W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

May 24, 2020 – 10:54 pm BST

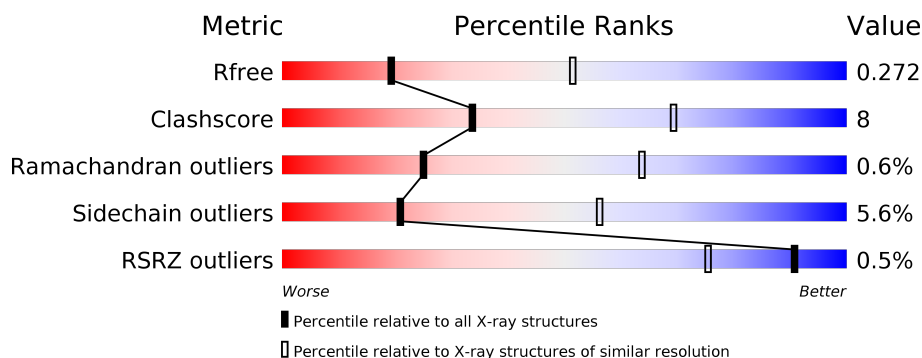|		
PDB ID	:	5UQ9
Title	:	Crystal structure of 6-phosphogluconate dehydrogenase with ((4R,5R)-5-(hyd roxycarbamoyl)-2,2-dimethyl-1,3-dioxolan-4-yl)methyl dihydrogen phosphate
Authors	:	Leonard, P.G.
Deposited on	:	2017-02-07
Resolution	:	3.00 Å(reported)

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 3.00 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		8
Ramachandran outliers		0.6%
Sidechain outliers		5.6%
RSRZ outliers		0.5%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	489	79% 17% •
1	B	489	% 79% 15% • •
1	C	489	71% 24% • •
1	D	489	76% 19% • •
1	E	489	77% 18% • •
1	F	489	76% 19% • •

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Mol	Chain	Length	Quality of chain
1	G	489	% ■ 63% 27% 5% 5%
1	H	489	% ■ 66% 26% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 29092 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 6-phosphogluconate dehydrogenase, decarboxylating.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	469	Total	C	N	O	S	0	0	0
			3642	2322	626	672	22			
1	B	470	Total	C	N	O	S	0	0	0
			3646	2324	627	673	22			
1	C	469	Total	C	N	O	S	0	0	0
			3642	2322	626	672	22			
1	D	469	Total	C	N	O	S	0	0	0
			3642	2322	626	672	22			
1	E	468	Total	C	N	O	S	0	0	0
			3635	2318	625	670	22			
1	F	469	Total	C	N	O	S	0	0	0
			3642	2322	626	672	22			
1	G	466	Total	C	N	O	S	0	0	0
			3613	2303	621	667	22			
1	H	466	Total	C	N	O	S	0	0	0
			3613	2303	621	667	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP P52209
A	-4	ALA	-	expression tag	UNP P52209
A	-3	MET	-	expression tag	UNP P52209
A	-2	ALA	-	expression tag	UNP P52209
A	-1	ASP	-	expression tag	UNP P52209
A	0	ILE	-	expression tag	UNP P52209
B	-5	GLY	-	expression tag	UNP P52209
B	-4	ALA	-	expression tag	UNP P52209
B	-3	MET	-	expression tag	UNP P52209
B	-2	ALA	-	expression tag	UNP P52209
B	-1	ASP	-	expression tag	UNP P52209
B	0	ILE	-	expression tag	UNP P52209
C	-5	GLY	-	expression tag	UNP P52209

