



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:44 am GMT

PDB ID : 4GHE
Title : Structure of Y257F variant of Homoprotocatechuate 2,3-Dioxygenase from B.fuscum in complex with 4-nitrocatechol at 1.60 Ang resolution
Authors : Kovaleva, E.G.; Lipscomb, J.D.
Deposited on : 2012-08-07
Resolution : 1.60 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

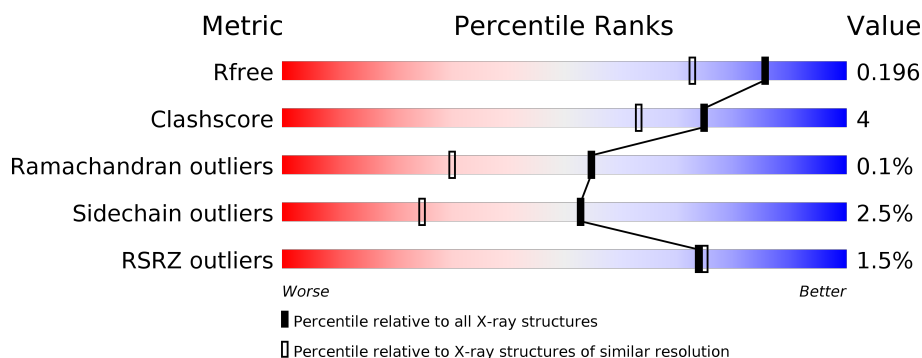
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (1.60-1.60)

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	365	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> </div>
1	B	365	<div> <div></div> <div> <div>89%</div> <div>10%</div> <div></div> </div> </div>
1	C	365	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>8%</div> <div></div> </div> </div>
1	D	365	<div> <div></div> <div> <div>88%</div> <div>10%</div> <div></div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	P6G	B	404	-	-	-	X
3	P6G	B	406	-	-	-	X
3	P6G	C	404	-	-	-	X
4	CL	C	405	-	-	X	-
6	4NC	C	403	-	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13530 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 Homoprotocatechuate 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	7	0
			2928	1840	519	562	7			
1	B	360	Total	C	N	O	S	0	8	0
			2968	1867	525	568	8			
1	C	351	Total	C	N	O	S	0	7	0
			2897	1823	511	555	8			
1	D	360	Total	C	N	O	S	0	8	0
			2971	1869	527	567	8			

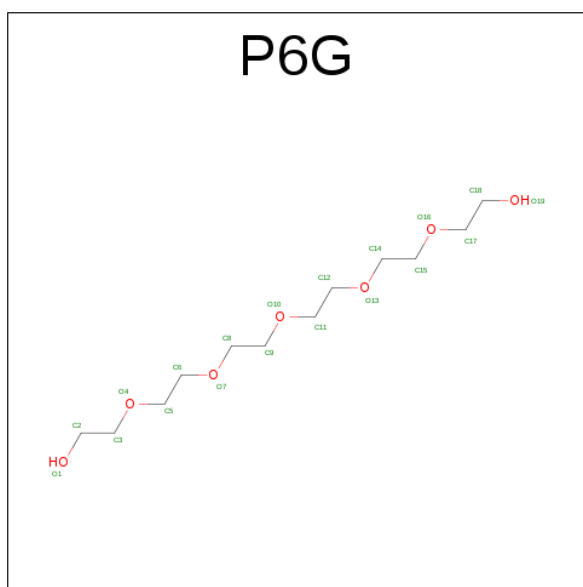
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	PHE	TYR	ENGINEERED MUTATION	UNP Q45135
B	257	PHE	TYR	ENGINEERED MUTATION	UNP Q45135
C	257	PHE	TYR	ENGINEERED MUTATION	UNP Q45135
D	257	PHE	TYR	ENGINEERED MUTATION	UNP Q45135

- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 3 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: C₁₂H₂₆O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	B	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	C	1	Total	C	O	0	0
			19	12	7		
3	D	1	Total	C	O	0	0
			19	12	7		

