



# Full wwPDB X-ray Structure Validation Report

Oct 2, 2014 – 11:49 PM EDT

PDB ID : 4CXY  
Title : Crystal structure of human FTO in complex with acylhydrazine inhibitor 21  
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Gao, Y.G.  
Deposited on : 2014-04-09  
Resolution : 2.65 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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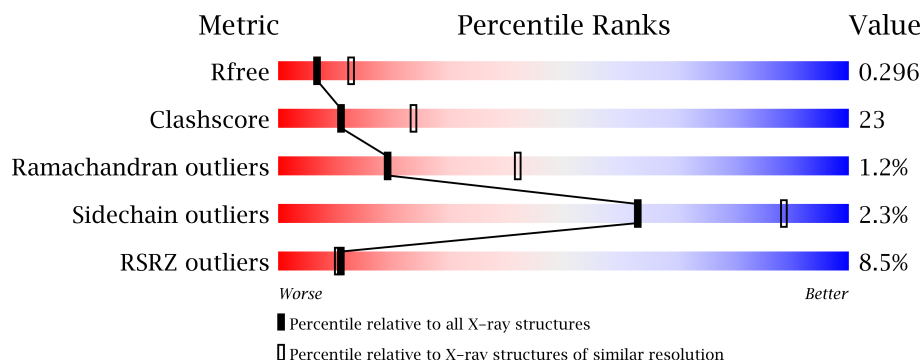
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.65 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))
$R_{free}$	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	495	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3658 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

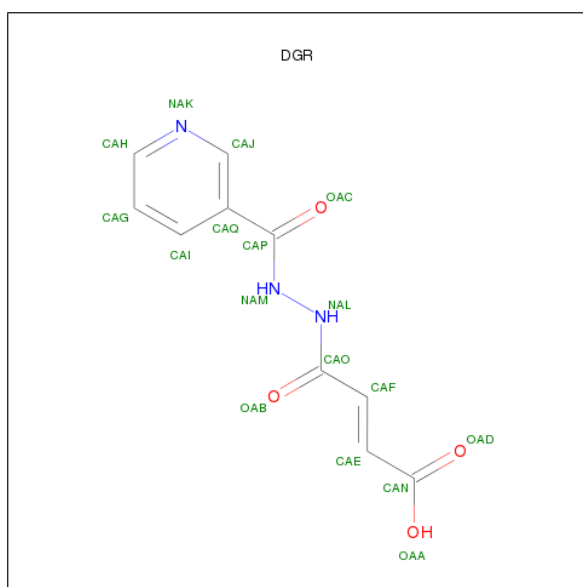
- Molecule 1 is a protein called ALPHA-KETOGLUTARATE-DEPENDENTDIOXYGENASE FTO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	436	3537	2243	610	662	22	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	MET	-	EXPRESSION TAG	UNP Q9C0B1
A	12	GLY	-	EXPRESSION TAG	UNP Q9C0B1
A	13	SER	-	EXPRESSION TAG	UNP Q9C0B1
A	14	SER	-	EXPRESSION TAG	UNP Q9C0B1
A	15	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	16	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	17	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	18	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	19	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	20	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	21	SER	-	EXPRESSION TAG	UNP Q9C0B1
A	22	SER	-	EXPRESSION TAG	UNP Q9C0B1
A	23	GLY	-	EXPRESSION TAG	UNP Q9C0B1
A	24	LEU	-	EXPRESSION TAG	UNP Q9C0B1
A	25	VAL	-	EXPRESSION TAG	UNP Q9C0B1
A	26	PRO	-	EXPRESSION TAG	UNP Q9C0B1
A	27	ARG	-	EXPRESSION TAG	UNP Q9C0B1
A	28	GLY	-	EXPRESSION TAG	UNP Q9C0B1
A	29	SER	-	EXPRESSION TAG	UNP Q9C0B1
A	30	HIS	-	EXPRESSION TAG	UNP Q9C0B1
A	31	MET	-	EXPRESSION TAG	UNP Q9C0B1

- Molecule 2 is (E)-4-(2-NICOTINOYLHYDRAZINYL)-4-OXOBUT-2-ENOICACID (three-letter code: DGR) (formula: C<sub>10</sub>H<sub>9</sub>N<sub>3</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	3	4		

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ni	0	0
			2	2		

- Molecule 4 is water.

