



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:20 PM UTC

PDB ID : 7UI3 / pdb_00007ui3
Title : Apo-form of Human Tryptophan 2,3-Dioxygenase Induced by NADH Binding
Authors : Yeh, S.-R.; Geeraerts, Z.
Deposited on : 2022-03-28
Resolution : 3.18 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

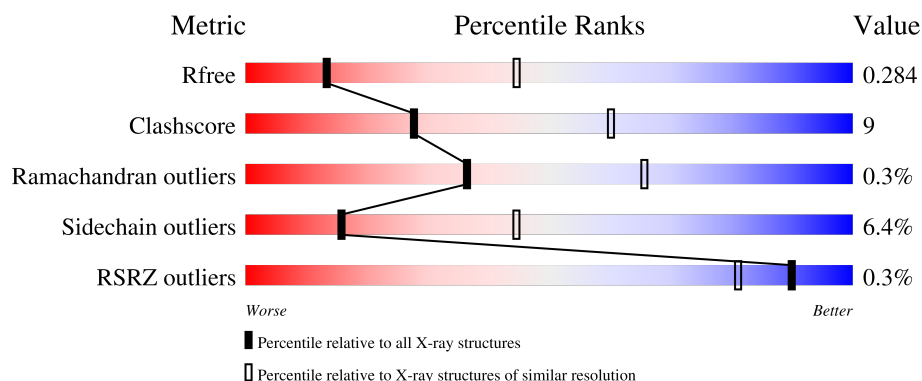
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 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	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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	380	
1	B	380	
1	C	380	
1	D	380	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17673 atoms, of which 8569 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 Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	309	Total	C	H	N	O	S	133	0	0
			4443	1452	2159	403	421	8			
1	B	302	Total	C	H	N	O	S	102	0	0
			4693	1524	2316	414	429	10			
1	C	293	Total	C	H	N	O	S	140	0	0
			4082	1357	1955	368	393	9			
1	D	303	Total	C	H	N	O	S	131	0	0
			4335	1436	2083	388	418	10			

There are 32 discrepancies between the modelled and reference sequences:

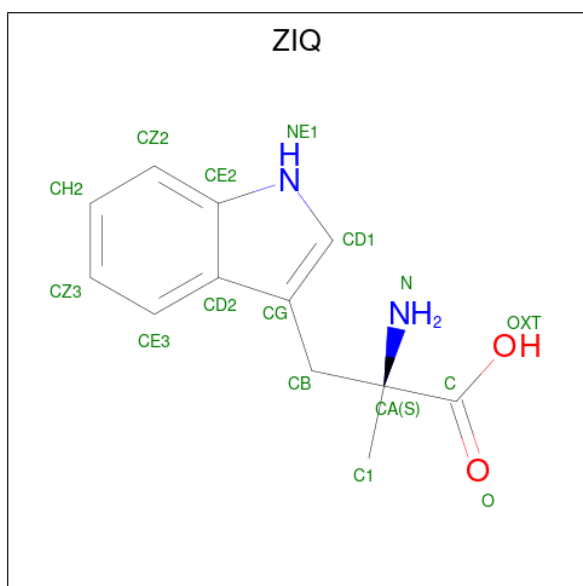
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

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Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