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	ALA	-	expression tag	UNP P52209
C	-3	MET	-	expression tag	UNP P52209
C	-2	ALA	-	expression tag	UNP P52209
C	-1	ASP	-	expression tag	UNP P52209
C	0	ILE	-	expression tag	UNP P52209
D	-5	GLY	-	expression tag	UNP P52209
D	-4	ALA	-	expression tag	UNP P52209
D	-3	MET	-	expression tag	UNP P52209
D	-2	ALA	-	expression tag	UNP P52209
D	-1	ASP	-	expression tag	UNP P52209
D	0	ILE	-	expression tag	UNP P52209
E	-5	GLY	-	expression tag	UNP P52209
E	-4	ALA	-	expression tag	UNP P52209
E	-3	MET	-	expression tag	UNP P52209
E	-2	ALA	-	expression tag	UNP P52209
E	-1	ASP	-	expression tag	UNP P52209
E	0	ILE	-	expression tag	UNP P52209
F	-5	GLY	-	expression tag	UNP P52209
F	-4	ALA	-	expression tag	UNP P52209
F	-3	MET	-	expression tag	UNP P52209
F	-2	ALA	-	expression tag	UNP P52209
F	-1	ASP	-	expression tag	UNP P52209
F	0	ILE	-	expression tag	UNP P52209
G	-5	GLY	-	expression tag	UNP P52209
G	-4	ALA	-	expression tag	UNP P52209
G	-3	MET	-	expression tag	UNP P52209
G	-2	ALA	-	expression tag	UNP P52209
G	-1	ASP	-	expression tag	UNP P52209
G	0	ILE	-	expression tag	UNP P52209
H	-5	GLY	-	expression tag	UNP P52209
H	-4	ALA	-	expression tag	UNP P52209
H	-3	MET	-	expression tag	UNP P52209
H	-2	ALA	-	expression tag	UNP P52209
H	-1	ASP	-	expression tag	UNP P52209
H	0	ILE	-	expression tag	UNP P52209

- Molecule 2 is [(4R,5R)-5-(hydroxycarbamoyl)-2,2-dimethyl-1,3-dioxolan-4-yl]methyl dihydrogen phosphate (three-letter code: 8HS) (formula: $C_7H_{14}NO_8P$).
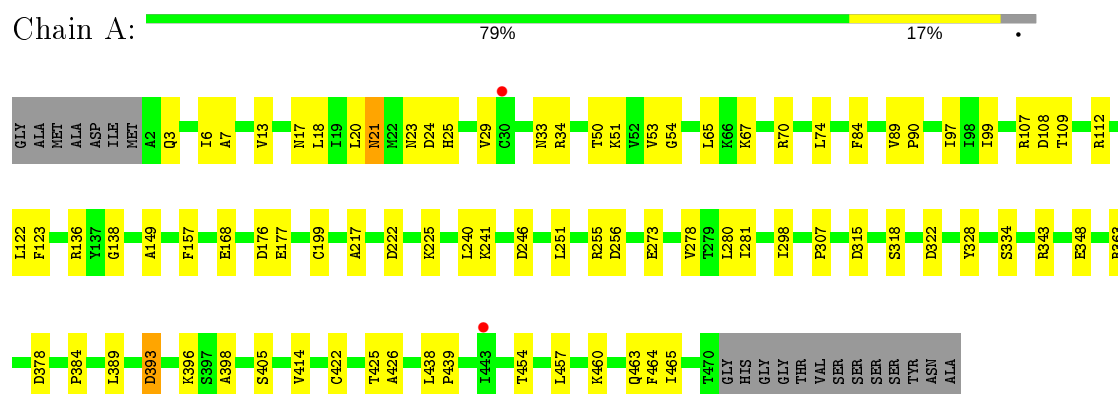
8HS
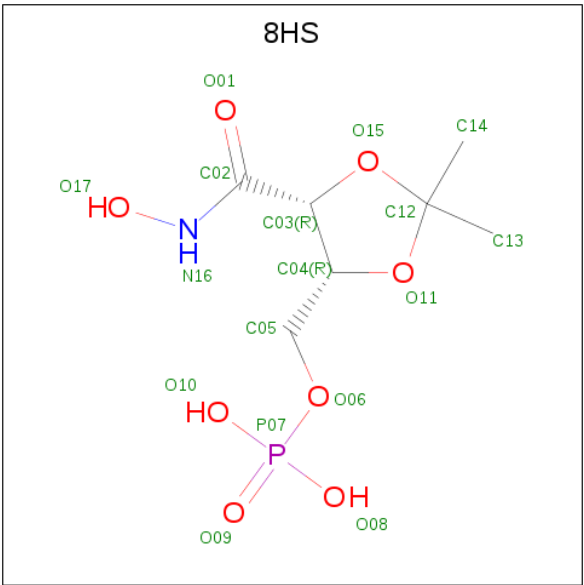
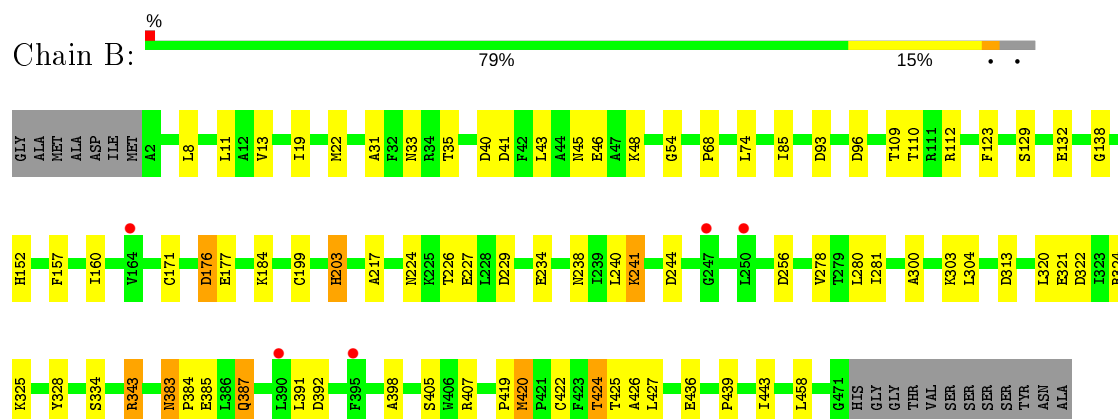| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	F	1	17	7	1	8	1	0	0

