



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 03:02 AM GMT

PDB ID : 1QXO
Title : Crystal structure of Chorismate synthase complexed with oxidized FMN and EPSP
Authors : Maclean, J.; Ali, S.
Deposited on : 2003-09-08
Resolution : 2.00 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

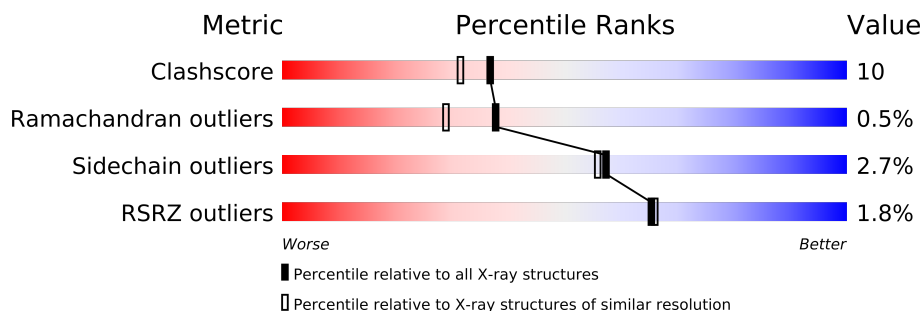
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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))
Clashscore	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	388	
1	B	388	
1	C	388	
1	D	388	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	NCO	A	2002	-	X
2	NCO	A	2004	-	X
2	NCO	A	2007	-	X
2	NCO	B	2003	-	X
2	NCO	B	2008	-	X
2	NCO	C	2005	-	X
2	NCO	D	2006	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
3	EDO	A	3001	-	X
3	EDO	A	3005	-	X
3	EDO	A	3006	-	X
3	EDO	B	3002	-	X
3	EDO	C	3003	-	X
3	EDO	D	3004	-	X
3	EDO	D	3007	-	X
4	FMN	C	4005	-	X
4	FMN	D	4006	-	X
5	EPS	B	5002	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14427 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	Se	0	8	0
			3037	1892	546	587	12			
1	B	388	Total	C	N	O	Se	0	8	0
			3043	1892	549	590	12			
1	C	388	Total	C	N	O	Se	0	8	0
			3035	1893	543	587	12			
1	D	388	Total	C	N	O	Se	0	4	0
			3022	1884	543	583	12			

There are 48 discrepancies between the modelled and reference sequences:

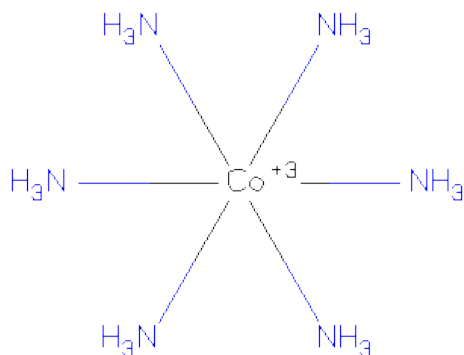
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
A	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6

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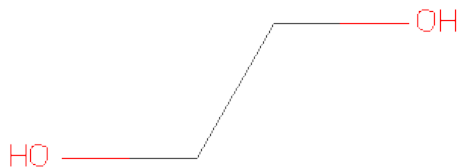
Chain	Residue	Modelled	Actual	Comment	Reference
B	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
B	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
C	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	1	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	49	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	74	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	88	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	138	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	155	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	273	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	298	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	310	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	321	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	348	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6
D	350	MSE	MET	MODIFIED RESIDUE	UNP P0A2Y6

