wwPDB X-ray Structure Validation Summary Report (i)

Aug 5, 2026 – 08:30 AM JST

PDB ID	:	5XBP / pdb_00005xbp
Title	:	Oxygenase component of 3-nitrotoluene dioxygenase from Diaphorobacter sp. strain DS2
Authors	:	Ramaswamy, S.; Kumari, A.; Singh, D.; Gurunath, R.
Deposited on	:	2017-03-21
Resolution	:	2.90 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

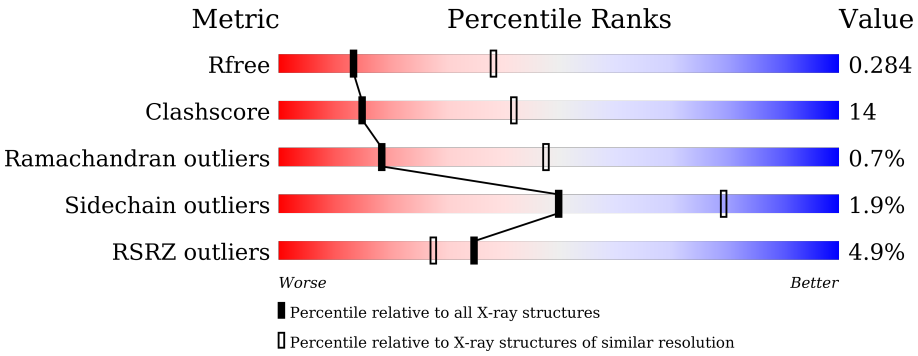
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 <=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	446	5% 68% 30% ·
1	D	446	6% 66% 32% ·
1	G	446	6% 66% 32% ·
2	C	193	2% 78% 20% ··
2	F	193	4% 78% 21% ··
2	I	193	3% 80% 18% ··

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15339 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 3NT oxygenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3480	2212	594	659	15			
1	D	444	Total	C	N	O	S	0	0	0
			3480	2212	594	659	15			
1	G	444	Total	C	N	O	S	0	0	0
			3480	2212	594	659	15			

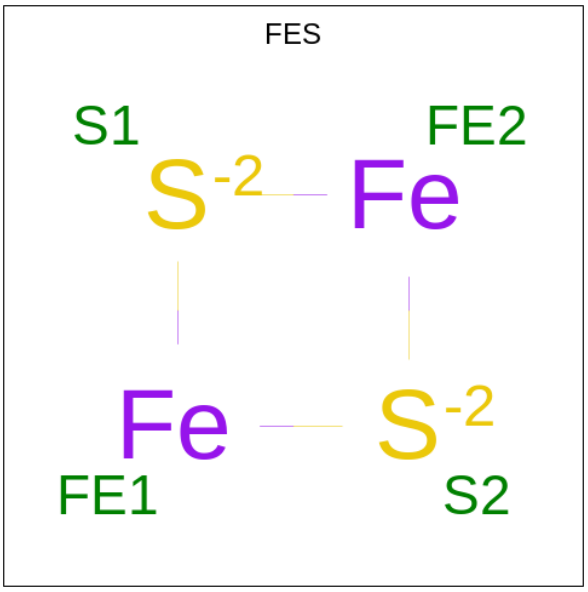
- Molecule 2 is a protein called 3NT oxygenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	192	Total	C	N	O	S	0	0	0
			1609	1017	294	294	4			
2	F	192	Total	C	N	O	S	0	0	0
			1609	1017	294	294	4			
2	I	192	Total	C	N	O	S	0	0	0
			1609	1017	294	294	4			

- Molecule 3 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Fe	0	0
			1	1		
3	D	1	Total	Fe	0	0
			1	1		
3	G	1	Total	Fe	0	0
			1	1		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 4 2 2	0	0
4	D	1	Total Fe S 4 2 2	0	0
4	G	1	Total Fe S 4 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	14	Total O 14 14	0	0
5	C	8	Total O 8 8	0	0
5	D	8	Total O 8 8	0	0
5	F	3	Total O 3 3	0	0
5	G	11	Total O 11 11	0	0
5	I	13	Total O 13 13	0	0