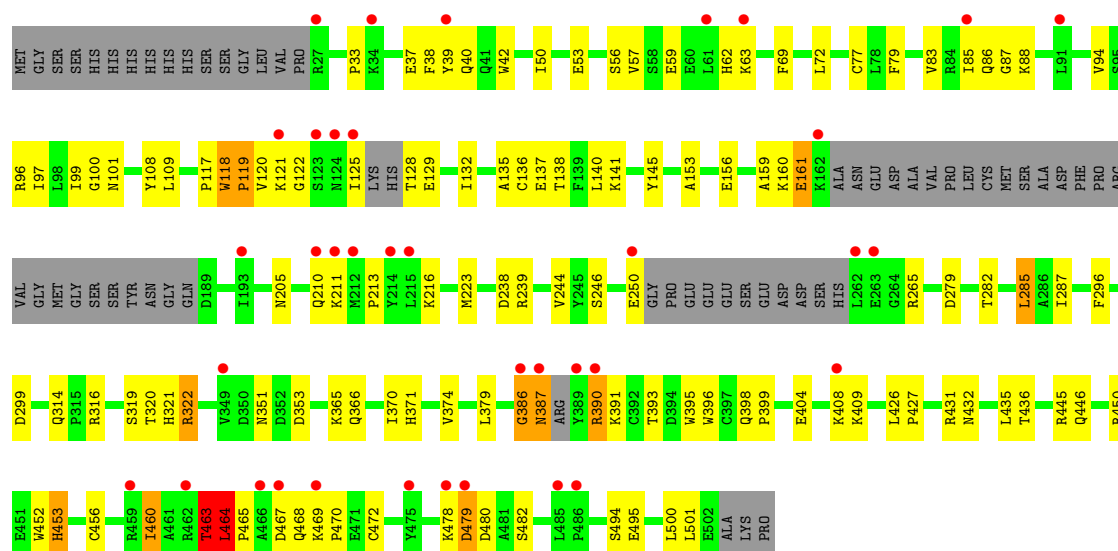
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		

### 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 errors 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: ALPHA-KETOGLUTARATE-DEPENDENTDIOXYGENASE FTO

Chain A: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.92Å 141.92Å 83.77Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.55 – 2.65 49.55 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.55-2.65) 99.7 (49.55-2.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.40 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.212 , 0.245 0.297 , 0.296	Depositor DCC
$R_{free}$ test set	915 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.6	EDS
Estimated twinning fraction	0.005 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.007 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.008 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.008 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.013 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.011 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.021 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 19267 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3658	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 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: DGR, NI

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	0.47	1/3620 (0.0%)	0.65	5/4907 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	119	PRO	N-CD	5.28	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	463	THR	N-CA-C	-8.04	89.29	111.00
1	A	464	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	118	TRP	C-N-CD	5.58	140.12	128.40
1	A	353	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	479	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	464	LEU	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3537	0	3437	158	2
2	A	17	0	0	0	0
3	A	2	0	0	0	0
4	A	102	0	0	18	0
All	All	3658	0	3437	158	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 23.

