wwPDB X-ray Structure Validation Summary Report (i)

Jan 30, 2021 – 03:21 PM EST

PDB ID	:	3FD8
Title	:	Crystal Structure of an oxidoreductase from Enterococcus faecalis
Authors	:	Damodharan, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2008-11-25
Resolution	:	2.45 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 following versions of software and data (see references (1)) were used in the production of this report:

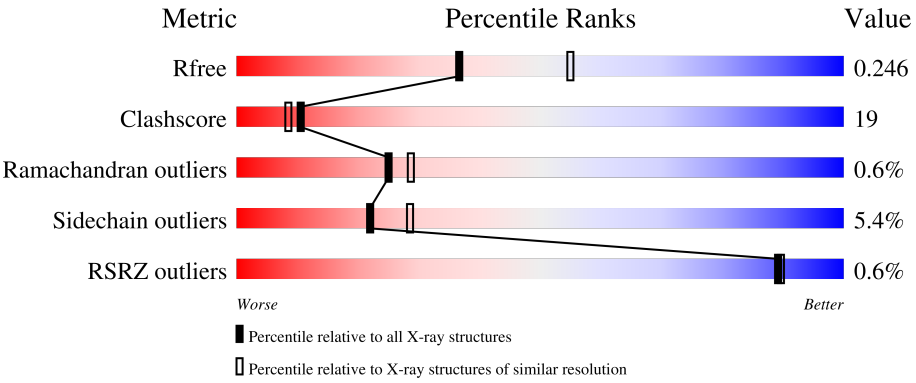
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	359	70% 26%
1	B	359	64% 30%
1	C	359	% 62% 32%
1	D	359	66% 28%
1	E	359	% 63% 30%

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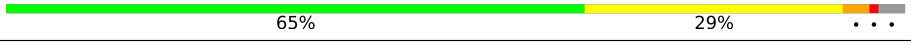
Mol	Chain	Length	Quality of chain
1	F	359	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 17472 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 Oxidoreductase, Gfo/Idh/MocA family.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	Se	0	0	0
			2767	1769	458	530	2	8			
1	B	348	Total	C	N	O	S	Se	0	0	0
			2767	1769	458	530	2	8			
1	C	347	Total	C	N	O	S	Se	0	0	0
			2758	1764	457	527	2	8			
1	D	349	Total	C	N	O	S	Se	0	0	0
			2773	1772	459	532	2	8			
1	E	349	Total	C	N	O	S	Se	0	0	0
			2775	1773	460	532	2	8			
1	F	349	Total	C	N	O	S	Se	0	0	0
			2773	1772	459	532	2	8			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q835X4
A	2	SER	-	expression tag	UNP Q835X4
A	3	LEU	-	expression tag	UNP Q835X4
A	352	GLU	-	expression tag	UNP Q835X4
A	353	GLY	-	expression tag	UNP Q835X4
A	354	HIS	-	expression tag	UNP Q835X4
A	355	HIS	-	expression tag	UNP Q835X4
A	356	HIS	-	expression tag	UNP Q835X4
A	357	HIS	-	expression tag	UNP Q835X4
A	358	HIS	-	expression tag	UNP Q835X4
A	359	HIS	-	expression tag	UNP Q835X4
B	1	MSE	-	expression tag	UNP Q835X4
B	2	SER	-	expression tag	UNP Q835X4
B	3	LEU	-	expression tag	UNP Q835X4
B	352	GLU	-	expression tag	UNP Q835X4
B	353	GLY	-	expression tag	UNP Q835X4
B	354	HIS	-	expression tag	UNP Q835X4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	355	HIS	-	expression tag	UNP Q835X4
B	356	HIS	-	expression tag	UNP Q835X4
B	357	HIS	-	expression tag	UNP Q835X4
B	358	HIS	-	expression tag	UNP Q835X4
B	359	HIS	-	expression tag	UNP Q835X4
C	1	MSE	-	expression tag	UNP Q835X4
C	2	SER	-	expression tag	UNP Q835X4
C	3	LEU	-	expression tag	UNP Q835X4
C	352	GLU	-	expression tag	UNP Q835X4
C	353	GLY	-	expression tag	UNP Q835X4
C	354	HIS	-	expression tag	UNP Q835X4
C	355	HIS	-	expression tag	UNP Q835X4
C	356	HIS	-	expression tag	UNP Q835X4
C	357	HIS	-	expression tag	UNP Q835X4
C	358	HIS	-	expression tag	UNP Q835X4
C	359	HIS	-	expression tag	UNP Q835X4
D	1	MSE	-	expression tag	UNP Q835X4
D	2	SER	-	expression tag	UNP Q835X4
D	3	LEU	-	expression tag	UNP Q835X4
D	352	GLU	-	expression tag	UNP Q835X4
D	353	GLY	-	expression tag	UNP Q835X4
D	354	HIS	-	expression tag	UNP Q835X4
D	355	HIS	-	expression tag	UNP Q835X4
D	356	HIS	-	expression tag	UNP Q835X4
D	357	HIS	-	expression tag	UNP Q835X4
D	358	HIS	-	expression tag	UNP Q835X4
D	359	HIS	-	expression tag	UNP Q835X4
E	1	MSE	-	expression tag	UNP Q835X4
E	2	SER	-	expression tag	UNP Q835X4
E	3	LEU	-	expression tag	UNP Q835X4
E	352	GLU	-	expression tag	UNP Q835X4
E	353	GLY	-	expression tag	UNP Q835X4
E	354	HIS	-	expression tag	UNP Q835X4
E	355	HIS	-	expression tag	UNP Q835X4
E	356	HIS	-	expression tag	UNP Q835X4
E	357	HIS	-	expression tag	UNP Q835X4
E	358	HIS	-	expression tag	UNP Q835X4
E	359	HIS	-	expression tag	UNP Q835X4
F	1	MSE	-	expression tag	UNP Q835X4
F	2	SER	-	expression tag	UNP Q835X4
F	3	LEU	-	expression tag	UNP Q835X4
F	352	GLU	-	expression tag	UNP Q835X4

