



# wwPDB X-ray Structure Validation Summary Report i

Feb 28, 2014 – 11:20 PM GMT

PDB ID : 3E4A  
Title : Human IDE-inhibitor complex at 2.6 angstrom resolution  
Authors : Malito, E.; Leissring, M.A.; Choi, S.; Cuny, G.D.; Tang, W.J.  
Deposited on : 2008-08-11  
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary 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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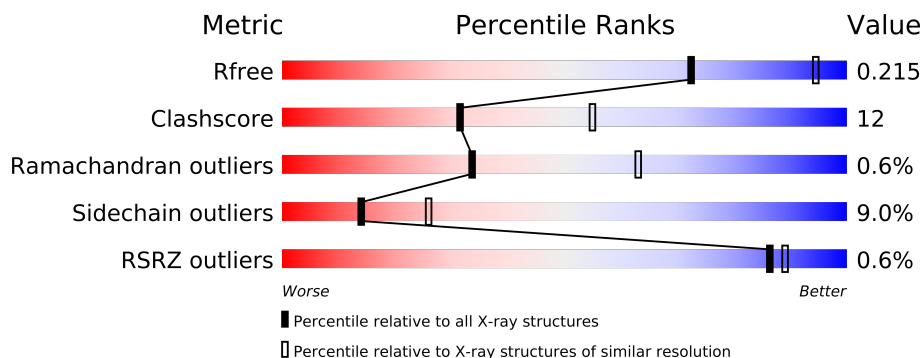
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
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)	:	stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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 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	1019	
1	B	1019	
2	F	3	
2	G	3	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	QIX	A	2001	-	X
4	QIX	B	2001	-	X
5	DIO	A	2003	-	X
5	DIO	B	2002	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	DIO	B	2003	-	X
5	DIO	B	2004	-	X
5	DIO	B	2005	-	X
5	DIO	B	2006	-	X
6	ACY	A	2010	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16294 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	961	Total	C	N	O	S	0	1	0
			7857	5058	1323	1454	22			
1	B	961	Total	C	N	O	S	0	1	0
			7857	5058	1323	1454	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	ILE	MET	ENGINEERED	UNP P14735
A	110	LEU	CYS	ENGINEERED	UNP P14735
A	111	GLN	GLU	ENGINEERED	UNP P14735
A	171	SER	CYS	ENGINEERED	UNP P14735
A	178	ALA	CYS	ENGINEERED	UNP P14735
A	257	VAL	CYS	ENGINEERED	UNP P14735
A	414	LEU	CYS	ENGINEERED	UNP P14735
A	555	ALA	VAL	ENGINEERED	UNP P14735
A	567	PHE	LYS	ENGINEERED	UNP P14735
A	568	PHE	LYS	ENGINEERED	UNP P14735
A	569	LEU	LYS	ENGINEERED	UNP P14735
A	573	ASN	CYS	ENGINEERED	UNP P14735
A	590	SER	CYS	ENGINEERED	UNP P14735
A	789	SER	CYS	ENGINEERED	UNP P14735
A	812	ALA	CYS	ENGINEERED	UNP P14735
A	819	ALA	CYS	ENGINEERED	UNP P14735
A	845	GLY	SER	ENGINEERED	UNP P14735
A	904	SER	CYS	ENGINEERED	UNP P14735
A	966	ASN	CYS	ENGINEERED	UNP P14735
A	974	ALA	CYS	ENGINEERED	UNP P14735
B	78	ILE	MET	ENGINEERED	UNP P14735
B	110	LEU	CYS	ENGINEERED	UNP P14735
B	111	GLN	GLU	ENGINEERED	UNP P14735
B	171	SER	CYS	ENGINEERED	UNP P14735
B	178	ALA	CYS	ENGINEERED	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
B	257	VAL	CYS	ENGINEERED	UNP P14735
B	414	LEU	CYS	ENGINEERED	UNP P14735
B	555	ALA	VAL	ENGINEERED	UNP P14735
B	567	PHE	LYS	ENGINEERED	UNP P14735
B	568	PHE	LYS	ENGINEERED	UNP P14735
B	569	LEU	LYS	ENGINEERED	UNP P14735
B	573	ASN	CYS	ENGINEERED	UNP P14735
B	590	SER	CYS	ENGINEERED	UNP P14735
B	789	SER	CYS	ENGINEERED	UNP P14735
B	812	ALA	CYS	ENGINEERED	UNP P14735
B	819	ALA	CYS	ENGINEERED	UNP P14735
B	845	GLY	SER	ENGINEERED	UNP P14735
B	904	SER	CYS	ENGINEERED	UNP P14735
B	966	ASN	CYS	ENGINEERED	UNP P14735
B	974	ALA	CYS	ENGINEERED	UNP P14735

