAL
1	A	179	LEU
1	A	184	THR
1	A	188	LYS
1	A	210	LYS
1	A	221	LEU
1	A	272	ARG
1	A	278	SER
1	A	285	VAL
1	A	345	LYS
1	A	367	VAL
1	A	372	TYR

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Mol	Chain	Res	Type
1	A	387	ASP
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	158	PRO
1	B	162	CYS
1	B	173	VAL
1	B	181	SER
1	B	184	THR
1	B	243	LEU
1	B	271	GLU
1	B	272	ARG
1	B	285	VAL
1	B	307	GLN
1	B	308	GLN
1	B	313	THR
1	B	318	LEU
1	B	372	TYR
1	B	381	LEU
1	B	385	LEU
1	B	387	ASP
1	B	388	MET
1	B	390	SER
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
1	A	341	ASN
1	B	94	ASN
1	B	302	HIS
1	B	405	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)

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	B	281	1	23,24,25	2.84	5 (21%)	25,32,34	1.51	3 (12%)
1	LLP	A	281	1	23,24,25	2.45	5 (21%)	25,32,34	1.64	5 (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
1	LLP	B	281	1	-	8/16/17/19	0/1/1/1
1	LLP	A	281	1	-	9/16/17/19	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	8.13	1.49	1.40
1	A	281	LLP	C3-C2	6.50	1.47	1.40
1	B	281	LLP	C4-C5	6.11	1.49	1.42
1	B	281	LLP	C4'-NZ	6.00	1.47	1.27
1	B	281	LLP	C4-C3	5.29	1.48	1.40
1	A	281	LLP	C4-C5	5.22	1.48	1.42
1	A	281	LLP	C4'-NZ	5.17	1.44	1.27
1	A	281	LLP	C4-C3	5.09	1.48	1.40
1	B	281	LLP	C4-C4'	3.03	1.52	1.46
1	A	281	LLP	C4-C4'	2.24	1.50	1.46

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	281	LLP	C4-C4'-NZ	-5.06	101.09	124.31
1	B	281	LLP	C4-C3-C2	-4.29	117.53	120.19
1	B	281	LLP	C4-C4'-NZ	-3.48	108.34	124.31
1	A	281	LLP	C6-N1-C2	2.78	124.32	119.17
1	B	281	LLP	C6-N1-C2	2.58	123.95	119.17
1	A	281	LLP	CE-NZ-C4'	2.39	126.24	118.90
1	A	281	LLP	C3-C2-N1	-2.20	117.93	120.77
1	A	281	LLP	CD-CE-NZ	-2.17	105.62	110.93

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
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	A	281	LLP	C5-C4-C4'-NZ
1	B	281	LLP	C3-C4-C4'-NZ
1	B	281	LLP	CD-CE-NZ-C4'
1	A	281	LLP	N-CA-CB-CG
1	A	281	LLP	CD-CE-NZ-C4'
1	A	281	LLP	CG-CD-CE-NZ
1	B	281	LLP	C5-C4-C4'-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 monosaccharides 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	A	503	-	5,5,5	0.15	0	5,5,5	0.56	0
2	EPE	B	501	-	15,15,15	1.78	1 (6%)	18,20,20	1.71	4 (22%)
4	GOL	B	503	-	5,5,5	0.38	0	5,5,5	0.26	0
2	EPE	A	501	-	15,15,15	2.09	1 (6%)	18,20,20	1.72	5 (27%)
3	PEG	A	502	-	6,6,6	0.78	0	5,5,5	0.74	0
3	PEG	B	502	-	6,6,6	0.60	0	5,5,5	0.64	0
4	GOL	A	504	-	5,5,5	0.28	0	5,5,5	0.97	0
4	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.60	0
4	GOL	B	504	-	5,5,5	0.34	0	5,5,5	0.67	0
4	GOL	A	506	-	5,5,5	0.42	0	5,5,5	0.45	0

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EPE	C10-S	-7.49	1.66	1.77
2	B	501	EPE	C10-S	-6.16	1.68	1.77