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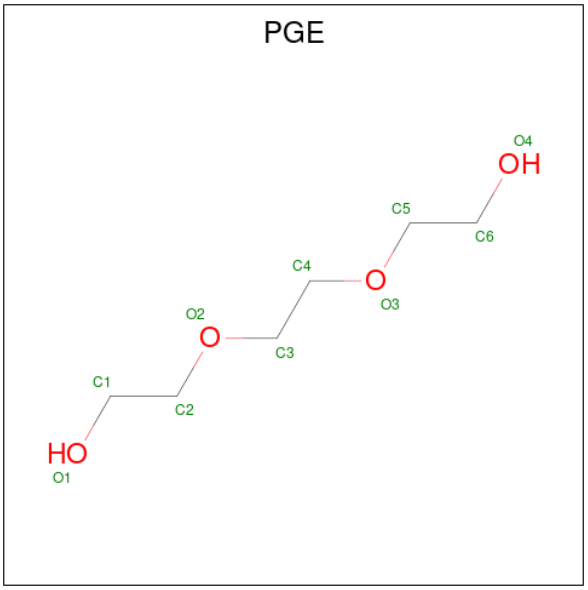
Chain	Residue	Modelled	Actual	Comment	Reference
F	353	GLY	-	expression tag	UNP Q835X4
F	354	HIS	-	expression tag	UNP Q835X4
F	355	HIS	-	expression tag	UNP Q835X4
F	356	HIS	-	expression tag	UNP Q835X4
F	357	HIS	-	expression tag	UNP Q835X4
F	358	HIS	-	expression tag	UNP Q835X4
F	359	HIS	-	expression tag	UNP Q835X4

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	F	1	Total C O 10 6 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	132	Total O 132 132	0	0
3	B	142	Total O 142 142	0	0
3	C	112	Total O 112 112	0	0