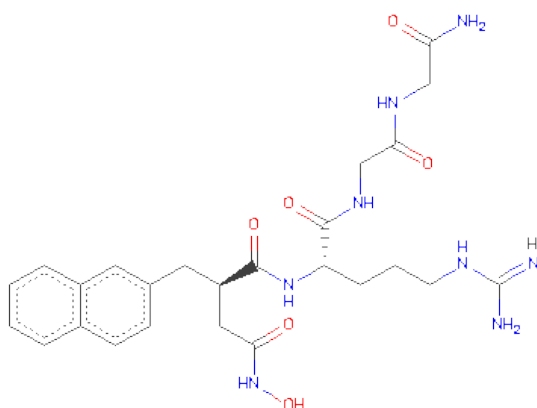
- Molecule 2 is a protein called HYDROXAMATE PEPTIDE III1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	G	3	Total	C	N	O	0	0	0
			15	9	3	3			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

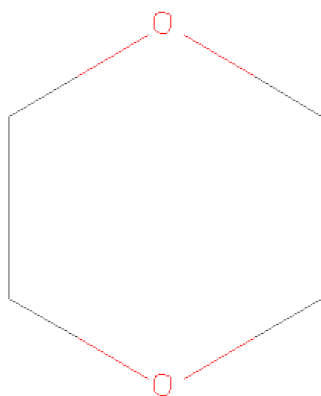
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N<sup>2</sup> -[(2R)-4-(HYDROXYAMINO)-2-(2-NAPHTHYLMETHYL)-4-OXOBUTANOYL]-L-ARGINYLGLYCYLGLYCINAMIDE (three-letter code: QIX) (formula: C<sub>25</sub>H<sub>34</sub>N<sub>8</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			39	25	8	6		
4	B	1	Total	C	N	O	0	0
			39	25	8	6		

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C<sub>4</sub>H<sub>8</sub>O<sub>2</sub>).



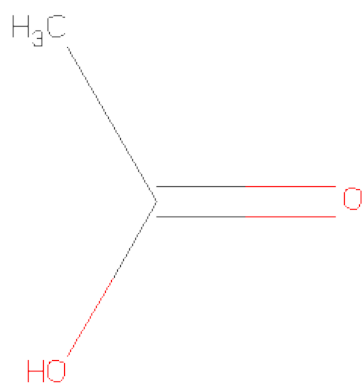
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			6	4	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		
5	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	214	Total O 214 214	0	0
7	B	158	Total O 158 158	0	0