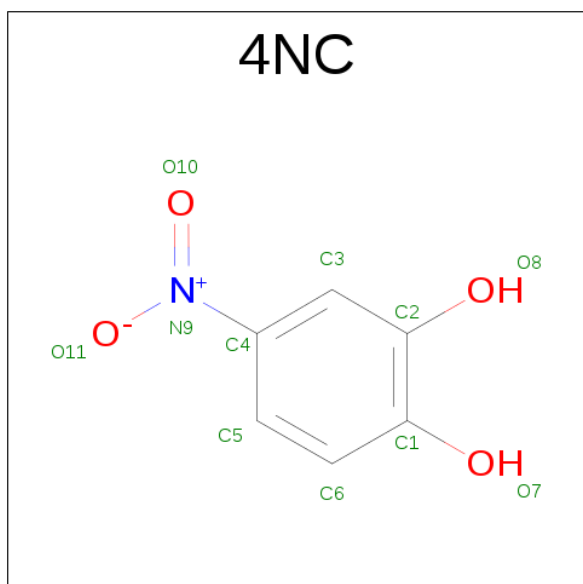
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	A	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is 4-NITROCATECHOL (three-letter code: 4NC) (formula: $C_6H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			11	6	1	4		

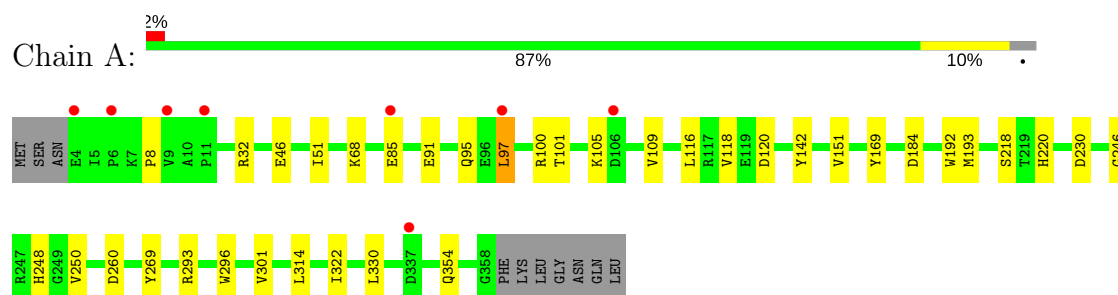
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	363	Total	O	0	0
			363	363		
7	B	428	Total	O	0	1
			429	429		
7	C	394	Total	O	0	5
			399	399		
7	D	422	Total	O	0	0
			422	422		

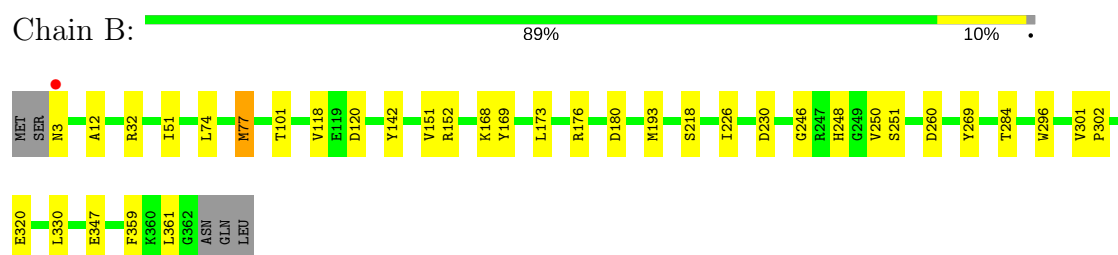
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

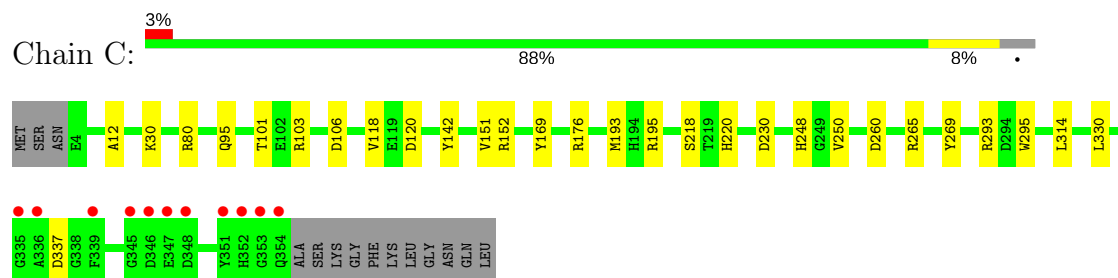
• Molecule 1: Homoprotocatechuate 2,3-dioxygenase