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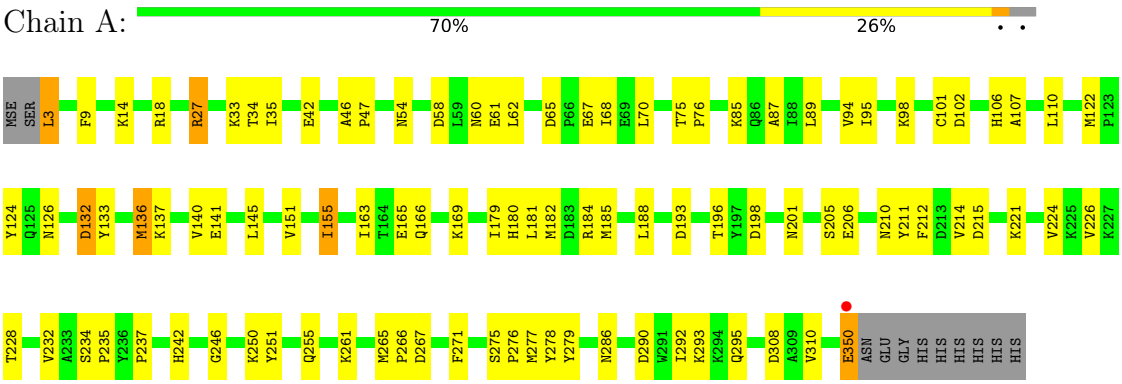
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	142	Total O 142 142	0	0
3	E	137	Total O 137 137	0	0
3	F	164	Total O 164 164	0	0

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.

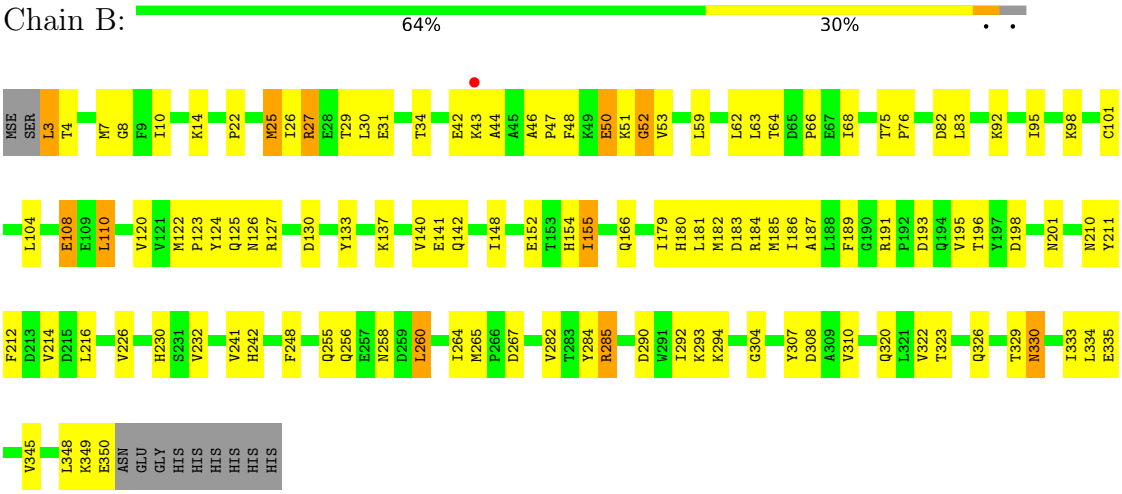
• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain A:



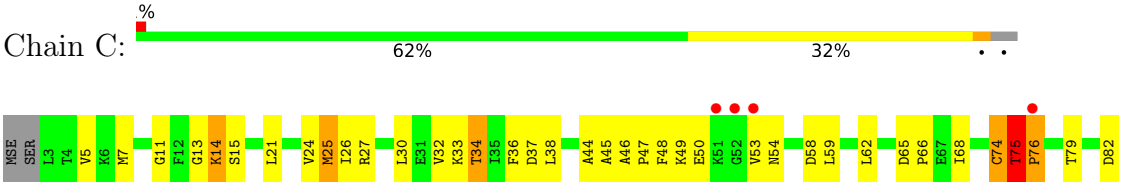
• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