All (158) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:LEU:HD21	1:A:469:LYS:CE	1.27	1.61
1:A:464:LEU:HD22	1:A:469:LYS:CG	1.35	1.52
1:A:118:TRP:CZ3	1:A:140:LEU:HD13	1.63	1.31
1:A:464:LEU:CD2	1:A:469:LYS:CG	2.11	1.26
1:A:390:ARG:HD2	1:A:390:ARG:O	1.12	1.24
1:A:464:LEU:CD2	1:A:469:LYS:HG3	1.69	1.23
1:A:464:LEU:CD2	1:A:469:LYS:CE	2.17	1.22
1:A:464:LEU:CD2	1:A:469:LYS:HE3	1.74	1.18
1:A:101:ASN:N	1:A:118:TRP:HE1	1.41	1.17
1:A:118:TRP:CE3	1:A:140:LEU:HD13	1.84	1.12
1:A:464:LEU:HD21	1:A:469:LYS:HE2	1.32	1.08
1:A:100:GLY:C	1:A:118:TRP:CD1	2.29	1.05
1:A:390:ARG:CD	1:A:390:ARG:O	2.05	1.05
1:A:85:ILE:HD11	1:A:109:LEU:CD1	1.85	1.05
1:A:101:ASN:OD1	1:A:118:TRP:HZ2	1.38	1.03
1:A:85:ILE:HD11	1:A:109:LEU:HD13	1.07	1.02
1:A:101:ASN:OD1	1:A:118:TRP:CZ2	2.14	1.00
1:A:101:ASN:N	1:A:118:TRP:NE1	2.10	1.00
1:A:465:PRO:HG2	1:A:468:GLN:HG2	1.43	0.97
1:A:118:TRP:CZ3	1:A:140:LEU:CD1	2.49	0.95
1:A:390:ARG:HD2	1:A:390:ARG:C	1.87	0.95
1:A:85:ILE:CD1	1:A:109:LEU:HD13	1.95	0.94
1:A:464:LEU:CD2	1:A:469:LYS:HG2	2.00	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:LEU:HD22	1:A:469:LYS:HG2	1.53	0.90
1:A:37:GLU:O	1:A:40:GLN:HG2	1.72	0.88
1:A:464:LEU:HD21	1:A:469:LYS:HE3	0.89	0.87
1:A:100:GLY:C	1:A:118:TRP:HD1	1.76	0.86
1:A:160:LYS:HA	1:A:161:GLU:HB3	1.59	0.85
1:A:463:THR:O	1:A:463:THR:HG23	1.74	0.84
1:A:117:PRO:HD2	1:A:393:THR:HG21	1.61	0.82
1:A:464:LEU:CD2	1:A:469:LYS:CD	2.57	0.82
1:A:464:LEU:HD21	1:A:469:LYS:CD	2.13	0.79
1:A:320:THR:OG1	1:A:322:ARG:NH1	2.17	0.78
1:A:404:GLU:HG2	1:A:408:LYS:HE3	1.67	0.76
1:A:118:TRP:CZ3	1:A:120:VAL:HG22	2.22	0.75
1:A:464:LEU:HD22	1:A:469:LYS:HG3	0.74	0.73
1:A:469:LYS:HD2	4:A:2095:HOH:O	1.88	0.73
1:A:118:TRP:CH2	1:A:120:VAL:HG22	2.24	0.72
1:A:469:LYS:CG	4:A:2095:HOH:O	2.38	0.71
1:A:465:PRO:CG	1:A:468:GLN:HG2	2.17	0.70
1:A:446:GLN:HE21	1:A:450:ARG:HE	1.40	0.70
1:A:467:ASP:OD1	1:A:468:GLN:N	2.26	0.69
1:A:79:PHE:HZ	1:A:391:LYS:HD3	1.58	0.69
1:A:371:HIS:HD2	1:A:445:ARG:CZ	2.07	0.68
1:A:100:GLY:C	1:A:118:TRP:NE1	2.46	0.67
1:A:117:PRO:CD	1:A:393:THR:HG21	2.23	0.66
1:A:99:ILE:HG23	4:A:2022:HOH:O	1.96	0.66
1:A:100:GLY:CA	1:A:118:TRP:CD1	2.79	0.66
1:A:101:ASN:CA	1:A:118:TRP:HE1	2.10	0.65
1:A:463:THR:O	1:A:463:THR:CG2	2.46	0.64
1:A:160:LYS:CA	1:A:161:GLU:HB3	2.27	0.64
1:A:77:CYS:HB3	1:A:97:ILE:HD12	1.79	0.64
1:A:387:ASN:CG	1:A:467:ASP:O	2.37	0.63
