



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 06:47 am GMT

PDB ID : 3UE8  
Title : Kynurenine Aminotransferase II Inhibitors  
Authors : Dounay, A.B.; Anderson, M.; Bechle, B.M.; Campbell, B.M.; Claffey, M.M.;  
Evdokimov, A.; Edelweiss, E.; Fonseca, K.R.; Gan, X.; Ghosh, S.; Hayward,  
M.M.; Horner, W.; Kim, J.Y.; McAllister, L.A.; Pandit, J.; Paradis, V.;  
Parikh, V.D.; Reese, M.R.; Rong, S.B.; Salafia, M.A.; Schuyten, K.; Strick,  
C.A.; Tuttle, J.B.; Valentine, J.; Wang, H.; Zawadzke, L.E.; Verhoest, P.R.  
Deposited on : 2011-10-28  
Resolution : 3.22 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : trunk28620  
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) : recalc28949

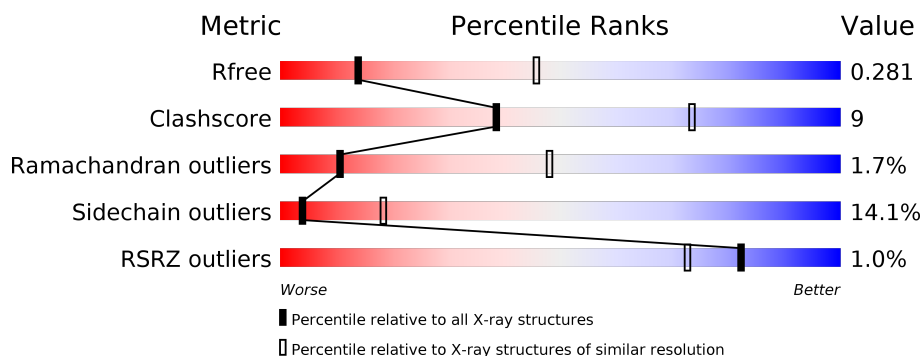
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.22 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	1036 (3.24-3.20)
Clashscore	112137	1161 (3.24-3.20)
Ramachandran outliers	110173	1140 (3.24-3.20)
Sidechain outliers	110143	1139 (3.24-3.20)
RSRZ outliers	101464	1040 (3.24-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	439	
1	B	439	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6485 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/alpha-aminoadipate aminotransferase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3188	2052	530	590	16			
1	B	414	Total	C	N	O	S	0	0	0
			3239	2081	541	600	17			

There are 28 discrepancies between the modelled and reference sequences:

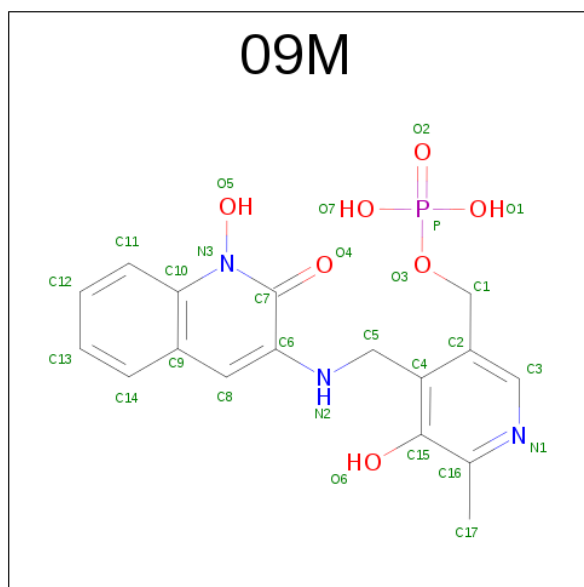
Chain	Residue	Modelled	Actual	Comment	Reference
A	426	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
A	427	VAL	-	EXPRESSION TAG	UNP Q8N5Z0
A	428	PRO	-	EXPRESSION TAG	UNP Q8N5Z0
A	429	ARG	-	EXPRESSION TAG	UNP Q8N5Z0
A	430	GLY	-	EXPRESSION TAG	UNP Q8N5Z0
A	431	SER	-	EXPRESSION TAG	UNP Q8N5Z0
A	432	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
A	433	GLU	-	EXPRESSION TAG	UNP Q8N5Z0
A	434	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	435	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	436	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	437	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	438	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
A	439	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	426	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
B	427	VAL	-	EXPRESSION TAG	UNP Q8N5Z0
B	428	PRO	-	EXPRESSION TAG	UNP Q8N5Z0
B	429	ARG	-	EXPRESSION TAG	UNP Q8N5Z0
B	430	GLY	-	EXPRESSION TAG	UNP Q8N5Z0
B	431	SER	-	EXPRESSION TAG	UNP Q8N5Z0
B	432	LEU	-	EXPRESSION TAG	UNP Q8N5Z0
B	433	GLU	-	EXPRESSION TAG	UNP Q8N5Z0
B	434	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	435	HIS	-	EXPRESSION TAG	UNP Q8N5Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	437	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	438	HIS	-	EXPRESSION TAG	UNP Q8N5Z0
B	439	HIS	-	EXPRESSION TAG	UNP Q8N5Z0