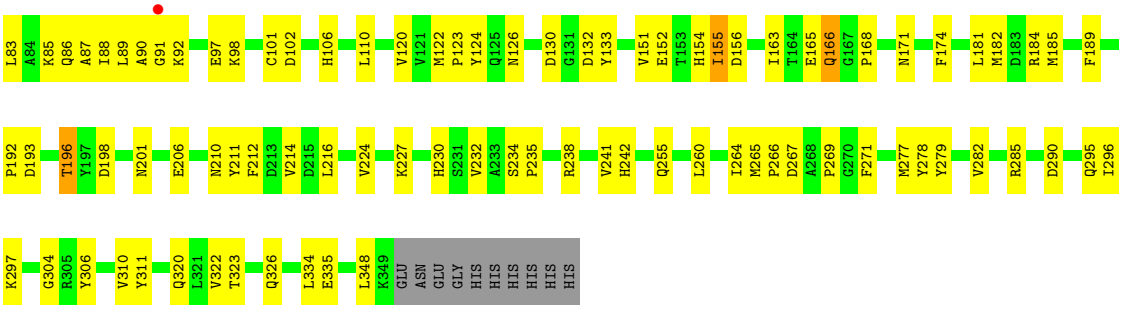
Chain B:



• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

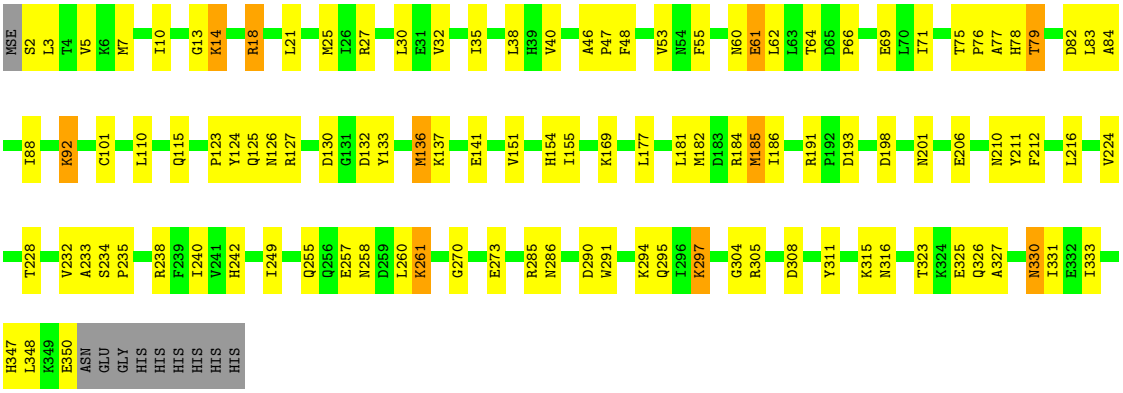
Chain C:





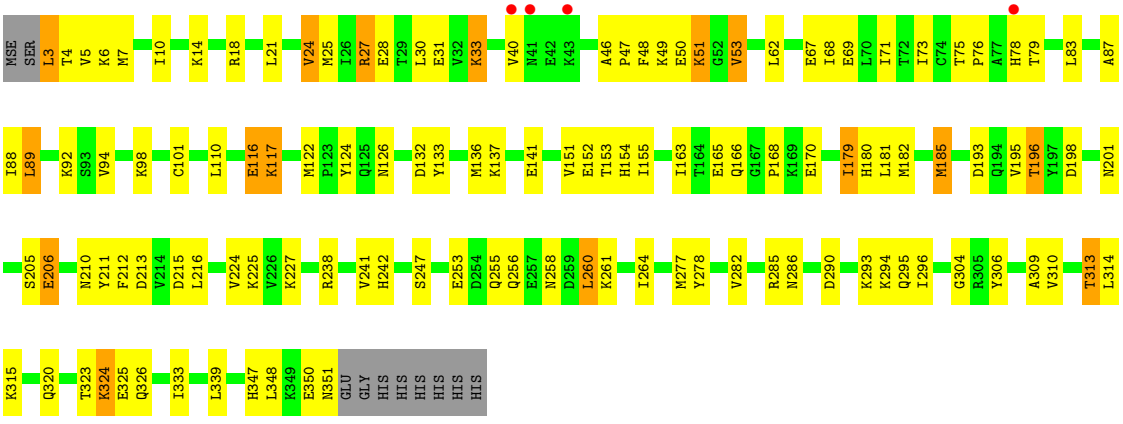
• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain D:



