



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 06:57 PM GMT

PDB ID : 4NBD
Title : Carbazole-bound oxygenase with Phe275 replaced by Trp and ferredoxin complex of carbazole 1,9a-dioxygenase (form2)
Authors : Ashikawa, Y.; Usami, Y.; Inoue, K.; Nojiri, H.
Deposited on : 2013-10-23
Resolution : 1.95 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

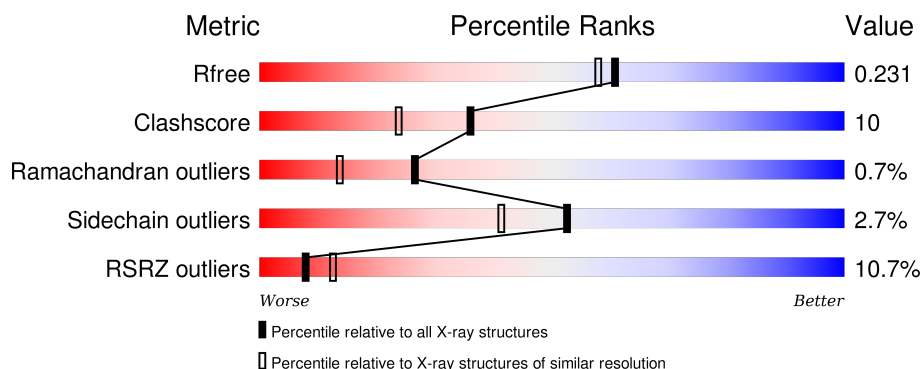
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 ≥ 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	392	<div> <div>5%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>
1	B	392	<div> <div>16%</div> <div>68%</div> <div>28%</div> <div>..</div> </div>
1	C	392	<div> <div>5%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
2	D	115	<div> <div>34%</div> <div>72%</div> <div>17%</div> <div>• 10%</div> </div>
2	E	115	<div> <div>7%</div> <div>77%</div> <div>16%</div> <div>7%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11827 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 Terminal oxygenase component of carbazole.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3092	1978	525	576	13			
1	B	384	Total	C	N	O	S	0	0	0
			3092	1978	525	576	13			
1	C	388	Total	C	N	O	S	0	0	0
			3131	2001	535	582	13			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	275	TRP	PHE	ENGINEERED MUTATION	UNP Q84II6
A	385	LEU	-	EXPRESSION TAG	UNP Q84II6
A	386	GLU	-	EXPRESSION TAG	UNP Q84II6
A	387	HIS	-	EXPRESSION TAG	UNP Q84II6
A	388	HIS	-	EXPRESSION TAG	UNP Q84II6
A	389	HIS	-	EXPRESSION TAG	UNP Q84II6
A	390	HIS	-	EXPRESSION TAG	UNP Q84II6
A	391	HIS	-	EXPRESSION TAG	UNP Q84II6
A	392	HIS	-	EXPRESSION TAG	UNP Q84II6
B	275	TRP	PHE	ENGINEERED MUTATION	UNP Q84II6
B	385	LEU	-	EXPRESSION TAG	UNP Q84II6
B	386	GLU	-	EXPRESSION TAG	UNP Q84II6
B	387	HIS	-	EXPRESSION TAG	UNP Q84II6
B	388	HIS	-	EXPRESSION TAG	UNP Q84II6
B	389	HIS	-	EXPRESSION TAG	UNP Q84II6
B	390	HIS	-	EXPRESSION TAG	UNP Q84II6
B	391	HIS	-	EXPRESSION TAG	UNP Q84II6
B	392	HIS	-	EXPRESSION TAG	UNP Q84II6
C	275	TRP	PHE	ENGINEERED MUTATION	UNP Q84II6
C	385	LEU	-	EXPRESSION TAG	UNP Q84II6
C	386	GLU	-	EXPRESSION TAG	UNP Q84II6
C	387	HIS	-	EXPRESSION TAG	UNP Q84II6
C	388	HIS	-	EXPRESSION TAG	UNP Q84II6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	389	HIS	-	EXPRESSION TAG	UNP Q84II6
C	390	HIS	-	EXPRESSION TAG	UNP Q84II6
C	391	HIS	-	EXPRESSION TAG	UNP Q84II6
C	392	HIS	-	EXPRESSION TAG	UNP Q84II6

