



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 23, 2023 – 03:56 PM EDT

PDB ID : 5TDV  
Title : Intermediate O<sub>2</sub> diiron complex in the Q228A variant of Toluene 4-moonoxygenase (T4moHD)  
Authors : Bailey, L.J.; Acheson, J.F.; Fox, B.G.  
Deposited on : 2016-09-19  
Resolution : 2.00 Å (reported)

This is a wwPDB X-ray Structure 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

<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>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35.1

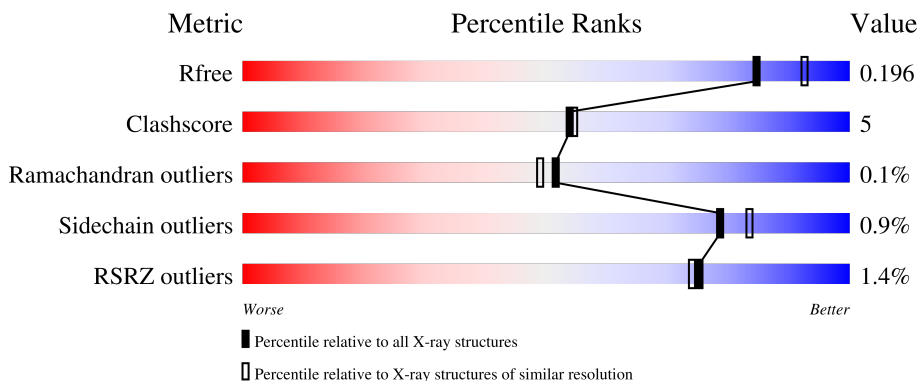
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



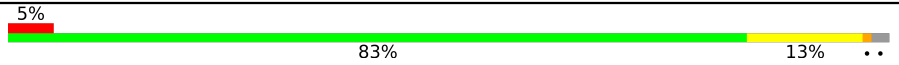

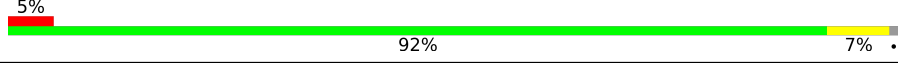
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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  $\geq 3$ , 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	500	 88% 10% ..
1	D	500	 86% 12% .
2	B	327	 83% 10% 7%
2	F	327	 82% 10% . 7%
3	C	84	 5% 86% 12% .

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Mol	Chain	Length	Quality of chain
3	G	84	 5% 83% 13% ..
4	E	103	 4% 88% 9% ..
4	H	103	 5% 92% 7% .

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 17695 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 Toluene-4-monooxygenase system protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	491	4059	2603	682	748	26	0	5	0
1	D	491	4077	2614	685	755	23	0	7	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ALA	GLN	engineered mutation	UNP Q00456
A	336	TRP	LEU	conflict	UNP Q00456
A	337	TYR	ASP	conflict	UNP Q00456
A	382	ASP	ASN	conflict	UNP Q00456
A	465	ASP	GLU	conflict	UNP Q00456
D	228	ALA	GLN	engineered mutation	UNP Q00456
D	336	TRP	LEU	conflict	UNP Q00456
D	337	TYR	ASP	conflict	UNP Q00456
D	382	ASP	ASN	conflict	UNP Q00456
D	465	ASP	GLU	conflict	UNP Q00456

- Molecule 2 is a protein called Toluene-4-monooxygenase system protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	305	2550	1615	442	478	15	0	3	0
2	F	305	2547	1612	444	476	15	0	4	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	239	TYR	TRP	conflict	UNP Q00460
F	239	TYR	TRP	conflict	UNP Q00460

- Molecule 3 is a protein called Toluene-4-monooxygenase system protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	82	Total 651	C 411	N 117	O 119	S 4	0	0	0
3	G	82	Total 664	C 419	N 118	O 122	S 5	0	2	0