- Molecule 2 is (5-HYDROXY-4-[[[(1-HYDROXY-2-OXO-1,2-DIHYDROQUINOLIN-3-YL)AMINO]METHYL]-6-METHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: 09M) (formula: C<sub>17</sub>H<sub>18</sub>N<sub>3</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			28	17	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			28	17	3	7	1		

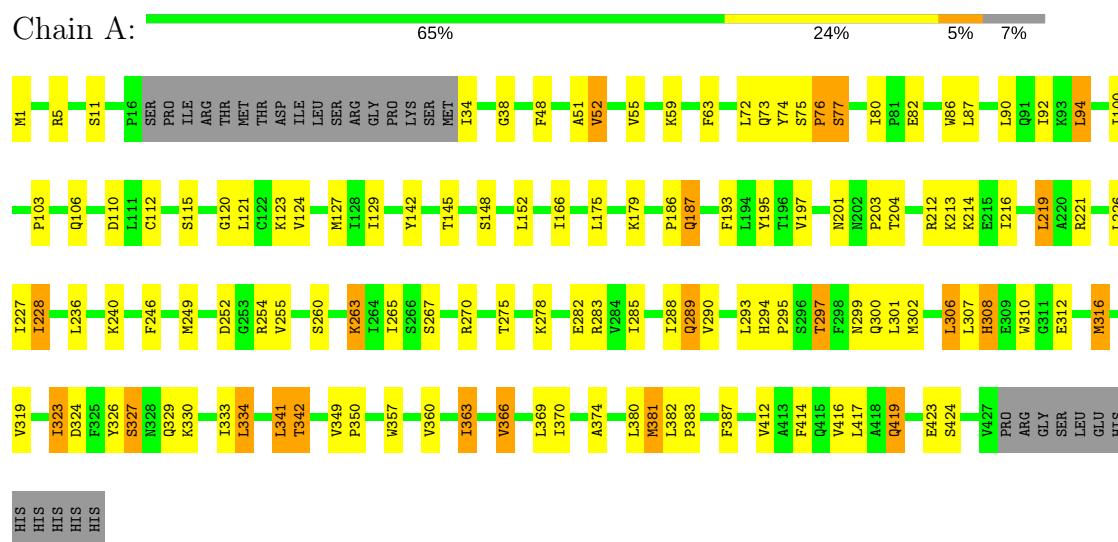
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

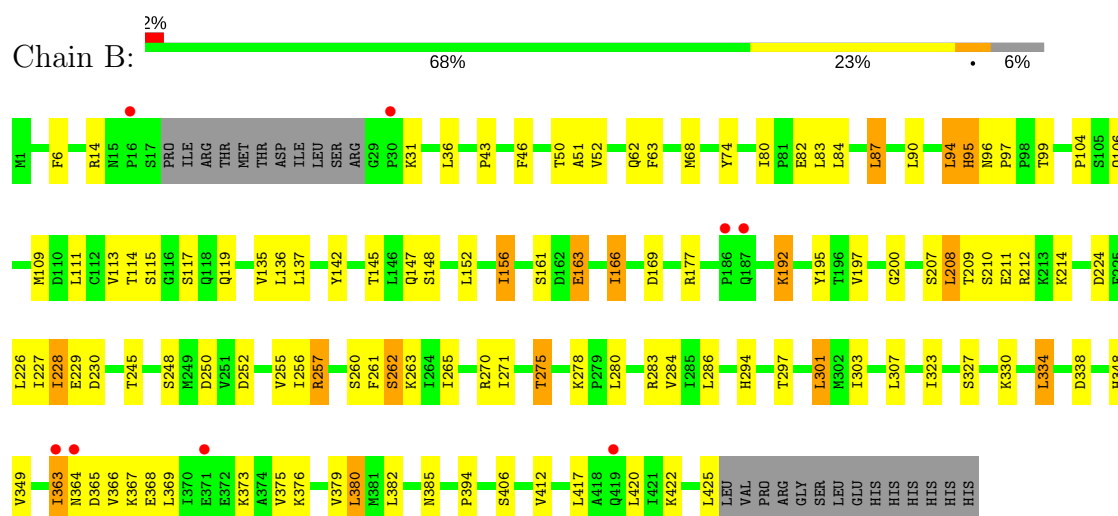
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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/alpha-aminoadipate aminotransferase, mitochondrial