- Molecule 2 is a protein called Ferredoxin CarAc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	103	Total	C	N	O	S	0	0	0
			759	477	127	148	7			
2	E	107	Total	C	N	O	S	0	0	0
			794	499	133	155	7			

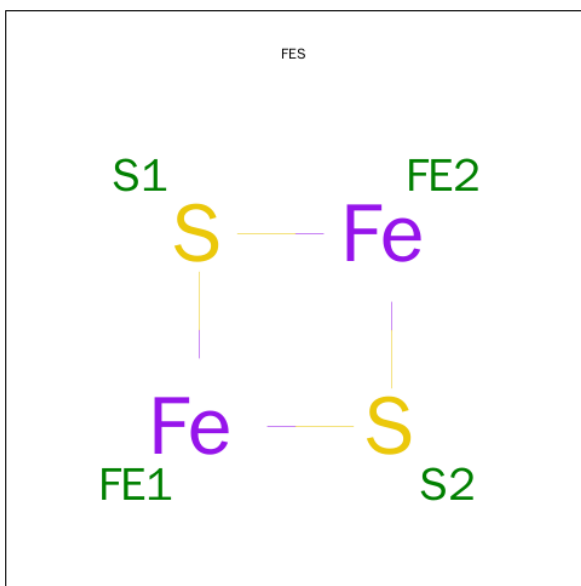
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	108	LEU	-	EXPRESSION TAG	UNP Q8GI16
D	109	GLU	-	EXPRESSION TAG	UNP Q8GI16
D	110	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	111	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	112	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	113	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	114	HIS	-	EXPRESSION TAG	UNP Q8GI16
D	115	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	108	LEU	-	EXPRESSION TAG	UNP Q8GI16
E	109	GLU	-	EXPRESSION TAG	UNP Q8GI16
E	110	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	111	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	112	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	113	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	114	HIS	-	EXPRESSION TAG	UNP Q8GI16
E	115	HIS	-	EXPRESSION TAG	UNP Q8GI16

- Molecule 3 is FE (II) ION (three-letter code: FE2) (formula: Fe).

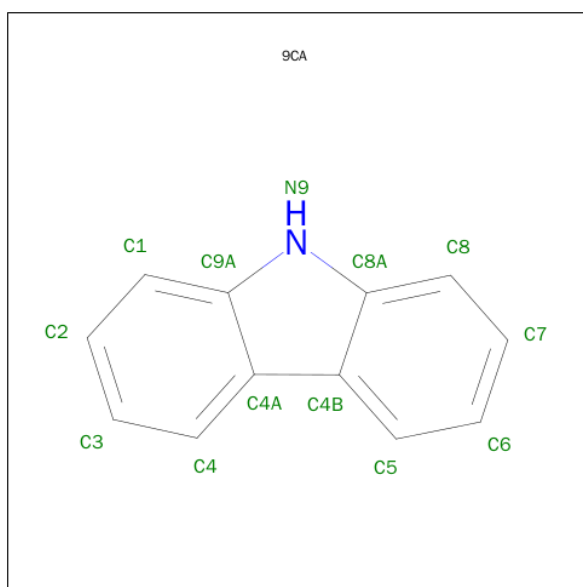
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Fe	0	0
			1	1		
3	A	1	Total	Fe	0	0
			1	1		
3	C	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	B	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		
4	D	1	Total	Fe	S	0	0
			4	2	2		
4	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 5 is 9H-CARBAZOLE (three-letter code: 9CA) (formula: $\text{C}_{12}\text{H}_9\text{N}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			13	12	1		
5	B	1	Total	C	N	0	0
			13	12	1		
5	C	1	Total	C	N	0	0
			13	12	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	287	Total	O	0	0
			287	287		
6	B	196	Total	O	0	0
			196	196		
6	C	335	Total	O	0	0
			335	335		
6	D	37	Total	O	0	0
			37	37		
6	E	42	Total	O	0	0
			42	42		

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.