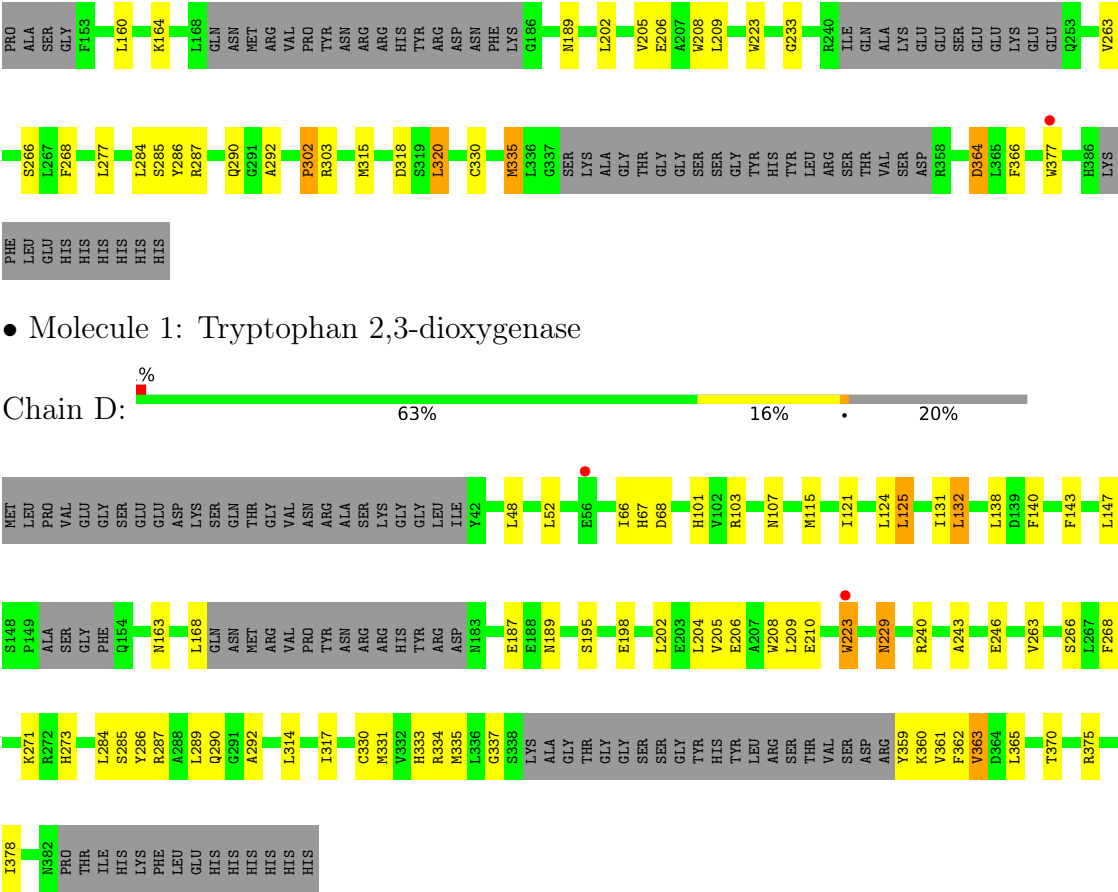
- Molecule 2 is alpha-methyl-L-tryptophan (CCD ID: ZIQ) (formula: $C_{12}H_{14}N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
2	B	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
2	C	1	Total	C	H	N	O	0	0
			30	12	14	2	2		
2	D	1	Total	C	H	N	O	0	0
			30	12	14	2	2		

- Molecule 1: Tryptophan 2,3-dioxygenase





• Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.85Å 156.26Å 88.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.18 19.97 – 3.18	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.97-3.18) 99.1 (19.97-3.18)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.244 , 0.278 0.245 , 0.284	Depositor DCC
R_{free} test set	1778 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	117.5	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17673	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZIQ

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	1.02	0/2330	1.63	0/3166
1	B	1.02	0/2425	1.58	1/3280 (0.0%)
1	C	1.05	0/2172	1.64	1/2958 (0.0%)
1	D	1.04	0/2300	1.63	0/3130
All	All	1.03	0/9227	1.62	2/12534 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	302	PRO	N-CA-C	-6.89	100.65	111.34
1	B	146	TYR	CA-C-O	-5.60	115.11	121.72