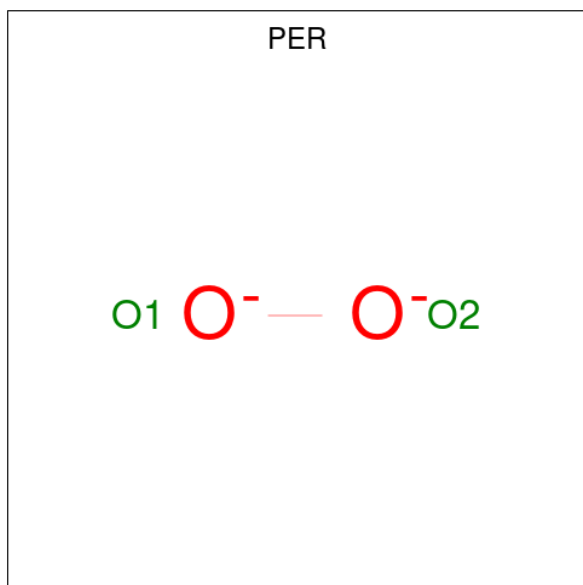
- Molecule 4 is a protein called Toluene-4-monooxygenase system protein D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	101	Total 819	C 511	N 145	O 160	S 3	0	2	0
4	H	102	Total 811	C 508	N 141	O 160	S 2	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	5	GLN	ASP	conflict	UNP Q00459
H	5	GLN	ASP	conflict	UNP Q00459

- Molecule 5 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total O 2 2	0	0

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Fe 2 2	0	0
6	D	2	Total Fe 2 2	0	0

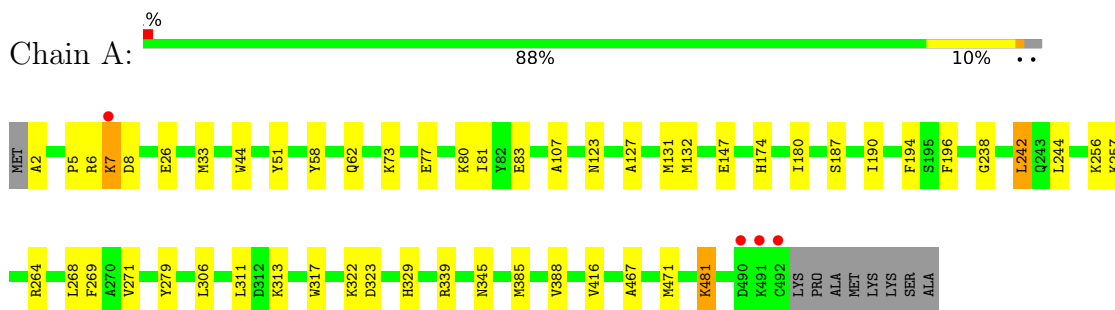
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	334	Total O 334 334	0	0
7	B	233	Total O 233 233	0	0
7	C	57	Total O 57 57	0	0
7	E	104	Total O 104 104	0	0
7	D	374	Total O 374 374	0	0
7	F	253	Total O 253 253	0	0
7	G	58	Total O 58 58	0	0
7	H	96	Total O 96 96	0	0

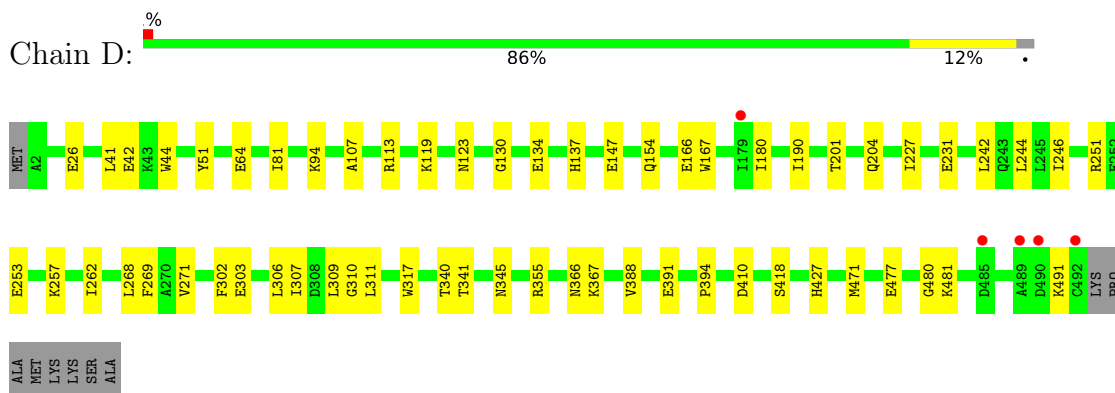
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