1:A:119:PRO:O	1:A:140:LEU:HD22	1.97	0.63
1:A:160:LYS:O	1:A:160:LYS:HD2	1.98	0.63
1:A:469:LYS:CD	4:A:2095:HOH:O	2.46	0.63
1:A:160:LYS:N	1:A:161:GLU:HA	2.14	0.62
1:A:118:TRP:HZ3	1:A:140:LEU:CD1	2.12	0.62
1:A:387:ASN:ND2	1:A:467:ASP:HB2	2.15	0.61
1:A:100:GLY:O	1:A:118:TRP:HD1	1.83	0.61
1:A:101:ASN:H	1:A:118:TRP:HE1	1.40	0.61
1:A:59:GLU:O	1:A:63:LYS:HG3	2.01	0.61
1:A:101:ASN:CA	1:A:118:TRP:NE1	2.64	0.60
1:A:100:GLY:O	1:A:118:TRP:CD1	2.54	0.59
1:A:319:SER:OG	1:A:321:HIS:NE2	2.33	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:404:GLU:O	1:A:408:LYS:HG3	2.04	0.58
1:A:87:GLY:O	1:A:88:LYS:HG2	2.04	0.58
1:A:465:PRO:HG2	1:A:468:GLN:CG	2.25	0.57
1:A:464:LEU:CD2	1:A:469:LYS:HE2	2.10	0.57
1:A:119:PRO:HD2	1:A:137:GLU:HA	1.87	0.57
1:A:279:ASP:OD2	1:A:282:THR:OG1	2.11	0.56
1:A:138:THR:O	1:A:141:LYS:N	2.39	0.56
1:A:69:PHE:HB3	4:A:2007:HOH:O	2.05	0.54
1:A:244:VAL:HG22	1:A:320:THR:HG22	1.89	0.54
1:A:480:ASP:OD1	1:A:482:SER:OG	2.19	0.53
1:A:387:ASN:CB	1:A:467:ASP:O	2.56	0.53
1:A:431:ARG:NH2	1:A:432:ASN:OD1	2.41	0.53
1:A:211:LYS:C	1:A:213:PRO:HD3	2.29	0.53
1:A:469:LYS:HG3	4:A:2095:HOH:O	2.03	0.53
1:A:446:GLN:HE21	1:A:450:ARG:NE	2.04	0.53
1:A:85:ILE:O	1:A:86:GLN:HB2	2.09	0.52
1:A:494:SER:OG	1:A:495:GLU:N	2.41	0.52
1:A:118:TRP:CE3	1:A:140:LEU:CD1	2.75	0.52
1:A:160:LYS:N	1:A:161:GLU:CA	2.73	0.52
1:A:371:HIS:HD2	1:A:445:ARG:NH2	2.08	0.51
1:A:453:HIS:HA	1:A:456:CYS:CB	2.40	0.51
1:A:210:GLN:CG	4:A:2038:HOH:O	2.58	0.51
1:A:452:TRP:O	1:A:456:CYS:HB2	2.11	0.51
1:A:210:GLN:CD	4:A:2038:HOH:O	2.49	0.51
1:A:223:MET:O	1:A:265:ARG:NE	2.39	0.50
1:A:426:LEU:HD12	1:A:427:PRO:HD2	1.94	0.50
1:A:87:GLY:O	1:A:88:LYS:CG	2.60	0.50
1:A:100:GLY:CA	1:A:118:TRP:HD1	2.22	0.50
1:A:86:GLN:O	1:A:88:LYS:HG3	2.12	0.49
1:A:101:ASN:HA	1:A:118:TRP:NE1	2.26	0.49
1:A:453:HIS:HA	1:A:456:CYS:HB3	1.93	0.49
1:A:96:ARG:HD3	4:A:2013:HOH:O	2.11	0.49
1:A:398:GLN:HB3	1:A:399:PRO:HD3	1.94	0.48
1:A:469:LYS:HB2	4:A:2095:HOH:O	2.12	0.48
1:A:42:TRP:HD1	1:A:42:TRP:O	1.97	0.48
1:A:100:GLY:HA2	1:A:118:TRP:CD1	2.49	0.47
1:A:118:TRP:HE3	1:A:140:LEU:HD22	1.78	0.47
1:A:101:ASN:OD1	1:A:118:TRP:CE2	2.66	0.47
1:A:128:THR:HG23	1:A:393:THR:OG1	2.15	0.47
1:A:50:ILE:HD12	1:A:153:ALA:HB1	1.95	0.47
1:A:120:VAL:HG12	1:A:121:LYS:N	2.30	0.47