- Molecule 2 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



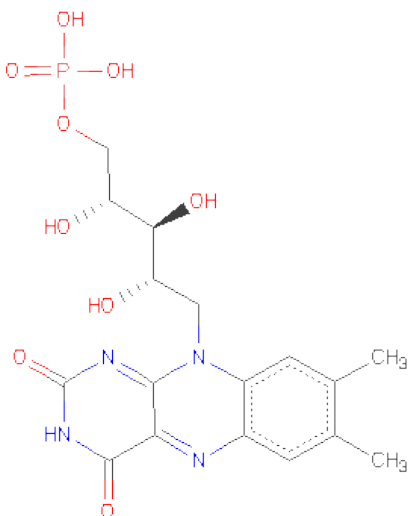
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	C	1	Total	Co	N	0	0
			7	1	6		
2	D	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	D	1	Total	Co	N	0	0
			7	1	6		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



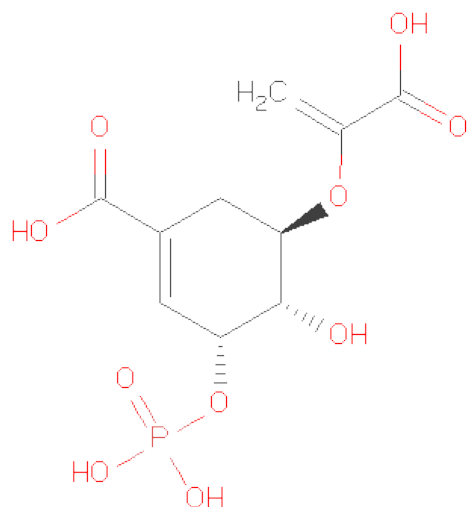
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 5 is 5-[(1-CARBOXYVINYL)OXY]-4-HYDROXY-3-(PHOSPHONOOXY)CYCLOHEX-1-ENE-1-CARBOXYLICACID (three-letter code: EPS) (formula: C₁₀H₁₃O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			21	10	10	1		
5	B	1	Total	C	O	P	0	0
			21	10	10	1		
5	C	1	Total	C	O	P	0	0
			21	10	10	1		
5	D	1	Total	C	O	P	0	0
			21	10	10	1		

- Molecule 6 is water.

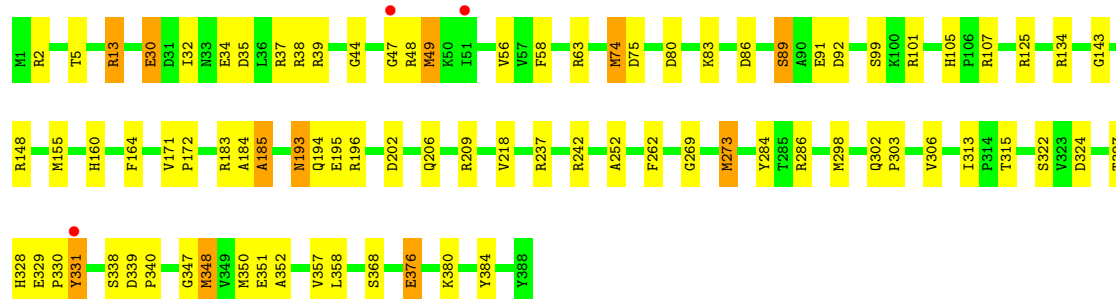
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	453	Total	O	0	0
			453	453		
6	B	528	Total	O	0	0
			528	528		
6	C	469	Total	O	0	0
			469	469		
6	D	479	Total	O	0	0
			479	479		

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.

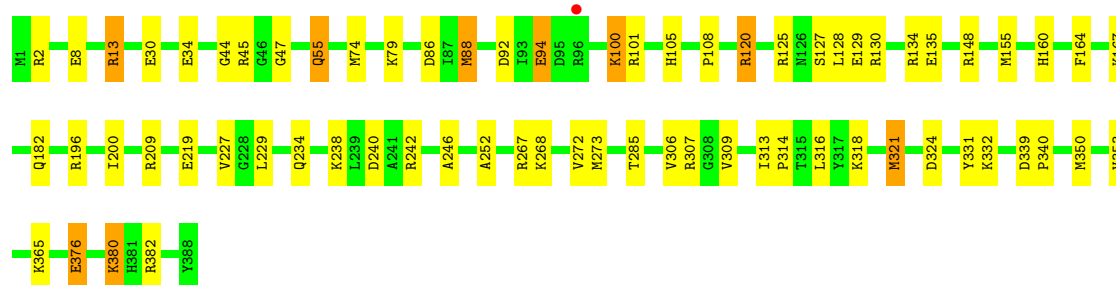
• Molecule 1: Chorismate synthase

Chain A: 