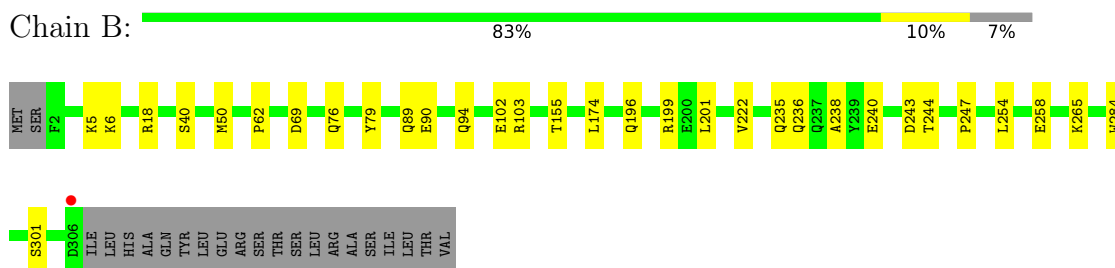
- Molecule 1: Toluene-4-monooxygenase system protein A



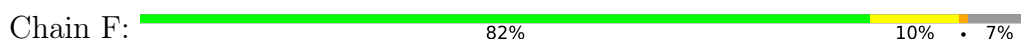
- Molecule 1: Toluene-4-monooxygenase system protein A

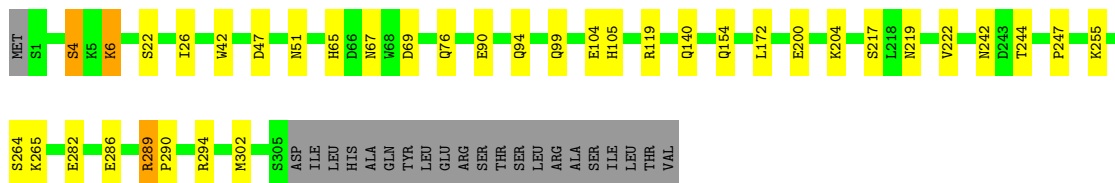


- Molecule 2: Toluene-4-monooxygenase system protein E

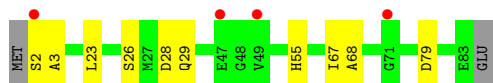
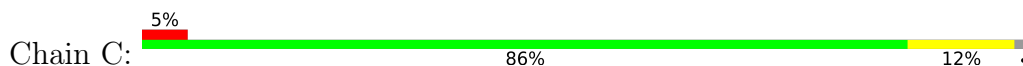


- Molecule 2: Toluene-4-monooxygenase system protein E

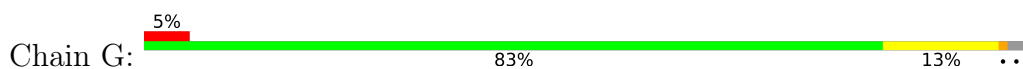




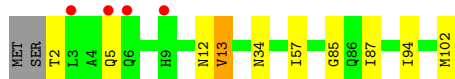
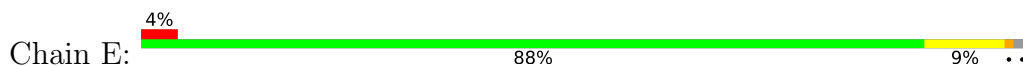
- Molecule 3: Toluene-4-monoxygenase system protein B



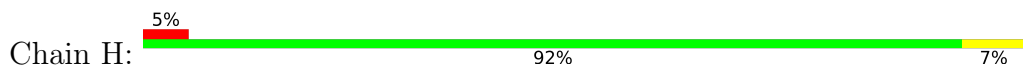
- Molecule 3: Toluene-4-monoxygenase system protein B



- Molecule 4: Toluene-4-monoxygenase system protein D



- Molecule 4: Toluene-4-monoxygenase system protein D





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.29Å 115.76Å 181.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.28 – 2.00 43.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.28-2.00) 98.7 (43.89-2.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.64 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (1.11rc1_2513)	Depositor
R, $R_{free}$	0.153 , 0.195 0.154 , 0.196	Depositor DCC
$R_{free}$ test set	7087 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	22.0	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	17695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.4916e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: PER, FE

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	0.39	0/4194	0.54	0/5695
1	D	0.43	0/4209	0.56	1/5719 (0.0%)
2	B	0.37	0/2627	0.51	0/3568
2	F	0.39	0/2624	0.55	3/3566 (0.1%)
3	C	0.31	0/663	0.51	0/898
3	G	0.43	0/679	0.60	1/920 (0.1%)
4	E	0.37	0/829	0.59	0/1119
4	H	0.36	0/824	0.57	0/1115
All	All	0.40	0/16649	0.55	5/22600 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	289	ARG	NE-CZ-NH2	-7.05	116.78	120.30
3	G	54	LYS	CD-CE-NZ	-6.42	96.94	111.70
2	F	289	ARG	NH1-CZ-NH2	5.64	125.60	119.40
1	D	306	LEU	CA-CB-CG	5.37	127.66	115.30
2	F	289	ARG	NE-CZ-NH1	-5.37	117.62	120.30