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	2284	2159	1990	39	0
1	B	2377	2316	2210	47	0
1	C	2127	1955	1767	35	0
1	D	2252	2083	1913	51	0
2	A	16	14	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	16	14	0	0	0
2	C	16	14	0	1	0
2	D	16	14	0	1	0
All	All	9104	8569	7880	152	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 (152) 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:131:ILE:O	1:A:134:THR:HG22	1.77	0.85
1:A:307:PRO:O	1:A:311:LEU:HD22	1.83	0.78
1:B:293:LEU:HD13	1:B:368:LEU:HD12	1.66	0.77
1:A:90:LEU:O	1:A:93:VAL:HG22	1.85	0.76
1:D:361:VAL:HG13	1:D:362:PHE:CD1	2.22	0.74
1:C:103:ARG:HA	2:C:401:ZIQ:OXT	1.87	0.74
1:C:136:THR:HG23	1:C:139:ASP:CG	2.12	0.74
1:A:310:LEU:HD23	1:A:310:LEU:O	1.90	0.71
1:A:93:VAL:HG11	1:A:115:MET:HE3	1.72	0.71
1:A:267:LEU:O	1:A:268:PHE:CD2	2.45	0.68
1:D:66:ILE:CB	1:D:143:PHE:HB3	2.25	0.66
1:D:115:MET:HE3	1:D:317:ILE:HD12	1.78	0.66
1:C:233:GLY:HA3	1:C:377:TRP:HE1	1.61	0.65
1:B:48:LEU:HA	1:B:51:VAL:HG22	1.78	0.65
1:B:289:LEU:HG	1:B:368:LEU:HD21	1.79	0.64
1:D:240:ARG:O	1:D:243:ALA:CB	2.47	0.63
1:B:337:GLY:HA3	1:D:370:THR:HB	1.79	0.63
1:C:120:VAL:HG12	1:D:131:ILE:HD13	1.81	0.63
1:B:296:TYR:O	1:B:299:ARG:HD2	1.99	0.63
1:A:297:PHE:CG	1:A:378:ILE:HD11	2.34	0.63
1:A:115:MET:HE2	1:A:115:MET:HA	1.80	0.62
1:A:134:THR:HG21	1:B:117:ARG:HG3	1.81	0.62
1:B:48:LEU:HB3	1:B:52:LEU:HD12	1.80	0.62
1:C:302:PRO:O	1:C:303:ARG:HB3	2.00	0.62
1:B:160:LEU:O	1:B:164:LYS:HE3	2.00	0.61
1:C:93:VAL:HG21	1:C:115:MET:HE3	1.82	0.61
1:A:131:ILE:HD13	1:B:120:VAL:HG12	1.82	0.61
1:C:115:MET:HA	1:C:115:MET:HE2	1.80	0.61
1:B:146:TYR:O	1:B:147:LEU:HB3	1.98	0.61
1:C:223:TRP:CG	1:C:290:GLN:OE1	2.54	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ARG:HH22	1:D:138:LEU:HB2	1.66	0.60
1:C:140:PHE:CG	1:C:335:MET:HG3	2.36	0.60
1:B:115:MET:HA	1:B:115:MET:HE2	1.83	0.60
1:C:48:LEU:HB3	1:C:52:LEU:HD23	1.83	0.59
1:D:48:LEU:HB3	1:D:52:LEU:HD23	1.85	0.59
1:A:89:GLU:OE1	1:B:67:HIS:HE1	1.86	0.59
1:C:287:ARG:HA	1:C:290:GLN:HE21	1.68	0.58
1:A:310:LEU:HD23	1:A:310:LEU:C	2.26	0.58
1:A:48:LEU:HB3	1:A:52:LEU:HD12	1.86	0.57
1:D:121:ILE:O	1:D:125:LEU:HD22	2.05	0.57
1:D:240:ARG:O	1:D:243:ALA:HB2	2.05	0.56
1:A:310:LEU:C	1:A:310:LEU:CD2	2.78	0.56
1:D:210:GLU:HA	1:D:287:ARG:HG3	1.87	0.56
1:B:93:VAL:HG21	1:B:115:MET:HE3	1.87	0.56
1:A:107:ASN:O	1:A:111:VAL:HG23	2.06	0.56
1:C:52:LEU:HA	1:C:55:GLN:HE21	1.71	0.55
1:A:59:SER:HA	1:A:62:LYS:HE2	1.88	0.55
1:A:82:TRP:CH2	1:B:131:ILE:HG21	2.42	0.54
1:D:334:ARG:NH1	1:D:335:MET:HE3	2.23	0.53
1:C:233:GLY:HA3	1:C:377:TRP:NE1	2.21	0.53
1:B:59:SER:HB3	1:B:64:ASN:O	2.08	0.53
1:C:284:LEU:HB2	1:C:364:ASP:OD1	2.09	0.53
1:A:59:SER:HB3	1:A:64:ASN:O	2.08	0.53
1:D:335:MET:HA	1:D:335:MET:HE2	1.91	0.53
1:D:209:LEU:HD12	1:D:292:ALA:N	2.25	0.52
1:C:209:LEU:HD12	1:C:292:ALA:N	2.25	0.52
1:B:65:LYS:C	1:B:66:ILE:HD12	2.36	0.51
1:D:223:TRP:CZ3	1:D:290:GLN:CB	2.94	0.51
1:C:160:LEU:O	1:C:164:LYS:HG2	2.12	0.50
1:A:162:GLU:O	1:A:165:ILE:HG12	2.11	0.50
1:B:370:THR:HG22	1:D:337:GLY:HA2	1.94	0.50
1:B:57:LEU:HD21	1:B:70:HIS:HA	1.93	0.50
1:B:66:ILE:HD12	1:B:66:ILE:N	2.26	0.50
1:B:72:PHE:O	1:B:75:THR:HG22	2.12	0.49
1:D:263:VAL:O	1:D:266:SER:OG	2.26	0.49
1:C:263:VAL:O	1:C:266:SER:OG	2.24	0.49
1:D:229:ASN:HD22	1:D:229:ASN:N	2.10	0.49
1:C:277:LEU:HD21	1:C:284:LEU:O	2.13	0.48
1:D:115:MET:HE3	1:D:317:ILE:CD1	2.42	0.48
1:B:335:MET:HA	1:B:335:MET:HE2	1.96	0.48
1:B:334:ARG:NH1	1:B:335:MET:HE3	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:HE1	1:A:310:LEU:HD12	1.96	0.48
1:B:69:GLU:HG2	1:B:73:ILE:CD1	2.44	0.47
1:C:268:PHE:HA	1:C:286:TYR:OH	2.13	0.47
1:A:45:TYR:OH	1:B:73:ILE:HD11	2.13	0.47