1:A:57:VAL:HB	1:A:62:HIS:NE2	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:VAL:HG12	1:A:96:ARG:HD2	1.97	0.47
1:A:136:CYS:HB3	4:A:2022:HOH:O	2.15	0.47
1:A:371:HIS:CD2	1:A:445:ARG:CZ	2.95	0.46
1:A:501:LEU:HD23	1:A:501:LEU:HA	1.83	0.46
1:A:365:LYS:HG3	1:A:366:GLN:N	2.29	0.46
1:A:478:LYS:C	1:A:480:ASP:H	2.19	0.46
1:A:460:ILE:HG12	1:A:460:ILE:O	2.16	0.45
1:A:159:ALA:C	1:A:161:GLU:HA	2.37	0.45
1:A:396:TRP:C	1:A:399:PRO:HD2	2.37	0.45
1:A:156:GLU:O	1:A:160:LYS:HB2	2.17	0.45
1:A:370:ILE:O	1:A:374:VAL:HG12	2.17	0.45
1:A:159:ALA:O	1:A:161:GLU:CB	2.65	0.45
1:A:120:VAL:HB	4:A:2023:HOH:O	2.17	0.44
1:A:395:TRP:CE3	1:A:395:TRP:O	2.70	0.44
1:A:96:ARG:NE	1:A:205:ASN:OD1	2.49	0.44
1:A:500:LEU:HD12	1:A:500:LEU:HA	1.82	0.44
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.67	0.44
1:A:464:LEU:HD23	1:A:469:LYS:HG2	1.95	0.43
1:A:453:HIS:HB2	1:A:472:CYS:SG	2.57	0.43
1:A:285:LEU:HD23	1:A:287:ILE:HD11	2.00	0.43
1:A:160:LYS:HB3	1:A:160:LYS:HE3	1.80	0.43
1:A:321:HIS:N	1:A:321:HIS:CD2	2.86	0.43
1:A:87:GLY:C	1:A:88:LYS:CG	2.87	0.43
1:A:246:SER:CB	1:A:316:ARG:HH21	2.32	0.43
1:A:210:GLN:HG3	4:A:2038:HOH:O	2.18	0.43
1:A:464:LEU:CG	1:A:469:LYS:HE3	2.45	0.43
1:A:160:LYS:CA	1:A:161:GLU:CB	2.94	0.42
1:A:250:GLU:OE1	1:A:314:GLN:NE2	2.52	0.42
1:A:386:GLY:O	1:A:387:ASN:C	2.57	0.42
1:A:464:LEU:CD1	1:A:469:LYS:HE3	2.50	0.42
1:A:108:TYR:HA	4:A:2018:HOH:O	2.20	0.42
1:A:50:ILE:HB	1:A:296:PHE:HB2	2.02	0.41
1:A:239:ARG:NH1	1:A:299:ASP:OD2	2.54	0.41
1:A:129:GLU:HG3	1:A:132:ILE:H	1.85	0.41
1:A:159:ALA:O	1:A:161:GLU:HB2	2.20	0.41
1:A:125:ILE:HG21	1:A:128:THR:HG22	2.03	0.41
1:A:135:ALA:O	1:A:138:THR:HB	2.21	0.41
1:A:465:PRO:CD	1:A:468:GLN:HG2	2.51	0.41
1:A:122:GLY:HA3	4:A:2024:HOH:O	2.21	0.41
1:A:121:LYS:H	1:A:121:LYS:HG3	1.67	0.41
1:A:464:LEU:HD11	1:A:469:LYS:HE3	2.03	0.41
1:A:72:LEU:N	4:A:2006:HOH:O	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:409:LYS:HE2	1:A:409:LYS:HB2	1.87	0.41
1:A:265:ARG:HB2	4:A:2055:HOH:O	2.20	0.41
1:A:33:PRO:HD3	1:A:38:PHE:CZ	2.56	0.40
1:A:351:ASN:O	1:A:409:LYS:NZ	2.54	0.40
1:A:56:SER:O	1:A:145:TYR:OH	2.34	0.40
1:A:94:VAL:HB	1:A:96:ARG:NH1	2.36	0.40
1:A:379:LEU:HD23	1:A:379:LEU:HA	1.92	0.40
1:A:431:ARG:O	1:A:435:LEU:HG	2.21	0.40
1:A:99:ILE:HD12	4:A:2015:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:TYR:OH	1:A:216:LYS:CA[6_445]	1.89	0.31
1:A:39:TYR:OH	1:A:216:LYS:CG[6_445]	2.17	0.03