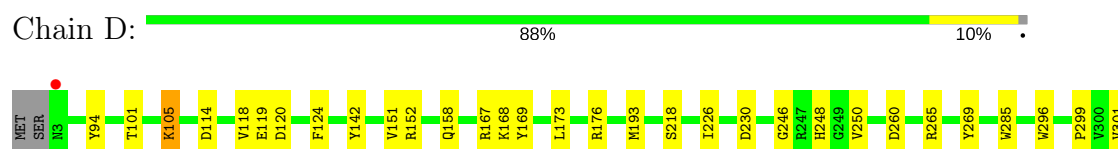
• Molecule 1: Homoprotocatechuate 2,3-dioxygenase



• Molecule 1: Homoprotocatechuate 2,3-dioxygenase



• Molecule 1: Homoprotocatechuate 2,3-dioxygenase



P302	
L314	
D348	
K357	
G358	
F359	
K360	
L361	
G362	
ASN	
GLN	
LEU	

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	110.51Å 150.12Å 96.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.30 – 1.60 42.30 – 1.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (42.30-1.60) 98.6 (42.30-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.155 , 0.186 0.166 , 0.196	Depositor DCC
R_{free} test set	10336 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	17.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13530	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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, 0.333 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: CA, FE2, 4NC, P6G, CL

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	0.66	1/3003 (0.0%)	0.80	2/4077 (0.0%)
1	B	0.67	0/3044	0.78	0/4131
1	C	0.72	1/2972 (0.0%)	0.86	6/4037 (0.1%)
1	D	0.72	0/3047	0.83	1/4134 (0.0%)
All	All	0.69	2/12066 (0.0%)	0.82	9/16379 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	TRP	CD2-CE2	5.58	1.48	1.41
1	C	295	TRP	CD2-CE2	5.08	1.47	1.41

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	D	265	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	C	293	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	293	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	293	ARG	NE-CZ-NH2	-5.83	117.39	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	2928	0	2766	20	0
1	B	2968	0	2809	22	0
1	C	2897	0	2738	14	0
1	D	2971	0	2816	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	26	0	0
3	B	57	0	78	1	0
3	C	38	0	52	6	0
3	D	19	0	26	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	5	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
6	C	11	0	3	6	0
7	A	363	0	0	5	0
7	B	429	0	0	2	0
7	C	399	0	0	5	0
7	D	422	0	0	6	0
All	All	13530	0	11314	85	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 4.

The worst 5 of 85 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)
6:C:403:4NC:N9	6:C:403:4NC:O10	1.57	1.37
6:C:403:4NC:N9	4:C:405:CL:CL	2.10	1.22
6:C:403:4NC:O10	4:C:405:CL:CL	0.64	1.01
1:A:8:PRO:HG3	1:A:97:LEU:HD13	1.54	0.89
1:A:100:ARG:HG2	1:A:314:LEU:HD12	1.58	0.84

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	360/365 (99%)	352 (98%)	8 (2%)	0	100	100
1	B	366/365 (100%)	357 (98%)	8 (2%)	1 (0%)	44	22
1	C	356/365 (98%)	348 (98%)	8 (2%)	0	100	100
1	D	366/365 (100%)	355 (97%)	11 (3%)	0	100	100
All	All	1448/1460 (99%)	1412 (98%)	35 (2%)	1 (0%)	55	30

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	SER

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	311/313 (99%)	303 (97%)	8 (3%)	51	23
1	B	316/313 (101%)	307 (97%)	9 (3%)	49	21
1	C	309/313 (99%)	301 (97%)	8 (3%)	51	23
1	D	316/313 (101%)	310 (98%)	6 (2%)	62	37
All	All	1252/1252 (100%)	1221 (98%)	31 (2%)	53	25