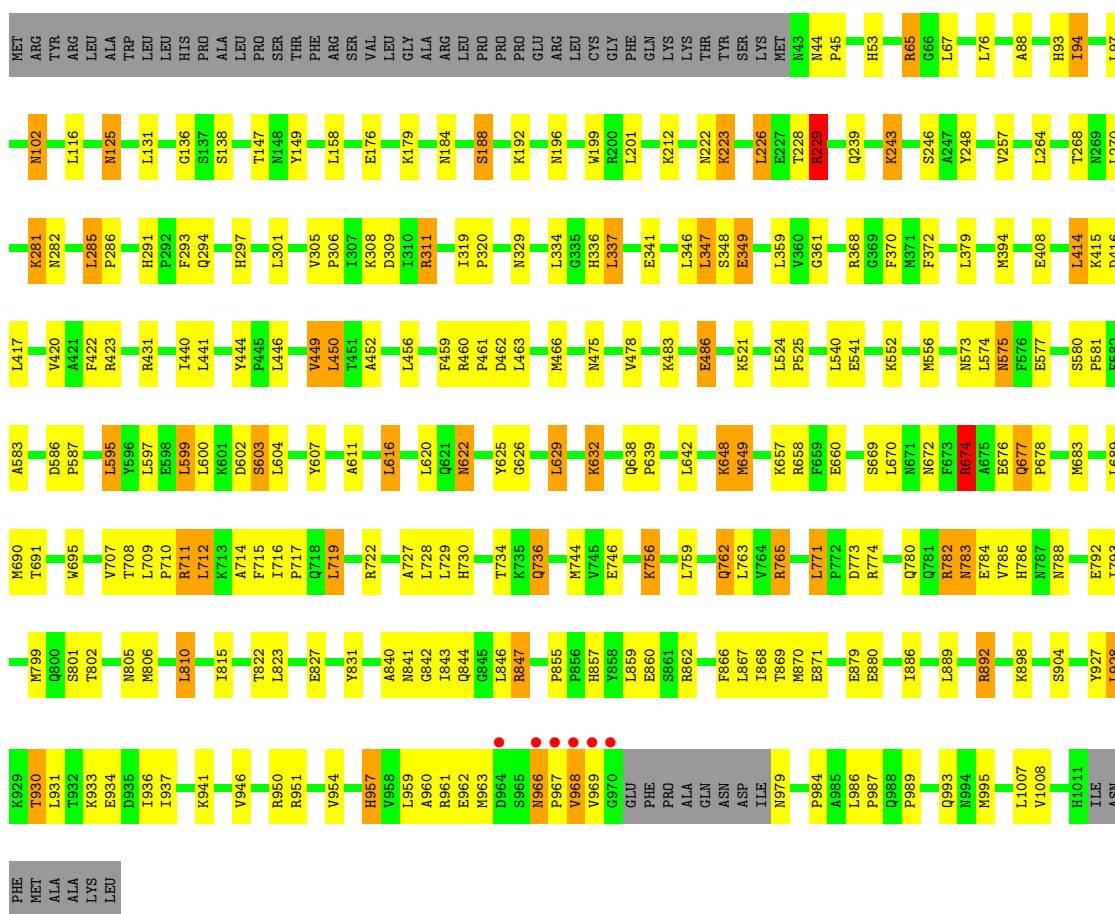


### 3 Residue-property plots

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.