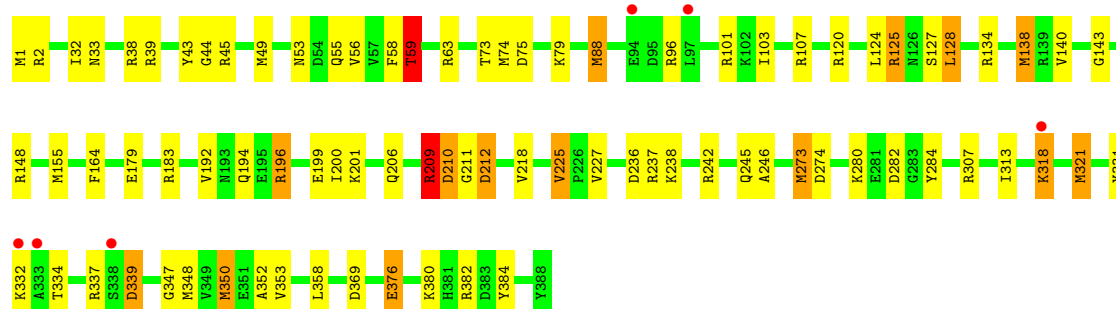
• Molecule 1: Chorismate synthase

Chain B: 



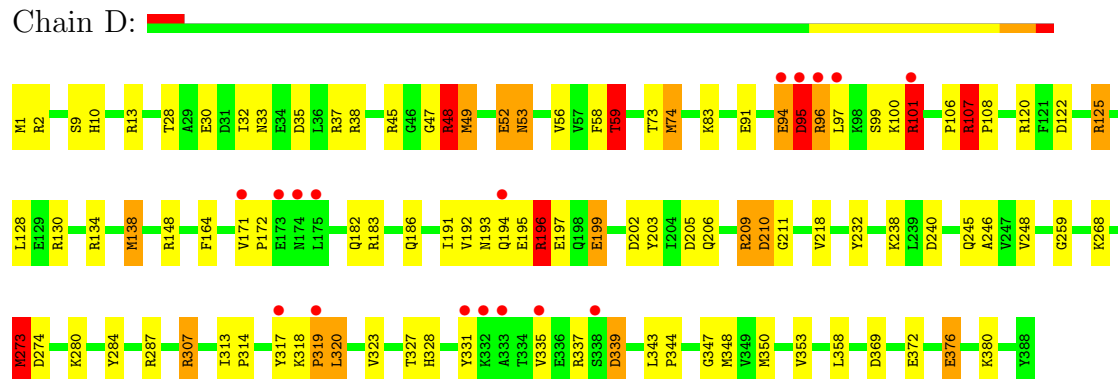
• Molecule 1: Chorismate synthase

Chain C: 



● Molecule 1: Chorismate synthase

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.06Å 124.58Å 85.16Å 90.00° 115.15° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.00) 70.3 (24.90-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.63 (at 1.99Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.222 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	7.8	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 84.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Outliers	0 of 102714 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14427	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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: FMN, NCO, EDO, EPS

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	0.75	5/3115 (0.2%)	1.43	38/4185 (0.9%)
1	B	0.79	4/3119 (0.1%)	1.37	26/4188 (0.6%)
1	C	0.78	8/3111 (0.3%)	1.49	38/4180 (0.9%)
1	D	0.78	4/3078 (0.1%)	1.62	53/4134 (1.3%)
All	All	0.78	21/12423 (0.2%)	1.48	155/16687 (0.9%)