- Molecule 1: Kynurenine/alpha-aminoadipate aminotransferase, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.62Å 116.60Å 129.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.43 – 3.22 28.54 – 3.22	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.43-3.22) 97.8 (28.54-3.22)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.07 (at 3.24Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, $R_{free}$	0.200 , 0.275 0.201 , 0.281	Depositor DCC
$R_{free}$ test set	790 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	56.9	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	6485	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 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: 09M, CL

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	0.54	0/3267	0.80	0/4443
1	B	0.50	0/3319	0.79	0/4505
All	All	0.52	0/6586	0.79	0/8948

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	3188	0	3169	65	0
1	B	3239	0	3243	52	0
2	A	28	0	17	6	0
2	B	28	0	18	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
All	All	6485	0	6447	111	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 9.

All (111) 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:129:ILE:HD11	1:A:193:PHE:HE1	1.39	0.87
1:A:142:TYR:HD1	1:A:145:THR:HG23	1.40	0.87
1:A:73:GLN:O	1:A:297:THR:HG21	1.81	0.80
1:B:256:ILE:HD11	1:B:280:LEU:HD23	1.67	0.75
1:A:145:THR:HG21	1:A:195:TYR:OH	1.89	0.72
1:A:129:ILE:HD11	1:A:193:PHE:CE1	2.24	0.71
1:B:104:PRO:HB3	1:B:278:LYS:HD3	1.75	0.68
1:A:52:VAL:HG13	1:B:52:VAL:HG13	1.76	0.68
1:A:214:LYS:HA	1:A:249:MET:HE1	1.77	0.66
1:A:333:ILE:HG13	1:A:414:PHE:HE1	1.61	0.65
1:A:142:TYR:CD1	1:A:145:THR:HG23	2.28	0.65
1:B:6:PHE:HA	1:B:192:LYS:HE3	1.79	0.64
1:A:34:ILE:HB	1:B:379:VAL:HG12	1.78	0.64
2:A:440:09M:H4	1:B:74:TYR:HH	1.44	0.64
1:B:95:HIS:HB2	1:B:248:SER:HB3	1.80	0.64
1:A:319:VAL:O	1:A:323:ILE:HG13	1.98	0.64
2:A:440:09M:O7	1:B:74:TYR:OH	2.12	0.63
1:A:197:VAL:HB	1:A:201:ASN:HD22	1.64	0.61
1:B:163:GLU:HG2	1:B:348:HIS:CE1	2.35	0.61
1:B:135:VAL:HG23	1:B:156:ILE:HG23	1.82	0.60
1:B:375:VAL:HA	1:B:380:LEU:HD11	1.82	0.60
1:B:142:TYR:O	1:B:145:THR:HG22	2.02	0.60
1:B:422:LYS:HA	1:B:425:LEU:HD12	1.84	0.59
1:B:51:ALA:HB3	1:B:63:PHE:HB2	1.84	0.59
1:A:120:GLY:O	1:A:124:VAL:HG23	2.03	0.58
1:A:75:SER:HB3	1:A:297:THR:HB	1.86	0.58
1:A:80:ILE:HG12	1:A:300:GLN:HB3	1.87	0.57
1:B:84:LEU:HD13	1:B:113:VAL:HG23	1.87	0.57
1:B:363:ILE:HG22	1:B:365:ASP:H	1.69	0.56
1:A:316:MET:HA	1:A:319:VAL:HG22	1.88	0.56
1:B:271:ILE:HG13	1:B:303:ILE:HD13	1.89	0.55
1:B:334:LEU:HD21	1:B:349:VAL:HG23	1.89	0.54
1:B:195:TYR:HD1	1:B:228:ILE:HD11	1.72	0.54
1:B:260:SER:OG	1:B:262:SER:HB2	2.08	0.54
1:A:270:ARG:HD3	1:B:294:HIS:CE1	2.43	0.54
1:A:186:PRO:O	1:A:187:GLN:HB2	2.07	0.54
1:A:115:SER:HA	1:A:270:ARG:O	2.08	0.54
1:B:87:LEU:HD11	1:B:261:PHE:HZ	1.73	0.53
1:A:48:PHE:HB2	1:A:72:LEU:HD11	1.89	0.53
1:A:263:LYS:NZ	2:A:440:09M:H14	2.24	0.53
1:B:63:PHE:CZ	1:B:301:LEU:HB3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LEU:HD12	1:A:219:LEU:HD22	1.92	0.51
1:A:227:ILE:HB	1:A:255:VAL:HG22	1.93	0.51