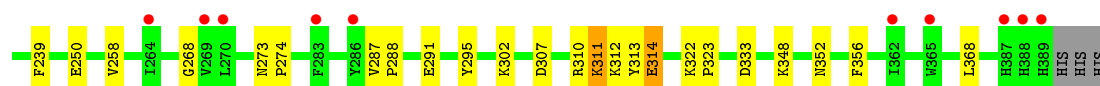
- Chain A:
-
- 5% 80% 17%

- Chain B:

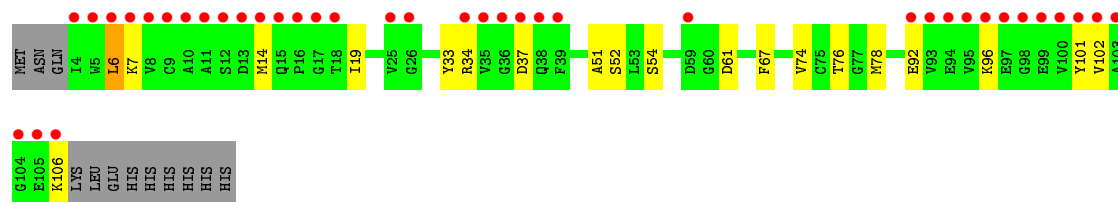
16% 68% 28%

Amino Acid	Count	Category
Met	1	Grey
A2	1	Green
G14	1	Red
G15	1	Green
A16	1	Green
P17	1	Green
F25	1	Green
H29	1	Green
Y30	1	Green
P31	1	Green
K36	1	Red
E37	1	Green
I38	1	Green
P43	1	Green
K44	1	Green
T45	1	Green
L46	1	Green
N56	1	Green
L65	1	Green
L65	1	Green
C69	1	Red
K85	1	Green
Y92	1	Green
H93	1	Green
A94	1	Green
L108	1	Green
T123	1	Green
K130	1	Green
F134	1	Red
I135	1	Green
Y136	1	Green
L137	1	Green
P142	1	Green
P143	1	Green
P144	1	Green
L145	1	Green
A146	1	Green
R147	1	Green
D148	1	Green
T149	1	Green
L154	1	Red
D155	1	Red
D156	1	Red
M159	1	Red
E159	1	Green
I160	1	Green
L161	1	Green
G162	1	Green
I167	1	Green
K168	1	Green
S169	1	Green
H170	1	Green
M171	1	Green
R172	1	Green
V175	1	Red
F179	1	Red
H183	1	Green
I184	1	Green
Y185	1	Green
I186	1	Green
S190	1	Green
I191	1	Red
L192	1	Green
V193	1	Green
K194	1	Red
D195	1	Red
N196	1	Green
D197	1	Green
L198	1	Green
G203	1	Green
F204	1	Red
A205	1	Green
P206	1	Green
G207	1	Green
G208	1	Red
D209	1	Green
R210	1	Green
K211	1	Red
Q212	1	Green
Q213	1	Green
T214	1	Red
R215	1	Red
D218	1	Red
D219	1	Red
D220	1	Red
V221	1	Red
V222	1	Red
G223	1	Green
R224	1	Green
Y228	1	Green
D229	1	Green
L230	1	Red
I231	1	Green
G232	1	Green
F233	1	Red
H234	1	Red
G235	1	Green
V236	1	Green
P237	1	Green
V238	1	Green
F239	1	Green
T242	1	Green
I243	1	Green
G244	1	Green
G245	1	Green
E246	1	Green
V247	1	Green
E255	1	Red
K256	1	Green
I257	1	Green
V258	1	Green
D261	1	Green
I262	1	Green
S263	1	Green
I264	1	Green
G268	1	Red
V269	1	Green
L270	1	Green
N273	1	Green
P274	1	Green
W275	1	Green
P276	1	Green
N277	1	Green
G278	1	Green
D279	1	Green
M280	1	Green
V281	1	Red
Q282	1	Green
W285	1	Green
V286	1	Green
V287	1	Red
P288	1	Green
E291	1	Green
N292	1	Green
T293	1	Green
H294	1	Green
Y295	1	Green
V296	1	Green
F297	1	Green
Q298	1	Green
T299	1	Green
L300	1	Green
G301	1	Red
K302	1	Green
P303	1	Green
C304	1	Green
A305	1	Green
N306	1	Green
P307	1	Green