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	2

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	MSE	CG-SE	13.31	2.40	1.95
1	D	273	MSE	CG-SE	13.14	2.40	1.95
1	C	273	MSE	CG-SE	12.20	2.37	1.95
1	D	49	MSE	CG-SE	9.80	2.28	1.95
1	B	88	MSE	CG-SE	9.58	2.28	1.95

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	48	ARG	NE-CZ-NH2	-20.75	109.92	120.30
1	D	196	ARG	NE-CZ-NH2	-17.53	111.53	120.30
1	D	196	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	D	2	ARG	NE-CZ-NH1	-13.76	113.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	ARG	NE-CZ-NH2	-13.60	113.50	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	10	HIS	Mainchain
1	D	248	VAL	Mainchain

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	3037	0	3050	49	0
1	B	3043	0	3053	48	0
1	C	3035	0	3054	71	0
1	D	3022	0	3038	86	0
2	A	21	0	0	0	0
2	B	14	0	0	0	0
2	C	14	0	0	0	0
2	D	14	0	0	1	0
3	A	12	0	18	4	0
3	B	4	0	6	1	0
3	C	4	0	6	2	0
3	D	8	0	12	2	0
4	A	31	0	19	5	0
4	B	31	0	19	4	0
4	C	62	0	38	7	0
4	D	62	0	38	6	0
5	A	21	0	8	0	0
5	B	21	0	8	1	0
5	C	21	0	8	0	0
5	D	21	0	8	0	0
6	A	453	0	0	7	0
6	B	528	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	469	0	0	16	0
6	D	479	0	0	16	0
All	All	14427	0	12383	255	0

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 10.

The worst 5 of 255 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:348:MSE:SE	1:D:348:MSE:CE	2.14	1.45
1:C:138:MSE:SE	1:C:138:MSE:CG	2.15	1.45
1:D:273:MSE:CE	1:D:273:MSE:SE	2.14	1.45
1:D:138:MSE:SE	1:D:138:MSE:CG	2.16	1.42
1:B:88:MSE:CE	1:B:88:MSE:SE	2.16	1.42

There are no symmetry-related clashes.

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	394/388 (102%)	386 (98%)	7 (2%)	1 (0%)	50	44
1	B	394/388 (102%)	387 (98%)	6 (2%)	1 (0%)	50	44
1	C	394/388 (102%)	383 (97%)	10 (2%)	1 (0%)	50	44
1	D	390/388 (100%)	375 (96%)	10 (3%)	5 (1%)	18	8
All	All	1572/1552 (101%)	1531 (97%)	33 (2%)	8 (0%)	38	29

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	GLY
1	D	319	PRO
1	D	47	GLY

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Mol	Chain	Res	Type
1	D	320	LEU
1	C	210	ASP

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	327/308 (106%)	321 (98%)	6 (2%)	71	73
1	B	327/308 (106%)	321 (98%)	6 (2%)	71	73
1	C	327/308 (106%)	321 (98%)	6 (2%)	71	73
1	D	323/308 (105%)	307 (95%)	16 (5%)	34	27
All	All	1304/1232 (106%)	1270 (97%)	34 (3%)	57	58

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	209	ARG
1	D	53	ASN
1	D	273	MSE
1	C	358	LEU
1	B	55	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	GLN
1	C	33	ASN
1	D	182	GLN
1	B	194	GLN
1	D	55	GLN