1:B:365:ASP:HB2	1:B:394:PRO:HB3	1.93	0.51
1:B:227:ILE:HB	1:B:255:VAL:HG22	1.93	0.51
1:A:103:PRO:HD2	1:A:106:GLN:HB2	1.93	0.51
1:A:330:LYS:HG3	1:A:350:PRO:HG2	1.93	0.50
1:A:260:SER:OG	2:A:440:09M:O2	2.22	0.49
1:A:92:ILE:HG12	1:A:100:ILE:HD12	1.93	0.49
1:A:121:LEU:HD23	1:A:228:ILE:HD11	1.93	0.49
1:B:263:LYS:NZ	2:B:440:09M:H14	2.28	0.49
1:B:245:THR:O	1:B:248:SER:OG	2.29	0.49
1:B:90:LEU:HG	1:B:94:LEU:HD12	1.94	0.49
1:A:294:HIS:HD2	1:A:295:PRO:O	1.96	0.49
1:B:261:PHE:HB3	1:B:265:ILE:HB	1.96	0.48
1:B:115:SER:HA	1:B:270:ARG:O	2.13	0.48
1:A:360:VAL:HG21	1:A:366:VAL:HG21	1.94	0.48
1:B:111:LEU:HG	1:B:275:THR:HG23	1.96	0.48
1:A:334:LEU:HD21	1:A:349:VAL:HG13	1.96	0.48
1:A:55:VAL:HG21	1:A:306:LEU:HD13	1.95	0.48
1:A:381:MET:HB3	1:B:36:LEU:HB2	1.96	0.48
1:B:209:THR:OG1	1:B:212:ARG:HG2	2.14	0.48
1:A:214:LYS:HA	1:A:249:MET:CE	2.44	0.48
1:A:333:ILE:HG13	1:A:414:PHE:CE1	2.46	0.47
1:A:75:SER:HB2	1:A:76:PRO:HD2	1.95	0.47
1:A:363:ILE:HD11	1:A:424:SER:HB2	1.95	0.47
1:B:200:GLY:H	1:B:207:SER:HB2	1.78	0.47
1:A:110:ASP:HB2	1:A:278:LYS:HA	1.96	0.47
1:A:212:ARG:O	1:A:216:ILE:HG13	2.14	0.47
1:B:166:ILE:HG23	1:B:208:LEU:HD11	1.95	0.47
1:B:43:PRO:HA	1:B:46:PHE:CD1	2.50	0.47
1:A:289:GLN:O	1:A:293:LEU:HD23	2.15	0.46
1:B:373:LYS:HB3	1:B:420:LEU:HD13	1.98	0.46
1:A:412:VAL:O	1:A:416:VAL:HG23	2.16	0.46
1:A:341:LEU:HD21	1:A:414:PHE:CD2	2.51	0.46
1:B:163:GLU:CG	1:B:348:HIS:CE1	2.98	0.46
1:A:370:ILE:HA	1:A:374:ALA:HB3	1.98	0.45
1:A:34:ILE:O	1:B:379:VAL:HA	2.16	0.45
1:B:97:PRO:HG2	1:B:109:MET:SD	2.56	0.45
1:A:267:SER:HB2	1:B:74:TYR:CZ	2.51	0.45
1:B:260:SER:HG	2:B:440:09M:H5	1.58	0.45
1:A:90:LEU:O	1:A:94:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:TYR:HA	1:A:329:GLN:HB2	1.99	0.44
1:A:416:VAL:O	1:A:419:GLN:HB2	2.17	0.44
1:B:271:ILE:HG13	1:B:303:ILE:CD1	2.47	0.44
2:A:440:09M:H3	2:A:440:09M:H13	1.73	0.44
1:A:299:ASN:HA	1:A:302:MET:HB2	2.00	0.43
1:A:74:TYR:HD1	1:A:294:HIS:HE1	1.66	0.43
1:B:229:GLU:HB3	1:B:257:ARG:HB2	2.00	0.43
1:A:203:PRO:HG3	1:A:387:PHE:CG	2.53	0.43
2:A:440:09M:H7	2:A:440:09M:H13	1.83	0.43
1:A:112:CYS:SG	1:A:285:ILE:HG12	2.58	0.43
1:A:51:ALA:HB3	1:A:63:PHE:HB2	2.01	0.42
1:B:263:LYS:HZ3	2:B:440:09M:H14	1.83	0.42
1:B:211:GLU:O	1:B:214:LYS:HB2	2.20	0.42
1:B:210:SER:O	1:B:214:LYS:HG3	2.19	0.42
1:A:213:LYS:HA	1:A:216:ILE:HD12	2.01	0.42
1:B:363:ILE:HG22	1:B:364:ASN:H	1.85	0.42
1:A:370:ILE:HG21	1:A:383:PRO:HG3	2.02	0.42
1:A:121:LEU:CD2	1:A:228:ILE:HD11	2.49	0.41
1:A:204:THR:HA	1:A:357:TRP:CB	2.50	0.41
1:A:290:VAL:HG11	1:B:147:GLN:HB3	2.00	0.41
1:A:246:PHE:HA	1:A:249:MET:HG2	2.03	0.41
1:A:186:PRO:O	1:A:187:GLN:CB	2.69	0.41
1:A:290:VAL:CG1	1:B:147:GLN:HB3	2.50	0.41
1:A:77:SER:HA	1:A:294:HIS:HB3	2.02	0.41
1:B:197:VAL:HA	1:B:230:ASP:O	2.21	0.41
1:A:73:GLN:HG3	1:A:74:TYR:N	2.36	0.40
1:A:86:TRP:HB2	1:A:308:HIS:CE1	2.56	0.40
1:A:324:ASP:HA	1:A:327:SER:HB2	2.04	0.40
1:B:114:THR:HB	1:B:119:GLN:HB3	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	406/439 (92%)	370 (91%)	28 (7%)	8 (2%)	9	44
1	B	410/439 (93%)	358 (87%)	46 (11%)	6 (2%)	12	51
All	All	816/878 (93%)	728 (89%)	74 (9%)	14 (2%)	11	48