1:B:268:PHE:HA	1:B:286:TYR:OH	2.14	0.47
1:B:217:PRO:O	1:B:221:ASN:HB3	2.15	0.47
1:D:101:HIS:HB3	1:D:107:ASN:ND2	2.30	0.47
1:C:49:GLU:OE1	1:C:50:LYS:HG3	2.15	0.47
1:B:299:ARG:NH2	1:D:138:LEU:HB2	2.29	0.47
1:D:52:LEU:HD22	1:D:52:LEU:N	2.30	0.47
1:D:240:ARG:O	1:D:243:ALA:HB3	2.15	0.47
1:A:45:TYR:CZ	1:B:147:LEU:HD22	2.49	0.46
1:C:88:TRP:CH2	1:D:67:HIS:HA	2.51	0.46
1:D:268:PHE:HA	1:D:286:TYR:OH	2.15	0.46
1:C:52:LEU:HA	1:C:55:GLN:NE2	2.30	0.46
1:A:121:ILE:HG12	1:B:131:ILE:HD12	1.97	0.46
1:D:361:VAL:HG13	1:D:362:PHE:HD1	1.79	0.46
1:B:277:LEU:HD22	1:B:282:ARG:HB2	1.96	0.46
1:A:89:GLU:CD	1:B:67:HIS:HE1	2.23	0.46
1:A:205:VAL:HG21	1:A:362:PHE:HE1	1.80	0.46
1:C:208:TRP:CE3	1:C:209:LEU:HD22	2.51	0.46
1:D:208:TRP:CE3	1:D:209:LEU:HD22	2.50	0.46
1:B:315:MET:HE3	1:B:366:PHE:CD1	2.51	0.45
1:B:293:LEU:HG	1:B:297:PHE:CE2	2.52	0.45
1:B:256:GLU:O	1:B:260:GLN:HG2	2.17	0.45
1:A:265:LEU:O	1:A:267:LEU:O	2.35	0.45
1:B:161:LEU:HD22	1:B:165:ILE:HD11	1.98	0.45
1:D:362:PHE:HB3	1:D:365:LEU:HD13	1.99	0.45
1:A:82:TRP:CZ3	1:B:131:ILE:HG21	2.52	0.44
1:A:124:LEU:C	1:A:124:LEU:HD13	2.42	0.44
1:B:156:LEU:O	1:B:160:LEU:HD13	2.17	0.44
1:C:83:PHE:O	1:C:87:LEU:HD23	2.18	0.44
1:C:206:GLU:OE2	1:C:285:SER:N	2.51	0.44
1:A:230:ILE:HA	1:A:377:TRP:CE3	2.52	0.44
1:A:202:LEU:C	1:A:202:LEU:HD13	2.43	0.44
1:D:375:ARG:O	1:D:378:ILE:HG12	2.18	0.44
1:A:227:GLU:O	1:A:230:ILE:HG13	2.18	0.44
1:D:124:LEU:C	1:D:124:LEU:HD13	2.43	0.43
1:C:88:TRP:HH2	1:D:67:HIS:HA	1.83	0.43
1:D:163:ASN:HD22	1:D:195:SER:HB2	1.83	0.43
1:A:93:VAL:HG21	1:A:115:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:O	1:D:132:LEU:HD13	2.18	0.43
1:D:202:LEU:C	1:D:202:LEU:HD13	2.43	0.43
1:A:378:ILE:HD12	1:A:378:ILE:HA	1.81	0.43
1:B:229:ASN:HD22	1:B:229:ASN:N	2.15	0.43
1:D:360:LYS:O	1:D:363:VAL:HG13	2.18	0.43
1:C:202:LEU:C	1:C:202:LEU:HD13	2.43	0.43
1:A:52:LEU:O	1:B:84:LYS:NZ	2.48	0.43
1:A:295:ILE:HG21	1:A:311:LEU:CD2	2.49	0.43
1:A:131:ILE:HD12	1:B:121:ILE:HG12	2.00	0.43
1:C:364:ASP:OD2	1:C:364:ASP:N	2.51	0.43
1:D:273:HIS:CE1	1:D:289:LEU:HD11	2.53	0.43
1:B:199:LYS:HA	1:B:203:GLU:OE2	2.19	0.42
1:D:246:GLU:O	1:D:246:GLU:HG2	2.19	0.42
1:D:206:GLU:OE2	1:D:285:SER:N	2.52	0.42
1:D:202:LEU:O	1:D:205:VAL:HG22	2.19	0.42
1:A:140:PHE:HA	1:A:143:PHE:CE1	2.55	0.42
1:A:206:GLU:OE2	1:A:285:SER:N	2.52	0.42
1:B:140:PHE:HA	1:B:143:PHE:CE1	2.54	0.42
1:C:140:PHE:CD2	1:C:335:MET:HG3	2.55	0.42
1:C:315:MET:HE3	1:C:366:PHE:CD2	2.54	0.42
1:C:122:LEU:HB2	1:C:320:LEU:HD23	2.02	0.42
1:B:161:LEU:HD22	1:B:165:ILE:CD1	2.49	0.42
1:C:121:ILE:HG12	1:D:131:ILE:HD12	2.02	0.42
1:D:187:GLU:OE1	1:D:187:GLU:N	2.49	0.42
1:A:299:ARG:HD3	1:A:308:PHE:CE1	2.55	0.41
1:C:140:PHE:HA	1:C:143:PHE:CE2	2.55	0.41
1:D:103:ARG:HA	2:D:401:ZIQ:O	2.20	0.41
1:D:205:VAL:O	1:D:209:LEU:HD23	2.20	0.41
1:C:205:VAL:O	1:C:209:LEU:HD23	2.20	0.41
1:D:132:LEU:HD12	1:D:331:MET:SD	2.60	0.41
1:B:370:THR:CG2	1:D:337:GLY:HA2	2.50	0.41
1:C:115:MET:O	1:C:118:VAL:HB	2.21	0.41
1:D:121:ILE:HG22	1:D:125:LEU:CD2	2.51	0.41
1:D:273:HIS:CE1	1:D:284:LEU:O	2.73	0.41
1:D:140:PHE:HA	1:D:143:PHE:CE1	2.56	0.40
1:D:333:HIS:HA	1:D:337:GLY:O	2.21	0.40
1:B:115:MET:O	1:B:118:VAL:HB	2.21	0.40
1:D:115:MET:HE2	1:D:314:LEU:CD2	2.51	0.40
1:D:124:LEU:HD13	1:D:124:LEU:O	2.21	0.40
1:B:250:LYS:O	1:B:254:VAL:HG23	2.22	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	301/380 (79%)	281 (93%)	19 (6%)	1 (0%)	36	66
1	B	294/380 (77%)	275 (94%)	18 (6%)	1 (0%)	36	66
1	C	283/380 (74%)	268 (95%)	14 (5%)	1 (0%)	30	60
1	D	295/380 (78%)	277 (94%)	18 (6%)	0	100	100
All	All	1173/1520 (77%)	1101 (94%)	69 (6%)	3 (0%)	36	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	LEU
1	C	42	TYR
1	A	154	GLN