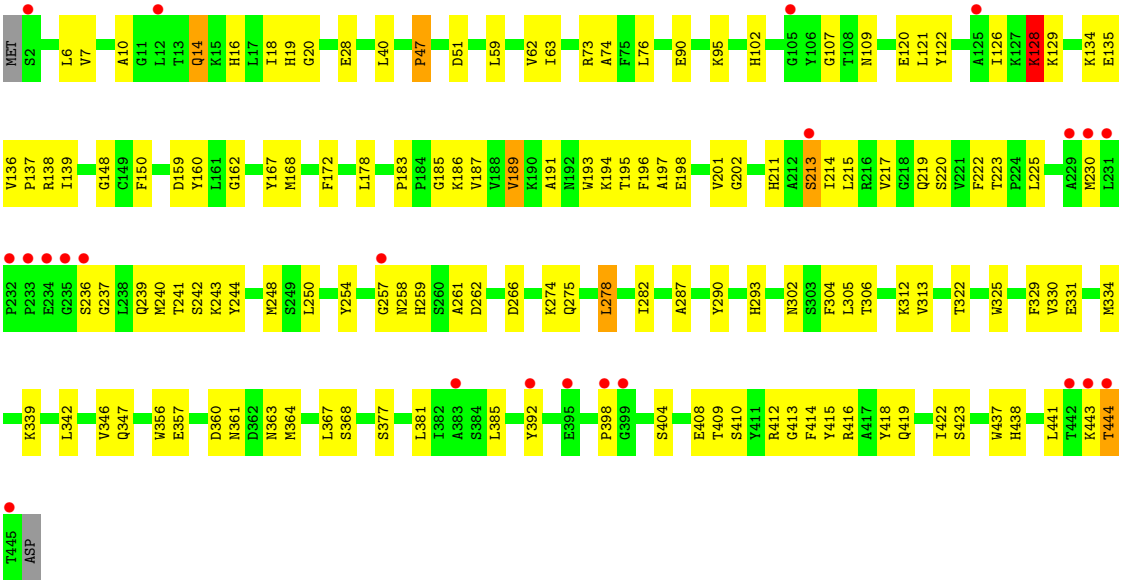
3 Residue-property plots (i)

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: 3NT oxygenase alpha subunit

Chain A:

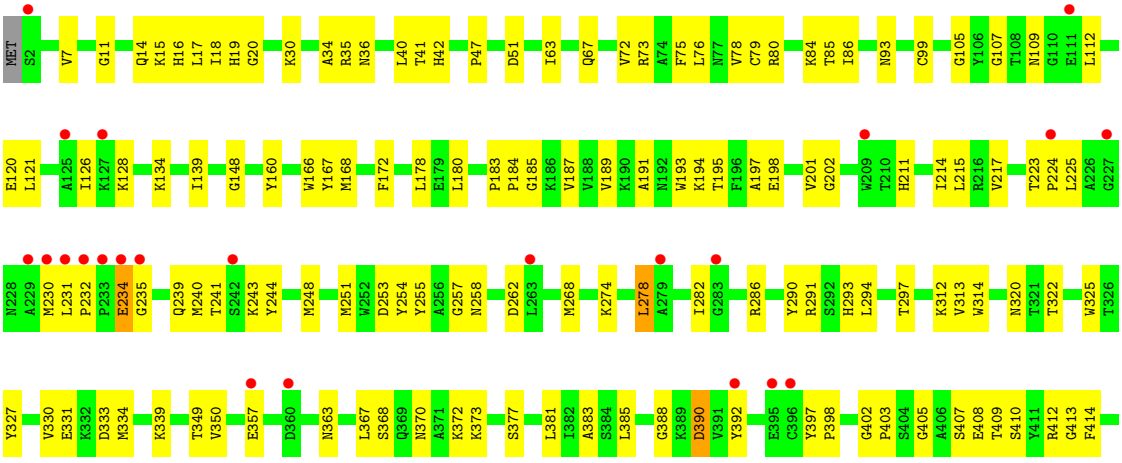


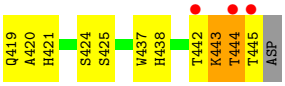


• Molecule 1: 3NT oxygenase alpha subunit

Chain D:



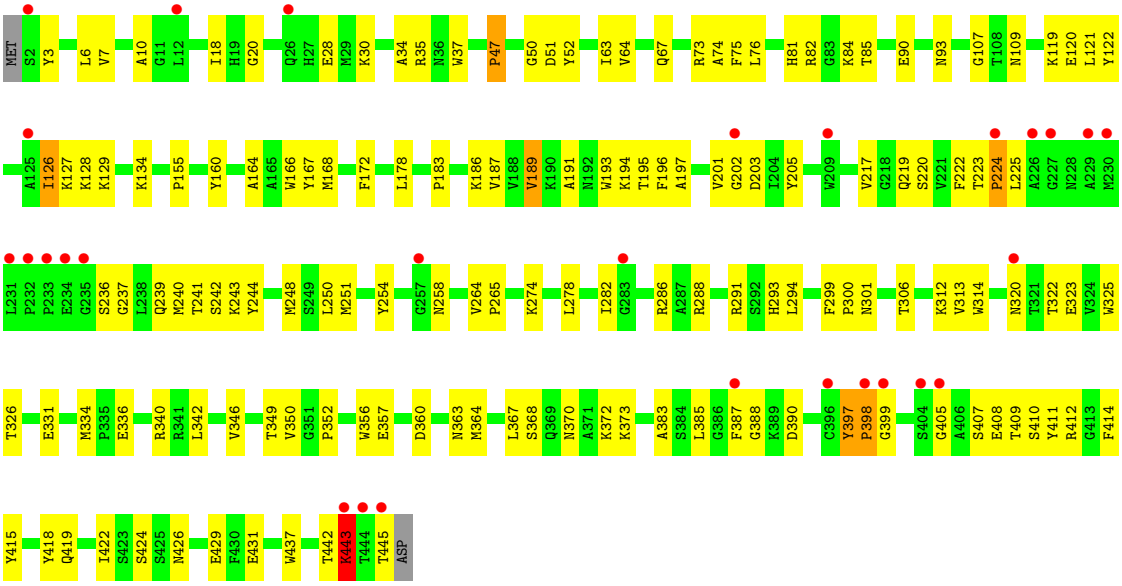




• Molecule 1: 3NT oxygenase alpha subunit

Chain G:

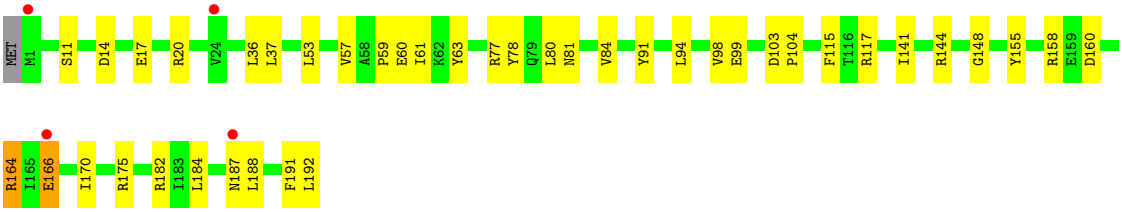




• Molecule 2: 3NT oxygenase beta subunit

Chain C:

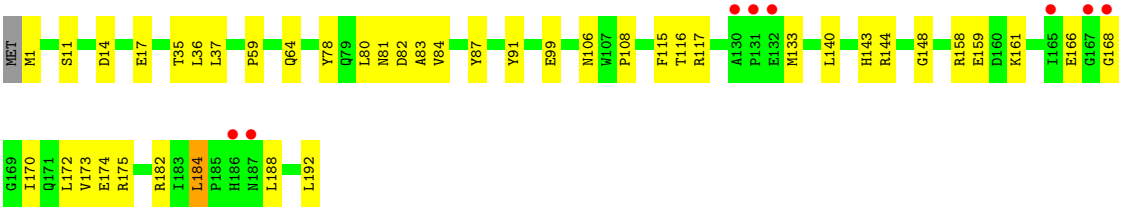




• Molecule 2: 3NT oxygenase beta subunit

Chain F:

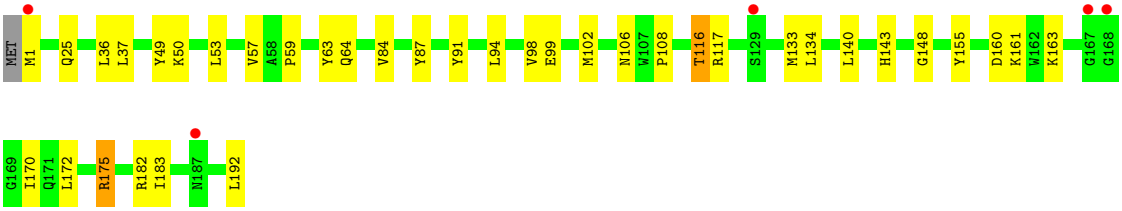




• Molecule 2: 3NT oxygenase beta subunit

Chain I:




MET M1 Q25 L36 L37 Y49 K50 L53 V57 A58 P59 Y63 Q64 V84 Y87 Y91 L94 V98 E99 M102 N106 W107 P108 T116 R117 S129 M133 L134 L140 H143 G148 Y155 D160 K161 W162 K163 G167 G168

G169 I170 Q171 L172 R175 R182 I183 N187 L192

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	178.80Å 178.80Å 242.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.71 – 2.90 47.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.1 (47.71-2.90) 84.7 (47.71-2.90)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.241 , 0.284 0.241 , 0.284	Depositor DCC
R_{free} test set	1920 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å^2)	35.2	Xtriage
Anisotropy	0.754	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	15339	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.94 % 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 1.2030e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE, 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	0.55	1/3577 (0.0%)	0.77	1/4850 (0.0%)
1	D	0.55	0/3577	0.80	3/4850 (0.1%)
1	G	0.60	3/3577 (0.1%)	0.81	7/4850 (0.1%)
2	C	0.66	2/1644 (0.1%)	0.83	1/2227 (0.0%)
2	F	0.56	1/1644 (0.1%)	0.77	0/2227
2	I	0.52	0/1644	0.78	1/2227 (0.0%)
All	All	0.57	7/15663 (0.0%)	0.79	13/21231 (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	D	0	1
1	G	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	155	PRO	CA-C	8.89	1.56	1.51
1	G	443	LYS	CA-C	-8.10	1.45	1.52
1	A	128	LYS	C-O	-5.88	1.16	1.24
2	C	164	ARG	C-O	-5.53	1.17	1.24
1	G	443	LYS	C-O	-5.20	1.19	1.24

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	443	LYS	CB-CA-C	-11.54	101.54	117.23
1	G	443	LYS	N-CA-C	8.74	123.28	108.67
1	D	235	GLY	N-CA-C	-8.59	92.82	113.18
1	G	397	TYR	CA-C-N	8.36	127.97	118.85
1	G	397	TYR	C-N-CA	8.36	127.97	118.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	234	GLU	Peptide
1	G	397	TYR	Peptide

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	3480	0	3313	119	1
1	D	3480	0	3315	106	0
1	G	3480	0	3314	124	0
2	C	1609	0	1590	35	1
2	F	1609	0	1590	30	0
2	I	1609	0	1590	33	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
4	A	4	0	0	0	0
4	D	4	0	0	0	0
4	G	4	0	0	1	0
5	A	14	0	0	1	0
5	C	8	0	0	0	0
5	D	8	0	0	0	0
5	F	3	0	0	1	0
5	G	11	0	0	0	0
5	I	13	0	0	2	0
All	All	15339	0	14712	414	1

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 14.