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	187	GLN
1	A	342	THR
1	B	250	ASP
1	A	240	LYS
1	B	14	ARG
1	B	224	ASP
1	B	106	GLN
1	A	76	PRO
1	A	59	LYS
1	B	152	LEU
1	A	369	LEU
1	A	38	GLY
1	B	96	ASN

### 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	349/383 (91%)	301 (86%)	48 (14%)	4	19
1	B	358/383 (94%)	306 (86%)	52 (14%)	4	17
All	All	707/766 (92%)	607 (86%)	100 (14%)	4	18

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ARG

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Mol	Chain	Res	Type
1	A	11	SER
1	A	52	VAL
1	A	82	GLU
1	A	87	LEU
1	A	94	LEU
1	A	123	LYS
1	A	127	MET
1	A	148	SER
1	A	152	LEU
1	A	166	ILE
1	A	179	LYS
1	A	219	LEU
1	A	221	ARG
1	A	226	LEU
1	A	228	ILE
1	A	236	LEU
1	A	252	ASP
1	A	254	ARG
1	A	263	LYS
1	A	265	ILE
1	A	275	THR
1	A	282	GLU
1	A	283	ARG
1	A	288	ILE
1	A	289	GLN
1	A	297	THR
1	A	301	LEU
1	A	306	LEU
1	A	307	LEU
1	A	308	HIS
1	A	310	TRP
1	A	312	GLU
1	A	316	MET
1	A	323	ILE
1	A	327	SER
1	A	334	LEU
1	A	341	LEU
1	A	342	THR
1	A	363	ILE
1	A	366	VAL
1	A	380	LEU
1	A	381	MET