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	203/348 (58%)	191 (94%)	12 (6%)	18	47
1	B	234/348 (67%)	217 (93%)	17 (7%)	13	40
1	C	179/348 (51%)	170 (95%)	9 (5%)	22	52
1	D	198/348 (57%)	184 (93%)	14 (7%)	13	41
All	All	814/1392 (58%)	762 (94%)	52 (6%)	16	44

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	LEU
1	A	122	LEU
1	A	160	LEU
1	A	190	GLU
1	A	204	LEU
1	A	218	HIS
1	A	300	GLU
1	A	310	LEU
1	A	311	LEU
1	A	318	ASP
1	A	320	LEU
1	A	378	ILE
1	B	65	LYS
1	B	138	LEU
1	B	161	LEU
1	B	164	LYS
1	B	209	LEU
1	B	216	GLU
1	B	249	GLU
1	B	251	GLU
1	B	253	GLN
1	B	278	SER
1	B	320	LEU
1	B	330	CYS
1	B	364	ASP
1	B	368	LEU
1	B	369	SER
1	B	372	LEU
1	B	382	ASN
1	C	49	GLU
1	C	55	GLN
1	C	136	THR
1	C	189	ASN
1	C	318	ASP
1	C	320	LEU
1	C	330	CYS
1	C	335	MET
1	C	364	ASP
1	D	68	ASP
1	D	125	LEU
1	D	132	LEU
1	D	147	LEU
1	D	168	LEU