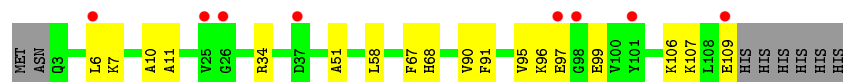
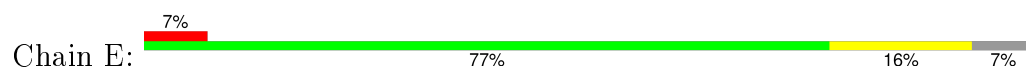
- Chain C:



• Molecule 2: Ferredoxin CarAc



• Molecule 2: Ferredoxin CarAc



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	98.34Å 88.20Å 108.11Å 90.00° 107.19° 90.00°	Depositor
Resolution (Å)	32.63 – 1.95 32.78 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (32.63-1.95) 99.1 (32.78-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.37 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.232 0.202 , 0.231	Depositor DCC
R_{free} test set	6392 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	34.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128028 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11827	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 9CA, FE2, FES

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	0.32	0/3175	0.62	1/4312 (0.0%)
1	B	0.28	0/3175	0.55	0/4312
1	C	0.34	0/3217	0.62	0/4369
2	D	0.29	0/775	0.55	0/1055
2	E	0.28	0/810	0.56	0/1101
All	All	0.31	0/11152	0.59	1/15149 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	220	ASP	N-CA-C	-5.13	97.15	111.00

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	3092	0	3004	49	0
1	B	3092	0	3004	91	0
1	C	3131	0	3031	46	0
2	D	759	0	732	14	0
2	E	794	0	770	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	1	0
4	D	4	0	0	0	0
4	E	4	0	0	1	0
5	A	13	0	9	0	0
5	B	13	0	9	0	0
5	C	13	0	9	0	0
6	A	287	0	0	3	0
6	B	196	0	0	3	0
6	C	335	0	0	5	0
6	D	37	0	0	1	0
6	E	42	0	0	0	0
All	All	11827	0	10568	206	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 10.

The worst 5 of 206 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:C:11:ARG:HH11	1:C:11:ARG:HB3	1.24	1.01
1:B:308:GLU:HG2	1:B:309:GLU:H	1.26	0.98
1:B:311:LYS:HA	1:B:311:LYS:HE3	1.54	0.89
1:C:233:GLU:HG2	6:C:622:HOH:O	1.75	0.86
1:B:306:ASN:ND2	1:B:308:GLU:HB3	1.94	0.82

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	382/392 (97%)	361 (94%)	17 (4%)	4 (1%)	19	8
1	B	382/392 (97%)	344 (90%)	34 (9%)	4 (1%)	19	8
1	C	386/392 (98%)	369 (96%)	15 (4%)	2 (0%)	34	21
2	D	101/115 (88%)	92 (91%)	9 (9%)	0	100	100
2	E	105/115 (91%)	100 (95%)	5 (5%)	0	100	100
All	All	1356/1406 (96%)	1266 (93%)	80 (6%)	10 (1%)	26	14

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	GLY
1	C	268	GLY
1	A	268	GLY
1	B	195	ASP
1	B	309	GLU