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Mol	Chain	Res	Type
1	A	382	LEU
1	A	417	LEU
1	A	419	GLN
1	A	423	GLU
1	B	31	LYS
1	B	50	THR
1	B	62	GLN
1	B	68	MET
1	B	80	ILE
1	B	82	GLU
1	B	83	LEU
1	B	87	LEU
1	B	94	LEU
1	B	95	HIS
1	B	99	THR
1	B	117	SER
1	B	136	LEU
1	B	137	LEU
1	B	148	SER
1	B	156	ILE
1	B	161	SER
1	B	163	GLU
1	B	166	ILE
1	B	169	ASP
1	B	177	ARG
1	B	192	LYS
1	B	208	LEU
1	B	226	LEU
1	B	228	ILE
1	B	252	ASP
1	B	257	ARG
1	B	262	SER
1	B	275	THR
1	B	283	ARG
1	B	284	VAL
1	B	286	LEU
1	B	297	THR
1	B	301	LEU
1	B	307	LEU
1	B	323	ILE
1	B	327	SER
1	B	330	LYS

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Mol	Chain	Res	Type
1	B	334	LEU
1	B	338	ASP
1	B	363	ILE
1	B	366	VAL
1	B	367	LYS
1	B	368	GLU
1	B	369	LEU
1	B	376	LYS
1	B	380	LEU
1	B	382	LEU
1	B	385	ASN
1	B	406	SER
1	B	412	VAL
1	B	417	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	147	GLN
1	A	155	ASN
1	A	201	ASN
1	A	237	GLN
1	A	294	HIS
1	A	308	HIS
1	B	44	ASN
1	B	91	GLN
1	B	130	ASN
1	B	147	GLN
1	B	187	GLN
1	B	199	ASN
1	B	201	ASN
1	B	237	GLN
1	B	294	HIS
1	B	299	ASN
1	B	348	HIS
1	B	364	ASN
1	B	415	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	09M	A	440	-	29,30,30	1.54	5 (17%)	35,44,44	1.26	4 (11%)
2	09M	B	440	-	29,30,30	1.39	2 (6%)	35,44,44	1.21	3 (8%)

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	09M	A	440	-	-	0/11/11/11	0/3/3/3
2	09M	B	440	-	-	0/11/11/11	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	440	09M	C7-N3	-4.67	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	440	09M	O3-C1	-3.36	1.31	1.44
2	A	440	09M	C8-C6	-3.00	1.31	1.37
2	A	440	09M	C6-N2	-2.50	1.32	1.39
2	A	440	09M	C10-N3	-2.22	1.34	1.39
2	B	440	09M	C10-N3	2.61	1.45	1.39
2	B	440	09M	C7-C6	6.13	1.48	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	440	09M	O3-C1-C2	-4.82	99.61	109.32
2	A	440	09M	C11-C10-N3	2.05	122.44	119.63
2	B	440	09M	C8-C6-C7	2.15	119.22	117.13
2	A	440	09M	C5-C4-C2	2.25	121.81	119.75
2	A	440	09M	C8-C6-C7	2.55	119.60	117.13
2	B	440	09M	C5-C4-C2	2.68	122.21	119.75
2	B	440	09M	C5-N2-C6	4.93	134.81	121.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	440	09M	6	0
2	B	440	09M	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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å <sup>2</sup> )	Q < 0.9
1	A	410/439 (93%)	-0.47	0	100   100	23, 47, 77, 97	0
1	B	414/439 (94%)	-0.28	8 (1%)	67   53	29, 59, 110, 145	0
All	All	824/878 (93%)	-0.38	8 (0%)	82   73	23, 52, 93, 145	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	30	PRO	3.1
1	B	371	GLU	2.7
1	B	187	GLN	2.4
1	B	364	ASN	2.4
1	B	363	ILE	2.2
1	B	16	PRO	2.1
1	B	186	PRO	2.0
1	B	419	GLN	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	09M	B	440	28/28	0.94	0.19	-0.07	40,53,77,78	0
2	09M	A	440	28/28	0.95	0.16	-0.72	35,43,58,62	0
3	CL	A	441	1/1	0.94	0.07	-	35,35,35,35	0
3	CL	B	441	1/1	0.89	0.11	-	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.