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	EPE	O2S-S-C10	4.45	112.27	106.92
2	A	501	EPE	C2-C3-N4	3.78	118.40	110.64
2	A	501	EPE	O1S-S-C10	3.27	110.85	106.92
2	A	501	EPE	C6-N1-C2	3.11	115.82	108.83
2	B	501	EPE	O1S-S-C10	2.79	110.27	106.92
2	A	501	EPE	C5-N4-C3	2.46	114.36	108.83
2	A	501	EPE	C3-C2-N1	2.35	115.47	110.64
2	B	501	EPE	C9-N1-C6	-2.32	105.30	111.23
2	B	501	EPE	O2S-S-O1S	-2.32	105.92	113.95

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
3	B	502	PEG	O2-C3-C4-O4
4	A	506	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
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

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Mol	Chain	Res	Type	Atoms
3	A	502	PEG	O1-C1-C2-O2
3	B	502	PEG	C1-C2-O2-C3
4	A	503	GOL	C1-C2-C3-O3
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	A	503	GOL	1	0
2	B	501	EPE	3	0
2	A	501	EPE	3	0
4	A	504	GOL	1	0
4	B	504	GOL	1	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%)	0.06	16 (3%)	39	32	23, 32, 61, 84	0
1	B	409/410 (99%)	0.25	29 (7%)	16	11	25, 35, 73, 94	0
All	All	818/820 (99%)	0.15	45 (5%)	25	19	23, 33, 64, 94	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	VAL	7.1
1	B	387	ASP	6.9
1	B	384	ASP	6.1
1	A	386	SER	5.9
1	B	383	ALA	5.7
1	B	62	ALA	5.6
1	B	389	ASN	5.4
1	B	386	SER	5.4
1	A	383	ALA	5.4
1	B	391	ASP	4.8
1	A	451	ASN	4.6
1	B	64	PRO	4.6
1	A	187	MET	4.6
1	A	387	ASP	4.5
1	B	388	MET	4.3
1	B	187	MET	4.3
1	A	55	VAL	4.2
1	B	334	ASP	4.2
1	B	385	LEU	3.8
1	B	52	ASN	3.8
1	B	390	SER	3.6
1	B	59	LYS	3.5
1	B	382	GLY	3.5
1	A	382	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	3.4
1	A	384	ASP	3.2
1	B	58	THR	3.2
1	B	51	SER	3.1
1	B	56	GLU	3.0
1	B	53	VAL	2.9
1	A	51	SER	2.9
1	A	64	PRO	2.8
1	A	391	ASP	2.6
1	B	122	GLN	2.6
1	A	185	ASP	2.6
1	B	185	ASP	2.5
1	B	249	VAL	2.4
1	A	59	LYS	2.3
1	B	65	SER	2.3
1	A	405	HIS	2.2
1	B	48	GLY	2.2
1	B	396	TYR	2.2
1	A	385	LEU	2.1
1	B	50	ASP	2.1
1	A	62	ALA	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(Å^2)	Q<0.9
1	LLP	A	281	24/25	0.98	0.17	25,26,27,27	0
1	LLP	B	281	24/25	0.98	0.21	28,29,29,29	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
3	PEG	B	502	7/7	0.83	0.18	42,43,43,43	0
4	GOL	B	503	6/6	0.84	0.27	48,50,51,51	0
4	GOL	A	505	6/6	0.91	0.18	50,51,51,51	0
3	PEG	A	502	7/7	0.92	0.14	37,38,38,38	0
4	GOL	A	506	6/6	0.92	0.21	44,45,45,45	0
2	EPE	B	501	15/15	0.92	0.15	53,55,59,59	0
4	GOL	B	504	6/6	0.93	0.14	37,38,39,39	0
4	GOL	A	503	6/6	0.94	0.17	44,44,45,45	0
4	GOL	A	504	6/6	0.94	0.34	43,43,44,44	0
2	EPE	A	501	15/15	0.95	0.14	50,52,53,54	0
5	CA	A	507	1/1	0.95	0.17	45,45,45,45	1
5	CA	A	509	1/1	0.96	0.07	51,51,51,51	0
5	CA	B	505	1/1	0.97	0.06	36,36,36,36	0
5	CA	A	508	1/1	0.98	0.04	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.