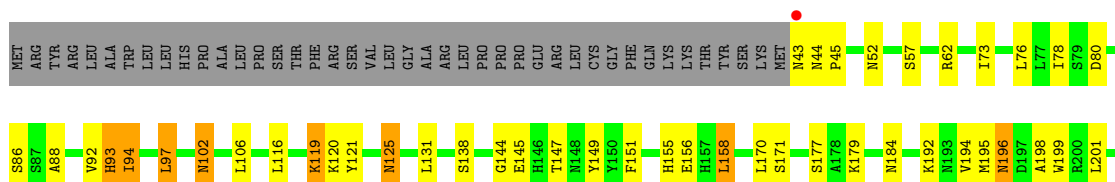
- Molecule 1: Insulin-degrading enzyme

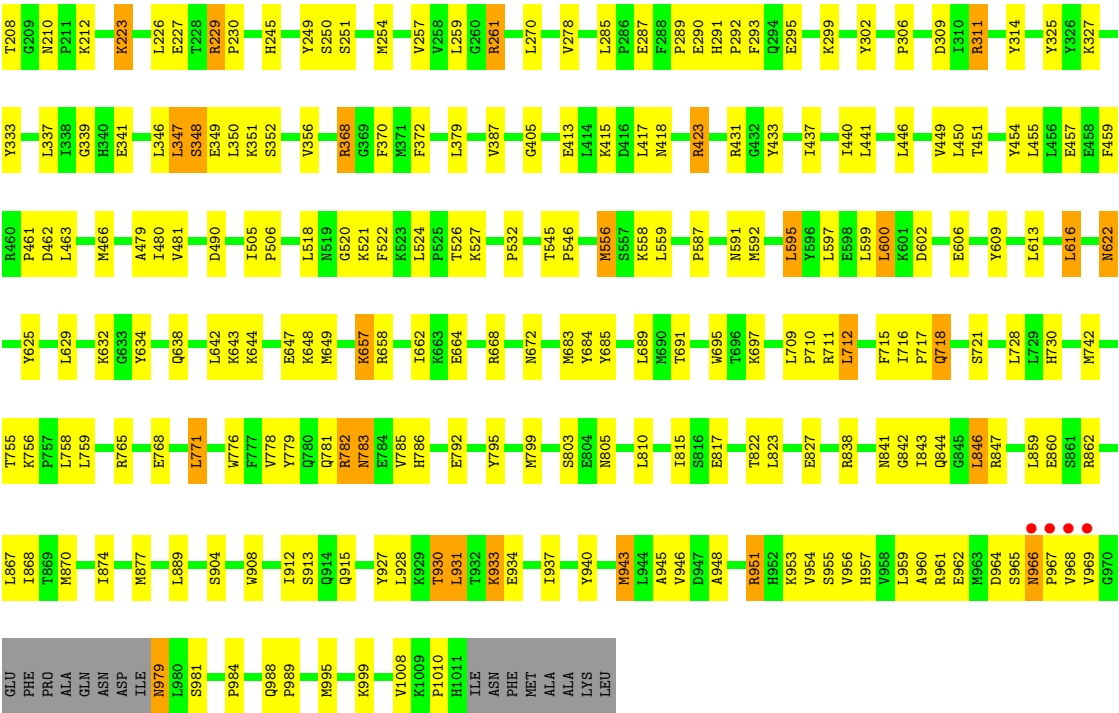
Chain A: 



- Molecule 1: Insulin-degrading enzyme

Chain B: 





● Molecule 2: HYDROXAMATE PEPTIDE II1

Chain F:



● Molecule 2: HYDROXAMATE PEPTIDE II1

Chain G:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	261.40Å 261.40Å 92.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.28 – 2.60 45.28 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.28-2.60) 97.3 (45.28-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.167 , 0.225 0.159 , 0.215	Depositor DCC
$R_{free}$ test set	5410 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 24.5	EDS
Estimated twinning fraction	0.019 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 106934 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	16294	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: ZN, DIO, ACY, QIX

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	0.98	5/8053 (0.1%)	0.98	13/10896 (0.1%)
1	B	0.92	0/8053	0.93	11/10896 (0.1%)
2	F	2.44	1/14 (7.1%)	1.87	0/18
2	G	2.42	1/14 (7.1%)	1.93	0/18
All	All	0.96	7/16134 (0.0%)	0.96	24/21828 (0.1%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	660	GLU	CG-CD	7.27	1.62	1.51
2	F	1	ALA	CA-CB	6.52	1.66	1.52
1	A	871	GLU	CG-CD	6.00	1.60	1.51
1	A	349	GLU	CG-CD	5.49	1.60	1.51
1	A	676	GLU	CG-CD	5.41	1.60	1.51

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ILE	CG1-CB-CG2	-6.73	96.60	111.40
1	A	674	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	A	414	LEU	CA-CB-CG	6.44	130.12	115.30
1	B	668	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	A	892	ARG	NE-CZ-NH2	6.34	123.47	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	7857	0	7791	186	1
1	B	7857	0	7791	180	0
2	F	15	0	17	1	0
2	G	15	0	17	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	39	0	32	3	0
4	B	39	0	32	4	0
5	A	12	0	16	12	0
5	B	30	0	40	3	0
6	A	32	0	32	0	0
6	B	24	0	24	2	0
7	A	214	0	0	7	0
7	B	158	0	0	7	0
All	All	16294	0	15792	369	1

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 12.

The worst 5 of 369 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:782:ARG:HG2	1:A:782:ARG:HH11	1.10	1.09
1:B:782:ARG:CG	1:B:782:ARG:HH11	1.67	1.05
1:B:116:LEU:HD21	4:B:2001:QIX:H25	1.26	1.05
1:A:782:ARG:HG2	1:A:782:ARG:NH1	1.67	1.01
1:B:841:ASN:H	5:B:2003:DIO:H11	1.28	0.99

All (1) 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:408:GLU:OE1	1:A:734:THR:OG1[2_564]	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	958/1019 (94%)	917 (96%)	39 (4%)	2 (0%)	56	82
1	B	958/1019 (94%)	919 (96%)	29 (3%)	10 (1%)	22	45
2	F	1/3 (33%)	0	1 (100%)	0	100	100
2	G	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1918/2044 (94%)	1837 (96%)	69 (4%)	12 (1%)	33	63