## 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	426/495 (86%)	392 (92%)	29 (7%)	5 (1%)	19	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	436	THR
1	A	479	ASP
1	A	386	GLY
1	A	83	VAL
1	A	460	ILE

### 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	385/436 (88%)	376 (98%)	9 (2%)	63 88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	GLU
1	A	161	GLU
1	A	238	ASP
1	A	285	LEU
1	A	322	ARG
1	A	387	ASN
1	A	390	ARG
1	A	453	HIS
1	A	463	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	314	GLN
1	A	371	HIS
1	A	387	ASN
1	A	446	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	DGR	A	1503	3	17,17,17	2.84	7 (41%)	21,21,21	2.22	8 (38%)

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	DGR	A	1503	3	-	0/14/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1503	DGR	CAF-CAE	5.77	1.49	1.32
2	A	1503	DGR	CAP-NAM	5.63	1.42	1.34
2	A	1503	DGR	CAO-NAL	4.51	1.42	1.35
2	A	1503	DGR	CAE-CAN	4.44	1.58	1.48
2	A	1503	DGR	OAB-CAO	-2.69	1.19	1.24
2	A	1503	DGR	OAA-CAN	-2.57	1.23	1.30
2	A	1503	DGR	CAJ-CAQ	2.41	1.43	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1503	DGR	CAQ-CAP-NAM	5.17	121.69	115.96
2	A	1503	DGR	CAO-NAL-NAM	5.01	126.98	119.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1503	DGR	CAE-CAF-CAO	-3.55	111.71	125.25
2	A	1503	DGR	OAA-CAN-OAD	3.07	129.46	122.58
2	A	1503	DGR	OAC-CAP-CAQ	-2.96	115.84	120.98
2	A	1503	DGR	CAF-CAE-CAN	-2.26	116.72	127.21
2	A	1503	DGR	CAP-NAM-NAL	-2.07	115.99	119.21
2	A	1503	DGR	OAB-CAO-NAL	-2.06	118.68	121.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	436/495 (88%)	0.70	37 (8%) 11 10	43, 79, 118, 143	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	LYS	7.2
1	A	214	TYR	6.2
1	A	459	ARG	4.0
1	A	123	SER	3.9
1	A	262	LEU	3.8
1	A	469	LYS	3.8
1	A	466	ALA	3.8
1	A	387	ASN	3.2
1	A	263	GLU	3.1
1	A	389	TYR	3.0
1	A	85	ILE	3.0
1	A	39	TYR	3.0
1	A	61	LEU	2.9
1	A	27	ARG	2.8
1	A	162	LYS	2.8
1	A	215	LEU	2.8
1	A	63	LYS	2.8
1	A	193	ILE	2.7
1	A	124	ASN	2.7
1	A	485	LEU	2.6
1	A	250	GLU	2.6
1	A	125	ILE	2.6
1	A	478	LYS	2.5
1	A	212	MET	2.5
1	A	467	ASP	2.5
1	A	479	ASP	2.5
1	A	121	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	386	GLY	2.3
1	A	34	LYS	2.3
1	A	390	ARG	2.2
1	A	349	VAL	2.2
1	A	91	LEU	2.1
1	A	462	ARG	2.1
1	A	486	PRO	2.1
1	A	408	LYS	2.1
1	A	210	GLN	2.0
1	A	475	TYR	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NI	A	1504	1/1	0.20	0.65	69,69,69,69	0
2	DGR	A	1503	17/17	0.21	-0.19	65,76,85,93	0
3	NI	A	1505	1/1	0.10	-6.91	126,126,126,126	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.