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	4059	0	3813	39	0
1	D	4077	0	3819	53	0
2	B	2550	0	2432	22	0
2	F	2547	0	2424	34	0
3	C	651	0	647	9	0
3	G	664	0	662	11	0
4	E	819	0	808	5	0
4	H	811	0	807	5	0
5	A	2	0	0	0	0
5	D	2	0	0	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
7	A	334	0	0	3	0
7	B	233	0	0	8	0
7	C	57	0	0	1	0
7	D	374	0	0	12	0
7	E	104	0	0	1	0
7	F	253	0	0	10	0
7	G	58	0	0	2	0
7	H	96	0	0	2	0
All	All	17695	0	15412	166	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 5.

The worst 5 of 166 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:D:231[B]:GLU:OE1	7:D:701:HOH:O	1.70	1.06
2:F:6:LYS:NZ	7:F:403:HOH:O	1.90	1.05
1:D:166:GLU:HA	1:D:471:MET:HG2	1.43	0.98
2:B:265:LYS:NZ	7:B:401:HOH:O	1.91	0.91
2:F:47:ASP:OD1	7:F:401:HOH:O	1.86	0.91

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	494/500 (99%)	480 (97%)	13 (3%)	1 (0%)	47	44
1	D	496/500 (99%)	481 (97%)	15 (3%)	0	100	100
2	B	306/327 (94%)	304 (99%)	2 (1%)	0	100	100
2	F	307/327 (94%)	304 (99%)	3 (1%)	0	100	100
3	C	80/84 (95%)	77 (96%)	3 (4%)	0	100	100
3	G	82/84 (98%)	77 (94%)	5 (6%)	0	100	100
4	E	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
4	H	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
All	All	1967/2028 (97%)	1922 (98%)	44 (2%)	1 (0%)	51	49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	419/422 (99%)	413 (99%)	6 (1%)	67	72
1	D	420/422 (100%)	416 (99%)	4 (1%)	76	81
2	B	278/296 (94%)	274 (99%)	4 (1%)	67	72
2	F	276/296 (93%)	274 (99%)	2 (1%)	84	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	72/75 (96%)	72 (100%)	0	100	100
3	G	75/75 (100%)	75 (100%)	0	100	100
4	E	86/87 (99%)	84 (98%)	2 (2%)	50	53
4	H	86/87 (99%)	86 (100%)	0	100	100
All	All	1712/1760 (97%)	1694 (99%)	18 (1%)	78	78

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	388[A]	VAL
2	F	6	LYS
2	F	4	SER
2	B	174[B]	LEU
1	D	123	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	345	ASN
3	G	40	ASN
2	F	51	ASN
2	F	241	ASN
1	D	379	ASN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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	$\# Z  > 2$
5	PER	D	601	6	0,1,1	-	-	-		
5	PER	A	601	6	0,1,1	-	-	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	491/500 (98%)	-0.34	4 (0%) 86 85	11, 22, 42, 62	0
1	D	491/500 (98%)	-0.27	5 (1%) 82 81	11, 22, 40, 60	0
2	B	305/327 (93%)	-0.40	1 (0%) 94 93	12, 27, 51, 82	0
2	F	305/327 (93%)	-0.45	0 100 100	12, 24, 46, 72	0
3	C	82/84 (97%)	0.21	4 (4%) 29 28	21, 38, 60, 74	0
3	G	82/84 (97%)	0.42	4 (4%) 29 28	20, 36, 58, 75	0
4	E	101/103 (98%)	-0.32	4 (3%) 38 37	12, 24, 48, 58	0
4	H	102/103 (99%)	-0.32	5 (4%) 29 28	14, 26, 53, 82	0
All	All	1959/2028 (96%)	-0.29	27 (1%) 75 74	11, 24, 48, 82	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	H	1	SER	5.2
4	E	5	GLN	3.7
1	D	492	CYS	3.6
1	A	7	LYS	3.5
1	D	489	ALA	3.3

### 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 monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	PER	D	601	2/2	0.93	0.29	29,29,29,47	0
5	PER	A	601	2/2	0.98	0.28	25,25,25,35	0
6	FE	A	602	1/1	1.00	0.10	17,17,17,17	0
6	FE	A	603	1/1	1.00	0.06	23,23,23,23	0
6	FE	D	602	1/1	1.00	0.08	15,15,15,15	0
6	FE	D	603	1/1	1.00	0.05	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.