3 Residue-property plots (i)

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.

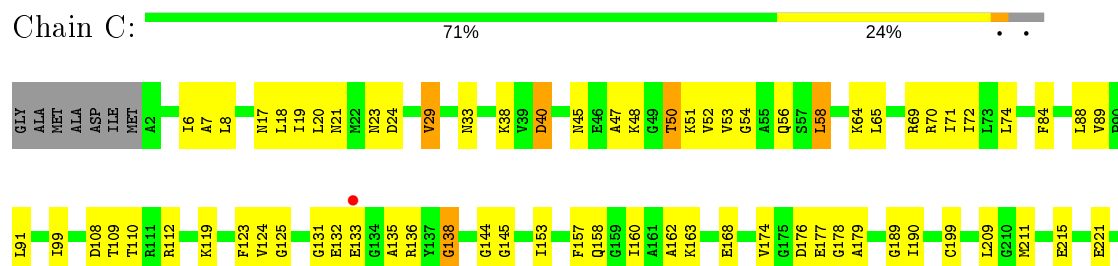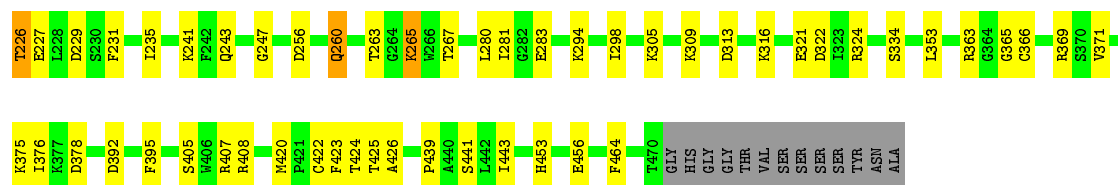- Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

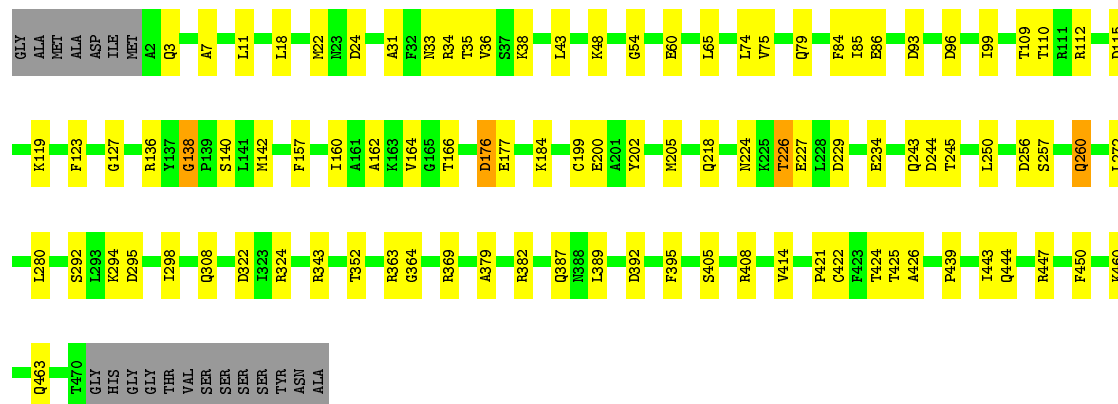- Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

- Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating
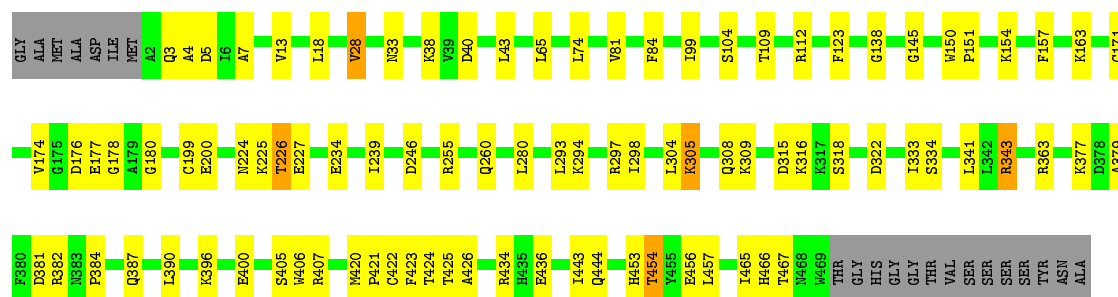
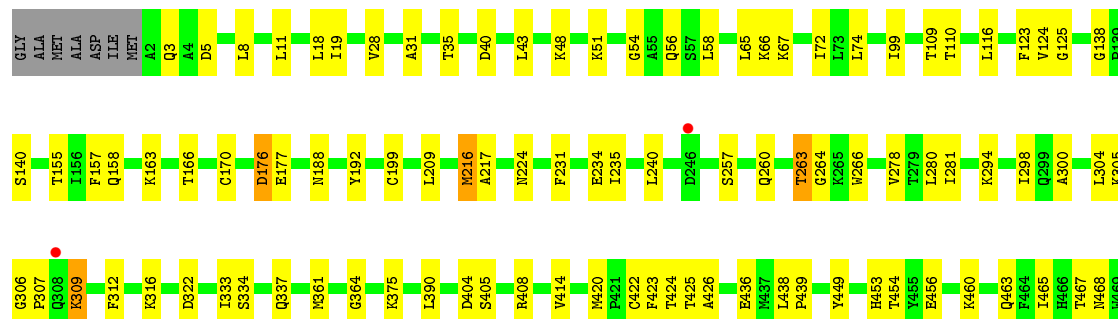• Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

Chain D:

• Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

Chain E:

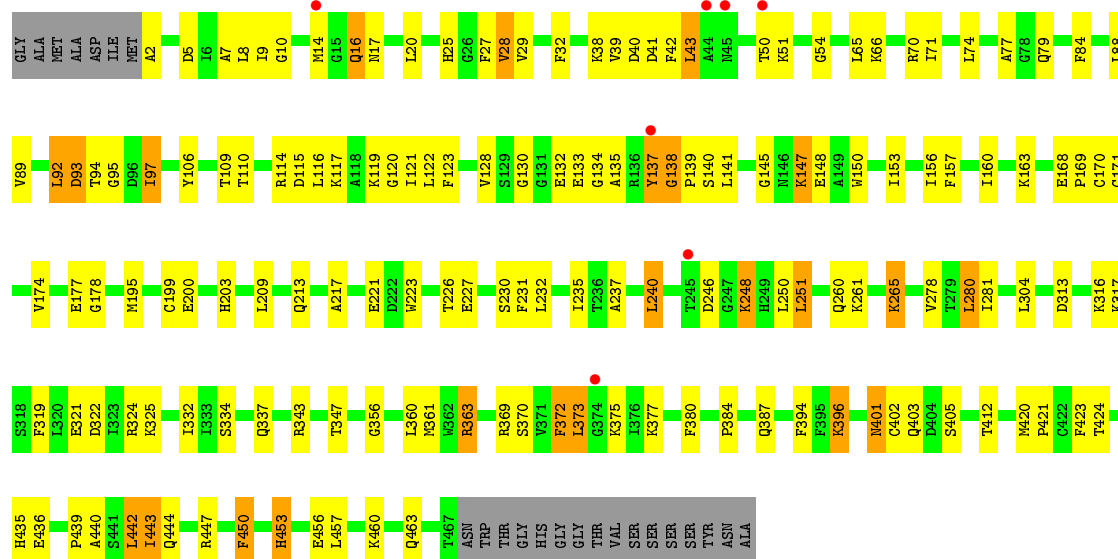• Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