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

Mol	Chain	Res	Type
1	B	193	MET
1	C	30	LYS
1	D	169	TYR
1	B	260	ASP
1	C	106	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
1	B	3	ASN
1	B	354	GLN
1	C	95	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 9 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	$\# Z > 2$
3	P6G	A	402	-	18,18,18	0.44	0	17,17,17	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	P6G	B	403	-	18,18,18	0.57	0	17,17,17	0.44	0
3	P6G	B	404	-	18,18,18	0.66	0	17,17,17	0.50	0
3	P6G	B	406	-	18,18,18	0.48	0	17,17,17	0.40	0
3	P6G	C	402	-	18,18,18	0.47	0	17,17,17	0.71	0
6	4NC	C	403	2	10,11,11	6.42	3 (30%)	13,15,15	1.30	2 (15%)
3	P6G	C	404	-	18,18,18	0.41	0	17,17,17	0.51	0
3	P6G	D	402	-	18,18,18	0.60	0	17,17,17	0.30	0

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
3	P6G	A	402	-	-	0/16/16/16	0/0/0/0
3	P6G	B	403	-	-	0/16/16/16	0/0/0/0
3	P6G	B	404	-	-	0/16/16/16	0/0/0/0
3	P6G	B	406	-	-	0/16/16/16	0/0/0/0
3	P6G	C	402	-	-	0/16/16/16	0/0/0/0
6	4NC	C	403	2	-	0/2/4/4	0/1/1/1
3	P6G	C	404	-	-	0/16/16/16	0/0/0/0
3	P6G	D	402	-	-	0/16/16/16	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	403	4NC	C4-N9	-4.40	1.37	1.45
6	C	403	4NC	C2-C1	4.43	1.47	1.40
6	C	403	4NC	O10-N9	19.16	1.57	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	403	4NC	C3-C4-N9	-2.85	116.38	118.81
6	C	403	4NC	C5-C4-N9	3.00	121.69	119.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	P6G	1	0
6	C	403	4NC	6	0
3	C	404	P6G	6	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	355/365 (97%)	-0.10	8 (2%) 61 61	12, 24, 46, 54	0
1	B	360/365 (98%)	-0.34	1 (0%) 93 93	11, 20, 33, 56	0
1	C	351/365 (96%)	-0.32	11 (3%) 49 48	10, 17, 32, 55	0
1	D	360/365 (98%)	-0.37	1 (0%) 93 93	10, 17, 31, 55	0
All	All	1426/1460 (97%)	-0.28	21 (1%) 74 75	10, 19, 38, 56	0

The worst 5 of 21 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	VAL	4.1
1	C	354	GLN	3.8
1	C	353	GLY	3.6
1	C	336	ALA	3.3
1	C	348	ASP	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 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(\AA^2)	Q<0.9
3	P6G	C	404	19/19	0.76	0.30	8.42	21,27,31,32	19
3	P6G	B	404	19/19	0.90	0.12	4.78	33,35,39,40	0
3	P6G	B	406	19/19	0.76	0.21	4.10	25,26,30,31	19
6	4NC	C	403	11/11	0.92	0.12	2.12	17,18,23,24	11
3	P6G	A	402	19/19	0.87	0.14	1.57	28,36,51,53	0
3	P6G	C	402	19/19	0.95	0.09	1.16	16,21,39,40	0
3	P6G	D	402	19/19	0.95	0.10	1.14	17,24,44,48	0
3	P6G	B	403	19/19	0.94	0.10	0.94	22,28,43,44	0
5	CA	B	402	1/1	0.99	0.03	-2.83	16,16,16,16	0
2	FE2	B	401	1/1	1.00	0.03	-3.89	23,23,23,23	0
2	FE2	C	401	1/1	1.00	0.05	-4.18	21,21,21,21	0
2	FE2	A	401	1/1	1.00	0.03	-4.42	24,24,24,24	0
2	FE2	D	401	1/1	1.00	0.04	-5.54	19,19,19,19	0
4	CL	B	405	1/1	0.99	0.06	-	21,21,21,21	0
4	CL	D	403	1/1	0.99	0.05	-	21,21,21,21	0
4	CL	C	405	1/1	1.00	0.19	-	7,7,7,7	1
4	CL	A	403	1/1	0.97	0.06	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.