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	968	VAL
1	B	52	ASN
1	B	965	SER
1	B	967	PRO
1	A	228	THR

### 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	855/906 (94%)	777 (91%)	78 (9%)	14	25
1	B	855/906 (94%)	780 (91%)	75 (9%)	14	27
All	All	1710/1812 (94%)	1557 (91%)	153 (9%)	14	26

5 of 153 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	898	LYS

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Mol	Chain	Res	Type
1	B	158	LEU
1	B	860	GLU
1	A	930	THR
1	A	1007	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	828	GLN
1	B	125	ASN
1	B	828	GLN
1	A	883	GLN
1	B	93	HIS

### 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 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	QIX	A	2001	3	40,40,40	3.69	20 (50%)	52,52,52	3.66	28 (53%)
5	DIO	A	2002	-	6,6,6	1.02	0	6,6,6	0.61	0
5	DIO	A	2003	-	6,6,6	1.04	0	6,6,6	0.56	0
6	ACY	A	2004	-	3,3,3	1.78	1 (33%)	3,3,3	1.42	0
6	ACY	A	2005	-	3,3,3	1.55	1 (33%)	3,3,3	0.67	0
6	ACY	A	2006	-	3,3,3	1.61	1 (33%)	3,3,3	1.34	0
6	ACY	A	2007	-	3,3,3	1.70	1 (33%)	3,3,3	0.92	0
6	ACY	A	2008	-	3,3,3	1.97	1 (33%)	3,3,3	1.67	1 (33%)
6	ACY	A	2009	-	3,3,3	1.75	1 (33%)	3,3,3	1.49	1 (33%)
6	ACY	A	2010	-	3,3,3	1.61	1 (33%)	3,3,3	1.25	0
6	ACY	A	2011	-	3,3,3	1.48	1 (33%)	3,3,3	0.59	0
4	QIX	B	2001	3	40,40,40	3.59	19 (47%)	52,52,52	3.23	25 (48%)
5	DIO	B	2002	-	6,6,6	0.67	0	6,6,6	0.30	0
5	DIO	B	2003	-	6,6,6	0.93	0	6,6,6	0.64	0
5	DIO	B	2004	-	6,6,6	1.16	0	6,6,6	0.59	0
5	DIO	B	2005	-	6,6,6	1.34	0	6,6,6	0.49	0
5	DIO	B	2006	-	6,6,6	1.04	0	6,6,6	0.28	0
6	ACY	B	2007	-	3,3,3	1.89	2 (66%)	3,3,3	1.49	0
6	ACY	B	2008	-	3,3,3	1.66	1 (33%)	3,3,3	0.81	0
6	ACY	B	2009	-	3,3,3	1.75	1 (33%)	3,3,3	1.17	0
6	ACY	B	2010	-	3,3,3	1.74	1 (33%)	3,3,3	1.07	0
6	ACY	B	2011	-	3,3,3	1.87	2 (66%)	3,3,3	0.98	0
6	ACY	B	2012	-	3,3,3	1.46	1 (33%)	3,3,3	1.02	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	QIX	A	2001	3	-	0/39/39/39	0/0/2/2
5	DIO	A	2002	-	-	0/0/6/6	0/1/1/1
5	DIO	A	2003	-	-	0/0/6/6	0/1/1/1
6	ACY	A	2004	-	-	0/0/0/0	0/0/0/0
6	ACY	A	2005	-	-	0/0/0/0	0/0/0/0
6	ACY	A	2006	-	-	0/0/0/0	0/0/0/0
6	ACY	A	2007	-	-	0/0/0/0	0/0/0/0
6	ACY	A	2008	-	-	0/0/0/0	0/0/0/0
6	ACY	A	2009	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ACY	A	2010	-	-	0/0/0/0	0/0/0/0
6	ACY	A	2011	-	-	0/0/0/0	0/0/0/0
4	QIX	B	2001	3	-	0/39/39/39	0/0/2/2
5	DIO	B	2002	-	-	0/0/6/6	0/1/1/1
5	DIO	B	2003	-	-	0/0/6/6	0/1/1/1
5	DIO	B	2004	-	-	0/0/6/6	0/1/1/1
5	DIO	B	2005	-	-	0/0/6/6	0/1/1/1
5	DIO	B	2006	-	-	0/0/6/6	0/1/1/1
6	ACY	B	2007	-	-	0/0/0/0	0/0/0/0
6	ACY	B	2008	-	-	0/0/0/0	0/0/0/0
6	ACY	B	2009	-	-	0/0/0/0	0/0/0/0
6	ACY	B	2010	-	-	0/0/0/0	0/0/0/0
6	ACY	B	2011	-	-	0/0/0/0	0/0/0/0
6	ACY	B	2012	-	-	0/0/0/0	0/0/0/0