Chain F:

T470 GLY HIS GLY THR VAL SER SER SER TYR ASN ALA

● Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

Chain G:

GLY ALA MET ALA ASP ILE MET A2 D5 I6 A7 L8 I9 G10 M14 G15 Q16 N17 L20 H25 G26 F27 V28 V29 F32 K38 V39 D40 D41 F42 L43 A44 N45 T50 K51 G54 L65 K66 R70 I71 L74 A77 G78 Q79 F84 L88

V89 L92 D93 T94 G95 D96 I97 Y106 T109 T110 R114 D115 L116 K117 A118 K119 G120 I121 L122 F123 V128 S129 G130 G131 E132 E133 G134 A135 R136 Y137 G138 P139 S140 L141 G145 N146 K147 E148 A149 W150 I153 I156 F157 I160 K163 E168 P169 C170 C171

V174 E177 G178 M195 C199 E200 H203 L209 Q213 A217 E221 D222 W223 T226 E227 S230 F231 L232 I235 T236 A237 L240 T245 D246 G247 K248 H249 L250 L251 Q260 K261 K265 V278 T279 L280 I281 L304 D313 K316 K317

S318 F319 L320 E321 D322 K323 R324 K325 I332 I333 S334 Q337 R343 T347 G356 L360 N361 M362 R363 R369 S370 V371 F372 L373 G374 F375 I376 K377 F380 P384 Q387 F394 F395 K396 N401 C402 Q403 D404 S405 T412 M420 P421 C422 F423 T424

H435 E436 P439 A440 S441 L442 I443 Q444 R447 F450 H453 E456 L457 K460 Q463 T467 ASN TRP THR GLY HIS GLY THR VAL SER SER SER TYR ASN ALA

● Molecule 1: 6-phosphogluconate dehydrogenase, decarboxylating

Chain H:

GLY ALA MET ALA ASP ILE MET A2 A7 L11 A12 V13 M14 G15 Q16 N17 L18 N21 M22 N23 D24 H25 A31 R34 T35 V36 D40 D41 F42 E46 T50 K51 V52 L58 K59 V62 S63 K64 L65 R69 L74 I85 V89 D93

D96 I99 R107 D108 T109 T110 R114 G125 S126 G127 V128 S129 G130 A135 R136 Y137 G138 P139 S140 L141 M142 I153 F157 I160 A161 A162 K163 V164 G167 C171 D176 E177 K184 Y192 C199 A217 Q218 D222 W223 N224 K225 L228 D229

S230 F231 L232 I233 E234 I235 T236 I239 L240 K241 F242 Q243 K248 L251 P252 K253 I254 R255 D256 S257 Q260 K261 G262 T263 G264 K265 E273 L280 E283 L293 K294 D295 E296 R297 I298 Q308 K309 D315 K316 K317 S318 F319 L320 E321 D322 I323 R324 K325 A326

S334 R363 G364 G365 C366 I367 I368 R369 S370 V371 F372 L373 G374 K375 F380 N383 L386 L390 V399 S405 W406 A409 P421 C422 F423 T424 T425 A426 Y430 D431 H435 P439 L442 F450 G451 A452 H453 T454 L457 F464 I465 H466 T467 ASN

TRP THR GLY HIS GLY THR VAL SER SER SER TYR ASN ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.31Å 164.93Å 133.20Å 90.00° 91.43° 90.00°	Depositor
Resolution (Å)	87.28 – 3.00	Depositor
	87.28 – 3.00	EDS
% Data completeness	99.8 (87.28-3.00)	Depositor
(in resolution range)	99.9 (87.28-3.00)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1.2155	Depositor
R, R_{free}	0.217 , 0.272	Depositor
	0.217 , 0.272	DCC
R_{free} test set	3911 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	59.6	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 32.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.030 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29092	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 8HS

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	0.24	0/3716	0.39	0/5009
1	B	0.24	0/3720	0.39	0/5014
1	C	0.24	0/3716	0.39	0/5009
1	D	0.24	0/3716	0.38	0/5009
1	E	0.24	0/3709	0.38	0/4999
1	F	0.24	0/3716	0.39	0/5009
1	G	0.24	0/3685	0.40	0/4965
1	H	0.24	0/3685	0.40	0/4965
All	All	0.24	0/29663	0.39	0/39979

There are no bond length outliers.