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	331/339 (98%)	323 (98%)	8 (2%)	57	47
1	B	331/339 (98%)	321 (97%)	10 (3%)	48	36
1	C	335/339 (99%)	326 (97%)	9 (3%)	52	41
2	D	81/93 (87%)	78 (96%)	3 (4%)	41	27
2	E	85/93 (91%)	84 (99%)	1 (1%)	78	75
All	All	1163/1203 (97%)	1132 (97%)	31 (3%)	52	41

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	195	ASP

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Mol	Chain	Res	Type
1	B	356	PHE
2	D	33	TYR
1	B	311	LYS
1	C	10	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	298	GLN
1	C	260	ASN
1	C	177	ASN
1	A	379	GLN
1	B	372	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	FES	A	502	1	0,4,4	0.00	-	0,4,4	0.00	-
5	9CA	A	503	-	15,15,15	1.26	1 (6%)	20,21,21	0.44	0
4	FES	B	502	1	0,4,4	0.00	-	0,4,4	0.00	-
5	9CA	B	503	-	15,15,15	1.25	1 (6%)	20,21,21	0.43	0
4	FES	C	502	1	0,4,4	0.00	-	0,4,4	0.00	-
5	9CA	C	503	-	15,15,15	1.25	1 (6%)	20,21,21	0.41	0
4	FES	D	201	2	0,4,4	0.00	-	0,4,4	0.00	-
4	FES	E	201	2	0,4,4	0.00	-	0,4,4	0.00	-

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	FES	A	502	1	-	0/0/4/4	0/1/1/1
5	9CA	A	503	-	-	0/0/0/0	0/3/3/3
4	FES	B	502	1	-	0/0/4/4	0/1/1/1
5	9CA	B	503	-	-	0/0/0/0	0/3/3/3
4	FES	C	502	1	-	0/0/4/4	0/1/1/1
5	9CA	C	503	-	-	0/0/0/0	0/3/3/3
4	FES	D	201	2	-	0/0/4/4	0/1/1/1
4	FES	E	201	2	-	0/0/4/4	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	503	9CA	C4B-C4A	-2.14	1.39	1.45
5	A	503	9CA	C4B-C4A	-2.12	1.39	1.45
5	C	503	9CA	C4B-C4A	-2.09	1.39	1.45

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	FES	1	0
4	E	201	FES	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	384/392 (97%)	0.21	18 (4%) 35 46	24, 34, 57, 65	0
1	B	384/392 (97%)	0.90	62 (16%) 3 4	27, 48, 66, 71	0
1	C	388/392 (98%)	0.10	19 (4%) 33 45	22, 33, 48, 66	0
2	D	103/115 (89%)	1.60	39 (37%) 0 0	33, 54, 66, 69	0
2	E	107/115 (93%)	0.45	8 (7%) 17 26	34, 50, 61, 69	0
All	All	1366/1406 (97%)	0.50	146 (10%) 8 12	22, 40, 64, 71	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	LEU	9.5
2	D	5	TRP	8.6
1	B	385	LEU	8.6
2	D	95	VAL	7.3
1	B	305	ALA	7.3

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 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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	9CA	A	503	13/13	0.85	0.16	0.64	52,55,56,56	0
5	9CA	C	503	13/13	0.97	0.18	0.11	23,26,27,28	0
4	FES	E	201	4/4	0.99	0.11	-0.07	35,36,37,38	0
5	9CA	B	503	13/13	0.88	0.14	-0.59	55,57,59,59	0
4	FES	A	502	4/4	0.99	0.14	-0.61	25,25,26,29	0
4	FES	C	502	4/4	0.99	0.12	-0.73	33,34,36,36	0
4	FES	B	502	4/4	1.00	0.13	-0.85	27,27,31,31	0
4	FES	D	201	4/4	0.99	0.06	-1.11	34,38,38,40	0
3	FE2	B	501	1/1	0.98	0.08	-1.35	70,70,70,70	0
3	FE2	A	501	1/1	0.99	0.05	-2.22	44,44,44,44	0
3	FE2	C	501	1/1	0.98	0.06	-3.12	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.