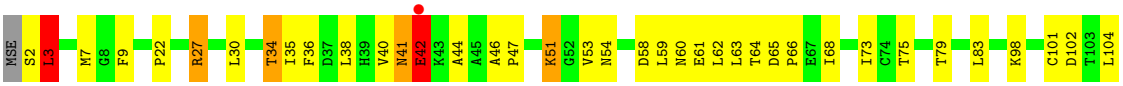
• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain E:



• Molecule 1: Oxidoreductase, Gfo/Idh/MocA family

Chain F:




E105 H106 A107 E108 E109 L110 M122 P123 Y124 Q125 N126 D132 Y133 M136 K137 E141 V151 H154 I155 Q166 F174 I179 H180 L181 M182 D183 R184 M185 I186 A187 L188 F189 T196 Y197 D198 N201 A207 N210 Y211 F212 L216 S220 K221 V224
H230 S231 V232 A233 P237 R238 F239 I240 F248 I249 K250 Y251 Q255 N258 D259 L260 M265 P266 F271 D274 M277 V282 T283 Y284 R285 D290 K293 T298 D308 A309 V310 Q320 T323 K324 E325 Q326 A327 L328 T329 N330 I331 E332 I333 L334
H347 L348 K349 E350 ASN GLU GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.57Å 151.32Å 161.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.45 48.80 – 2.45	Depositor EDS
% Data completeness (in resolution range)	91.4 (48.14-2.45) 95.2 (48.80-2.45)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.57 (at 2.45Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.196 , 0.240 0.202 , 0.246	Depositor DCC
R_{free} test set	4544 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	23.6	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 40.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	17472	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: PGE

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	0.35	0/2826	0.64	0/3815
1	B	0.36	0/2826	0.65	1/3815 (0.0%)
1	C	0.35	0/2817	0.69	1/3803 (0.0%)
1	D	0.36	0/2832	0.66	0/3823
1	E	0.37	0/2834	0.67	0/3826
1	F	0.38	0/2832	0.68	0/3823
All	All	0.36	0/16967	0.66	2/22905 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	75	THR	N-CA-C	7.36	130.86	111.00
1	B	52	GLY	N-CA-C	5.03	125.69	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	2767	0	2692	82	0
1	B	2767	0	2692	102	0
1	C	2758	0	2686	111	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2773	0	2697	105	0
1	E	2775	0	2698	129	0
1	F	2773	0	2697	100	0
2	B	10	0	14	1	0
2	C	10	0	14	5	0
2	F	10	0	14	2	0
3	A	132	0	0	5	0
3	B	142	0	0	8	0
3	C	112	0	0	9	0
3	D	142	0	0	10	0
3	E	137	0	0	7	0
3	F	164	0	0	5	0
All	All	17472	0	16204	608	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 19.