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	QIX	C14-N16	11.75	1.44	1.32
4	A	2001	QIX	C14-N16	11.11	1.44	1.32
4	A	2001	QIX	C43-N45	8.15	1.52	1.33
4	B	2001	QIX	C29-N31	7.94	1.50	1.33
4	A	2001	QIX	C02-N04	7.62	1.49	1.33

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	QIX	C18-C19-C28	13.11	135.55	121.25
4	B	2001	QIX	C18-C12-C13	-10.24	98.74	111.39
4	A	2001	QIX	C18-C12-C13	-9.24	99.97	111.39
4	A	2001	QIX	C18-C19-C20	-8.84	103.55	120.90
4	B	2001	QIX	C18-C19-C28	8.59	130.62	121.25

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	961/1019 (94%)	-0.66	6 (0%) 86 89	16, 33, 55, 100	0
1	B	961/1019 (94%)	-0.64	5 (0%) 88 90	24, 37, 58, 102	0
2	F	3/3 (100%)	0.55	0 100 100	52, 52, 55, 56	0
2	G	3/3 (100%)	0.61	0 100 100	42, 42, 45, 51	0
All	All	1928/2044 (94%)	-0.65	11 (0%) 86 89	16, 35, 57, 102	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	966	ASN	5.5
1	B	966	ASN	5.0
1	A	968	VAL	3.4
1	A	967	PRO	3.3
1	B	968	VAL	3.3

### 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
5	DIO	B	2003	6/6	0.21	16.38	35,56,63,86	0
5	DIO	B	2006	6/6	0.24	8.50	69,76,87,90	0
5	DIO	A	2003	6/6	0.21	8.45	31,43,51,60	0
6	ACY	A	2010	4/4	0.18	7.86	33,53,56,58	0
4	QIX	A	2001	39/39	0.19	5.64	33,53,81,84	0
5	DIO	B	2004	6/6	0.16	4.99	51,64,67,78	0
4	QIX	B	2001	39/39	0.19	4.95	40,58,90,102	0
5	DIO	B	2005	6/6	0.22	3.24	55,70,84,95	0
5	DIO	B	2002	6/6	0.16	2.55	33,38,46,54	0
6	ACY	B	2010	4/4	0.14	1.81	29,52,60,63	0
6	ACY	A	2011	4/4	0.14	1.52	24,37,42,51	0
6	ACY	B	2012	4/4	0.14	1.52	42,51,56,59	0
6	ACY	A	2009	4/4	0.14	1.23	45,49,60,65	0
5	DIO	A	2002	6/6	0.12	1.12	45,59,65,67	0
3	ZN	B	2000	1/1	0.11	0.46	32,32,32,32	0
6	ACY	A	2008	4/4	0.15	0.34	41,43,53,60	0
6	ACY	B	2007	4/4	0.18	-0.04	43,60,65,75	0
6	ACY	A	2007	4/4	0.13	-0.09	38,51,60,66	0
3	ZN	A	2000	1/1	0.11	-0.27	31,31,31,31	0
6	ACY	A	2006	4/4	0.12	-0.34	32,62,70,82	0
6	ACY	B	2008	4/4	0.12	-0.55	56,61,68,69	0
6	ACY	A	2004	4/4	0.12	-0.56	51,60,64,74	0
6	ACY	B	2011	4/4	0.12	-1.07	28,53,55,70	0
6	ACY	B	2009	4/4	0.12	-1.18	34,48,57,58	0
6	ACY	A	2005	4/4	0.11	-2.82	42,53,61,68	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.