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 ⓘ

26 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	NCO	A	2002	-	6,6,6	0.46	0	0,15,15	0.00	-
2	NCO	A	2004	-	6,6,6	0.43	0	0,15,15	0.00	-
2	NCO	A	2007	-	6,6,6	0.48	0	0,15,15	0.00	-
3	EDO	A	3001	-	3,3,3	0.58	0	2,2,2	0.54	0
3	EDO	A	3005	-	3,3,3	0.76	0	2,2,2	0.53	0
3	EDO	A	3006	-	3,3,3	0.92	0	2,2,2	1.23	0
4	FMN	A	4001	-	33,33,33	1.79	9 (27%)	46,50,50	2.03	10 (21%)
5	EPS	A	5001	-	21,21,21	4.73	15 (71%)	31,31,31	3.78	18 (58%)
2	NCO	B	2003	-	6,6,6	0.58	0	0,15,15	0.00	-
2	NCO	B	2008	-	6,6,6	0.44	0	0,15,15	0.00	-
3	EDO	B	3002	-	3,3,3	0.61	0	2,2,2	0.80	0
4	FMN	B	4002	-	33,33,33	1.46	6 (18%)	46,50,50	2.54	11 (23%)
5	EPS	B	5002	-	21,21,21	4.69	16 (76%)	31,31,31	4.45	21 (67%)
2	NCO	C	2001	-	6,6,6	0.63	0	0,15,15	0.00	-
2	NCO	C	2005	-	6,6,6	0.53	0	0,15,15	0.00	-
3	EDO	C	3003	-	3,3,3	0.54	0	2,2,2	0.65	0
4	FMN	C	4003	-	33,33,33	1.69	8 (24%)	46,50,50	1.98	9 (19%)
4	FMN	C	4005	-	33,33,33	1.52	6 (18%)	46,50,50	1.90	7 (15%)
5	EPS	C	5003	-	21,21,21	4.75	15 (71%)	31,31,31	4.04	20 (64%)
2	NCO	D	2006	-	6,6,6	0.46	0	0,15,15	0.00	-
2	NCO	D	2009	-	6,6,6	0.55	0	0,15,15	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	3004	-	3,3,3	0.64	0	2,2,2	0.13	0
3	EDO	D	3007	-	3,3,3	0.63	0	2,2,2	0.63	0
4	FMN	D	4004	-	33,33,33	1.55	7 (21%)	46,50,50	1.98	13 (28%)
4	FMN	D	4006	-	33,33,33	1.55	6 (18%)	46,50,50	2.36	8 (17%)
5	EPS	D	5004	-	21,21,21	4.64	15 (71%)	31,31,31	4.10	18 (58%)

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	NCO	A	2002	-	-	0/0/0/0	0/0/0/0
2	NCO	A	2004	-	-	0/0/0/0	0/0/0/0
2	NCO	A	2007	-	-	0/0/0/0	0/0/0/0
3	EDO	A	3001	-	-	0/1/1/1	0/0/0/0
3	EDO	A	3005	-	-	0/1/1/1	0/0/0/0
3	EDO	A	3006	-	-	0/1/1/1	0/0/0/0
4	FMN	A	4001	-	-	0/18/18/18	0/0/3/3
5	EPS	A	5001	-	-	0/16/33/33	0/1/1/1
2	NCO	B	2003	-	-	0/0/0/0	0/0/0/0
2	NCO	B	2008	-	-	0/0/0/0	0/0/0/0
3	EDO	B	3002	-	-	0/1/1/1	0/0/0/0
4	FMN	B	4002	-	-	0/18/18/18	0/0/3/3
5	EPS	B	5002	-	-	0/16/33/33	0/1/1/1
2	NCO	C	2001	-	-	0/0/0/0	0/0/0/0
2	NCO	C	2005	-	-	0/0/0/0	0/0/0/0
3	EDO	C	3003	-	-	0/1/1/1	0/0/0/0
4	FMN	C	4003	-	-	0/18/18/18	0/0/3/3
4	FMN	C	4005	-	-	0/18/18/18	0/0/3/3
5	EPS	C	5003	-	-	0/16/33/33	0/1/1/1
2	NCO	D	2006	-	-	0/0/0/0	0/0/0/0
2	NCO	D	2009	-	-	0/0/0/0	0/0/0/0
3	EDO	D	3004	-	-	0/1/1/1	0/0/0/0
3	EDO	D	3007	-	-	0/1/1/1	0/0/0/0
4	FMN	D	4004	-	-	0/18/18/18	0/0/3/3
4	FMN	D	4006	-	-	0/18/18/18	0/0/3/3
5	EPS	D	5004	-	-	0/16/33/33	0/1/1/1