The worst 5 of 414 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:G:167:TYR:CE1	1:G:398:PRO:CG	2.10	1.26
1:G:167:TYR:CE1	1:G:398:PRO:HG3	1.81	1.14
1:G:167:TYR:CE1	1:G:398:PRO:HG2	1.65	1.08
1:D:349:THR:HG22	1:D:350:VAL:HG23	1.39	1.03
2:C:37:LEU:HD12	2:C:158:ARG:NH2	1.72	1.03

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:ASP:OD2	2:C:166:GLU:O[6_554]	1.98	0.22

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	442/446 (99%)	406 (92%)	33 (8%)	3 (1%)	18 48
1	D	442/446 (99%)	406 (92%)	30 (7%)	6 (1%)	9 30
1	G	442/446 (99%)	410 (93%)	28 (6%)	4 (1%)	14 41
2	C	190/193 (98%)	181 (95%)	9 (5%)	0	100 100
2	F	190/193 (98%)	183 (96%)	7 (4%)	0	100 100
2	I	190/193 (98%)	183 (96%)	7 (4%)	0	100 100
All	All	1896/1917 (99%)	1769 (93%)	114 (6%)	13 (1%)	18 48

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	443	LYS
1	D	257	GLY
1	G	47	PRO
1	A	47	PRO
1	D	47	PRO

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	364/366 (100%)	355 (98%)	9 (2%)	42	74
1	D	364/366 (100%)	354 (97%)	10 (3%)	39	73
1	G	364/366 (100%)	358 (98%)	6 (2%)	55	83
2	C	175/176 (99%)	172 (98%)	3 (2%)	53	82
2	F	175/176 (99%)	174 (99%)	1 (1%)	78	93
2	I	175/176 (99%)	173 (99%)	2 (1%)	65	88
All	All	1617/1626 (99%)	1586 (98%)	31 (2%)	50	79

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

Mol	Chain	Res	Type
1	D	189	VAL
1	G	368	SER
1	D	368	SER
2	I	37	LEU
1	G	127	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	109	ASN
1	G	199	ASN
2	I	143	HIS
1	G	143	HIS

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Mol	Chain	Res	Type
1	G	378	ASN

5.3.3 RNA

There are no RNA molecules 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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	G	502	1	0,4,4	-	-	-		
4	FES	D	502	1	0,4,4	-	-	-		
4	FES	A	502	1	0,4,4	-	-	-		

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	G	502	1	-	-	0/1/1/1
4	FES	D	502	1	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FES	A	502	1	-	-	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	502	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

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, 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	444/446 (99%)	0.47	23 (5%)	33	26	24, 38, 62, 108	0
1	D	444/446 (99%)	0.59	26 (5%)	28	22	25, 40, 64, 106	0
1	G	444/446 (99%)	0.57	28 (6%)	26	20	22, 39, 64, 103	0
2	C	192/193 (99%)	0.07	4 (2%)	63	54	19, 33, 54, 67	0
2	F	192/193 (99%)	0.13	8 (4%)	40	32	20, 36, 61, 79	0
2	I	192/193 (99%)	0.14	5 (2%)	57	48	17, 34, 61, 83	0
All	All	1908/1917 (99%)	0.41	94 (4%)	35	27	17, 38, 63, 108	0

The worst 5 of 94 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	445	THR	6.4
1	D	230	MET	5.6
1	A	233	PRO	5.6
1	G	229	ALA	5.4
1	D	233	PRO	5.1

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 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(Å^2)	Q<0.9
3	FE	D	501	1/1	0.96	0.15	71,71,71,71	0
3	FE	A	501	1/1	0.98	0.08	51,51,51,51	0
3	FE	G	501	1/1	0.98	0.09	54,54,54,54	0
4	FES	D	502	4/4	0.98	0.11	65,66,69,73	0
4	FES	G	502	4/4	0.98	0.09	56,61,66,75	0
4	FES	A	502	4/4	0.99	0.10	60,60,67,70	0

6.5 Other polymers (i)

There are no such residues in this entry.