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Mol	Chain	Res	Type
1	D	189	ASN
1	D	198	GLU
1	D	204	LEU
1	D	223	TRP
1	D	229	ASN
1	D	271	LYS
1	D	330	CYS
1	D	359	TYR
1	D	363	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	309	GLN
1	B	67	HIS
1	B	98	GLN
1	B	128	GLN
1	B	229	ASN
1	B	253	GLN
1	C	55	GLN
1	C	70	HIS
1	C	128	GLN
1	C	141	ASN
1	C	163	ASN
1	C	290	GLN
1	D	47	HIS
1	D	53	ASN
1	D	70	HIS
1	D	116	HIS
1	D	163	ASN
1	D	229	ASN
1	D	309	GLN
1	D	367	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ZIQ	A	401	-	14,17,17	0.65	0	20,25,25	0.94	1 (5%)
2	ZIQ	B	401	-	14,17,17	0.65	0	20,25,25	1.14	3 (15%)
2	ZIQ	C	401	-	14,17,17	0.63	0	20,25,25	1.11	2 (10%)
2	ZIQ	D	401	-	14,17,17	0.61	0	20,25,25	1.08	2 (10%)

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	ZIQ	A	401	-	-	2/11/11/11	0/2/2/2
2	ZIQ	B	401	-	-	6/11/11/11	0/2/2/2
2	ZIQ	C	401	-	-	1/11/11/11	0/2/2/2
2	ZIQ	D	401	-	-	2/11/11/11	0/2/2/2

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	ZIQ	O-C-CA	-3.12	117.18	122.78
2	C	401	ZIQ	O-C-CA	-3.12	117.19	122.78
2	B	401	ZIQ	O-C-CA	-3.06	117.29	122.78
2	A	401	ZIQ	O-C-CA	-2.76	117.83	122.78
2	C	401	ZIQ	C1-CA-CB	-2.59	107.18	110.82
2	D	401	ZIQ	C1-CA-CB	-2.50	107.32	110.82
2	B	401	ZIQ	C1-CA-CB	-2.49	107.33	110.82
2	B	401	ZIQ	CB-CA-C	2.30	112.26	109.10

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	ZIQ	O-C-CA-N
2	D	401	ZIQ	O-C-CA-CB
2	D	401	ZIQ	OXT-C-CA-CB
2	A	401	ZIQ	CA-CB-CG-CD2
2	B	401	ZIQ	OXT-C-CA-C1
2	B	401	ZIQ	O-C-CA-CB
2	B	401	ZIQ	OXT-C-CA-CB
2	B	401	ZIQ	O-C-CA-C1
2	B	401	ZIQ	CA-CB-CG-CD2
2	A	401	ZIQ	CA-CB-CG-CD1
2	B	401	ZIQ	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ZIQ	1	0
2	D	401	ZIQ	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	309/380 (81%)	-0.22	0 100 100	81, 121, 173, 211	0
1	B	302/380 (79%)	-0.24	1 (0%) 90 81	70, 103, 150, 183	0
1	C	293/380 (77%)	-0.17	1 (0%) 90 81	80, 127, 171, 214	0
1	D	303/380 (79%)	-0.24	2 (0%) 84 69	82, 124, 165, 204	0
All	All	1207/1520 (79%)	-0.22	4 (0%) 90 81	70, 120, 167, 214	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	TRP	2.7
1	B	356	SER	2.6
1	D	223	TRP	2.0
1	D	56	GLU	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 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
2	ZIQ	C	401	16/16	0.89	0.10	115,120,133,136	0
2	ZIQ	D	401	16/16	0.89	0.09	125,131,135,135	0
2	ZIQ	B	401	16/16	0.94	0.07	82,86,95,97	0
2	ZIQ	A	401	16/16	0.96	0.06	82,89,94,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.