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	5004	EPS	O3-C3	-11.51	1.26	1.45
5	B	5002	EPS	O3-C3	-11.22	1.26	1.45
5	C	5003	EPS	O3-C3	-11.00	1.27	1.45
5	C	5003	EPS	C7-C9	-10.35	1.39	1.49
5	A	5001	EPS	C7-C9	-10.26	1.39	1.49

The worst 5 of 135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4006	FMN	C4A-C10-N10	-11.05	115.00	120.51
5	B	5002	EPS	O12-C10-O11	-10.77	98.13	123.62
5	A	5001	EPS	P-O3-C3	-10.64	99.96	122.04
5	D	5004	EPS	O12-C10-O11	-10.56	98.61	123.62
4	B	4002	FMN	C4A-C10-N10	-10.41	115.31	120.51

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, 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	388/388 (100%)	-0.11	3 (0%) 83 84	15, 22, 44, 65	0
1	B	388/388 (100%)	-0.19	1 (0%) 91 93	15, 22, 36, 59	0
1	C	388/388 (100%)	-0.04	6 (1%) 70 70	15, 23, 50, 79	0
1	D	388/388 (100%)	0.05	17 (4%) 33 32	15, 23, 51, 83	0
All	All	1552/1552 (100%)	-0.07	27 (1%) 65 67	15, 22, 46, 83	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	SER	5.1
1	C	333	ALA	4.8
1	C	97	LEU	4.4
1	D	96	ARG	4.3
1	D	94	GLU	4.3

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	EDO	C	3003	4/4	0.33	29.34	26,32,32,33	0
2	NCO	A	2007	7/7	0.37	28.95	80,80,80,80	0
2	NCO	B	2003	7/7	0.21	14.17	40,41,41,42	0
2	NCO	C	2005	7/7	0.22	11.16	52,53,53,53	0
3	EDO	A	3006	4/4	0.23	9.83	38,38,39,39	0
3	EDO	B	3002	4/4	0.21	9.66	23,27,29,29	0
3	EDO	D	3007	4/4	0.18	9.53	28,29,30,33	0
3	EDO	A	3005	4/4	0.18	8.18	31,31,33,35	0
4	FMN	C	4005	31/31	0.26	7.90	46,53,62,63	0
2	NCO	D	2006	7/7	0.26	6.15	47,47,47,48	0
2	NCO	B	2008	7/7	0.23	5.57	73,73,74,74	0
2	NCO	A	2002	7/7	0.40	5.01	86,86,86,86	0
3	EDO	A	3001	4/4	0.20	4.64	25,29,30,34	0
3	EDO	D	3004	4/4	0.16	4.38	20,26,28,28	0
2	NCO	A	2004	7/7	0.18	2.43	39,40,41,42	0
4	FMN	D	4006	31/31	0.18	2.34	46,50,51,51	0
5	EPS	B	5002	21/21	0.17	2.33	21,27,37,39	0
5	EPS	A	5001	21/21	0.14	1.10	19,26,41,42	0
5	EPS	D	5004	21/21	0.16	0.71	22,33,43,44	0
5	EPS	C	5003	21/21	0.15	0.21	23,29,42,43	0
2	NCO	C	2001	7/7	0.13	-0.14	34,34,35,36	0
4	FMN	C	4003	31/31	0.10	-0.34	18,22,25,28	0
4	FMN	D	4004	31/31	0.10	-0.48	16,20,24,26	0
2	NCO	D	2009	7/7	0.11	-0.62	25,26,28,29	0
4	FMN	A	4001	31/31	0.10	-0.72	17,20,23,24	0
4	FMN	B	4002	31/31	0.10	-1.26	17,20,22,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.