The worst 5 of 608 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:E:185:MSE:HG2	1:E:224:VAL:HG11	1.23	1.18
1:D:185:MSE:HG2	1:D:224:VAL:HG11	1.30	1.13
1:E:182:MSE:HE1	1:E:333:ILE:HG21	1.33	1.11
1:C:182:MSE:HE2	1:C:216:LEU:HD21	1.19	1.10
1:F:155:ILE:HD13	1:F:181:LEU:HD21	1.22	1.10

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	346/359 (96%)	329 (95%)	16 (5%)	1 (0%)	41	49
1	B	346/359 (96%)	326 (94%)	19 (6%)	1 (0%)	41	49
1	C	345/359 (96%)	327 (95%)	13 (4%)	5 (1%)	11	9
1	D	347/359 (97%)	329 (95%)	17 (5%)	1 (0%)	41	49
1	E	347/359 (97%)	328 (94%)	17 (5%)	2 (1%)	25	29
1	F	347/359 (97%)	326 (94%)	18 (5%)	3 (1%)	17	19
All	All	2078/2154 (96%)	1965 (95%)	100 (5%)	13 (1%)	25	29

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	75	THR
1	F	41	ASN
1	A	155	ILE
1	B	155	ILE
1	E	51	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	297/298 (100%)	286 (96%)	11 (4%)	34	45
1	B	297/298 (100%)	282 (95%)	15 (5%)	24	31
1	C	296/298 (99%)	282 (95%)	14 (5%)	26	34
1	D	298/298 (100%)	278 (93%)	20 (7%)	16	20
1	E	298/298 (100%)	276 (93%)	22 (7%)	13	16
1	F	298/298 (100%)	283 (95%)	15 (5%)	24	32
All	All	1784/1788 (100%)	1687 (95%)	97 (5%)	22	28

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	60	ASN

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Mol	Chain	Res	Type
1	D	261	LYS
1	F	188	LEU
1	D	62	LEU
1	D	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	217	HIS
1	C	316	ASN
1	F	230	HIS
1	C	255	GLN
1	D	115	GLN

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)

3 ligands are modelled in this entry.

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	PGE	B	360	-	9,9,9	0.63	0	8,8,8	1.41	2 (25%)
2	PGE	C	360	-	9,9,9	0.64	0	8,8,8	1.47	2 (25%)
2	PGE	F	360	-	9,9,9	0.74	0	8,8,8	1.46	2 (25%)

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	PGE	B	360	-	-	6/7/7/7	-
2	PGE	C	360	-	-	4/7/7/7	-
2	PGE	F	360	-	-	5/7/7/7	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	360	PGE	C3-O2-C2	2.63	124.69	113.29
2	C	360	PGE	C5-O3-C4	2.56	124.36	113.29
2	B	360	PGE	C5-O3-C4	2.52	124.21	113.29
2	F	360	PGE	C5-O3-C4	2.44	123.86	113.29
2	C	360	PGE	C3-O2-C2	2.44	123.84	113.29

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	360	PGE	O2-C3-C4-O3
2	B	360	PGE	O3-C5-C6-O4
2	C	360	PGE	C6-C5-O3-C4
2	B	360	PGE	O1-C1-C2-O2
2	C	360	PGE	O2-C3-C4-O3

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	360	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	360	PGE	5	0
2	F	360	PGE	2	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, 95^{th} 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	340/359 (94%)	-0.30	1 (0%) 94 94	12, 25, 46, 57	0
1	B	340/359 (94%)	-0.31	1 (0%) 94 94	10, 22, 40, 58	0
1	C	339/359 (94%)	-0.06	5 (1%) 73 71	12, 27, 47, 61	0
1	D	341/359 (94%)	-0.30	0 100 100	11, 22, 40, 57	0
1	E	341/359 (94%)	-0.29	4 (1%) 79 77	9, 22, 40, 64	0
1	F	341/359 (94%)	-0.38	1 (0%) 94 94	11, 19, 36, 65	0
All	All	2042/2154 (94%)	-0.27	12 (0%) 89 89	9, 22, 43, 65	0

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	52	GLY	4.1
1	E	41	ASN	3.2
1	C	51	LYS	3.2
1	B	43	LYS	3.1
1	E	43	LYS	2.9

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 monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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
2	PGE	F	360	10/10	0.84	0.22	30,31,37,39	0
2	PGE	C	360	10/10	0.91	0.18	31,34,35,37	0
2	PGE	B	360	10/10	0.91	0.18	31,32,35,36	0

6.5 Other polymers

There are no such residues in this entry.