There are no bond angle outliers.

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	3642	0	3640	52	0
1	B	3646	0	3643	47	0
1	C	3642	0	3640	74	0
1	D	3642	0	3640	58	0
1	E	3635	0	3633	55	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3642	0	3640	61	1
1	G	3613	0	3617	96	0
1	H	3613	0	3617	104	0
2	F	17	0	0	0	0
All	All	29092	0	29070	494	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 8.

The worst 5 of 494 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:246:ASP:OD2	1:G:248:LYS:NZ	1.92	1.03
1:A:438:LEU:N	1:B:256:ASP:OD2	2.06	0.88
1:C:221:GLU:OE2	1:C:241:LYS:NZ	2.06	0.88
1:G:226:THR:OG1	1:G:227:GLU:OE2	1.92	0.88
1:C:366:CYS:O	1:C:369:ARG:NH1	2.08	0.85

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:E:316:LYS:NZ	1:F:40:ASP:OD2[1_455]	1.83	0.37

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	467/489 (96%)	442 (95%)	24 (5%)	1 (0%)	47	82
1	B	468/489 (96%)	440 (94%)	24 (5%)	4 (1%)	17	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	467/489 (96%)	442 (95%)	23 (5%)	2 (0%)	34	72
1	D	467/489 (96%)	440 (94%)	25 (5%)	2 (0%)	34	72
1	E	466/489 (95%)	443 (95%)	22 (5%)	1 (0%)	47	82
1	F	467/489 (96%)	447 (96%)	18 (4%)	2 (0%)	34	72
1	G	464/489 (95%)	417 (90%)	42 (9%)	5 (1%)	14	50
1	H	464/489 (95%)	437 (94%)	23 (5%)	4 (1%)	17	55
All	All	3730/3912 (95%)	3508 (94%)	201 (5%)	21 (1%)	25	64

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	384	PRO
1	H	231	PHE
1	H	452	ALA
1	G	450	PHE
1	D	308	GLN

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	380/393 (97%)	368 (97%)	12 (3%)	39	74
1	B	380/393 (97%)	364 (96%)	16 (4%)	30	66
1	C	380/393 (97%)	359 (94%)	21 (6%)	21	57
1	D	380/393 (97%)	365 (96%)	15 (4%)	32	69
1	E	379/393 (96%)	358 (94%)	21 (6%)	21	57
1	F	380/393 (97%)	362 (95%)	18 (5%)	26	63
1	G	377/393 (96%)	333 (88%)	44 (12%)	5	22
1	H	377/393 (96%)	353 (94%)	24 (6%)	17	51
All	All	3033/3144 (96%)	2862 (94%)	171 (6%)	21	56

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	309	LYS
1	F	216	MET
1	H	222	ASP
1	E	343	ARG
1	F	35	THR

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	C	453	HIS
1	G	25	HIS
1	F	453	HIS
1	C	23	ASN
1	F	224	ASN

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)

1 ligand is 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	8HS	F	501	-	17,17,17	4.31	6 (35%)	22,26,26	1.27	4 (18%)

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	8HS	F	501	-	-	4/12/26/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	8HS	C02-N16	10.62	1.47	1.33
2	F	501	8HS	O15-C03	-9.57	1.24	1.43
2	F	501	8HS	O15-C12	7.40	1.57	1.43
2	F	501	8HS	O11-C12	-5.72	1.32	1.43
2	F	501	8HS	O01-C02	-2.91	1.17	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	8HS	C13-C12-C14	-2.78	107.56	113.19
2	F	501	8HS	O01-C02-N16	-2.60	119.91	123.27
2	F	501	8HS	O11-C04-C03	2.55	106.27	101.94
2	F	501	8HS	O15-C12-O11	2.09	107.87	105.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	501	8HS	C05-O06-P07-O08
2	F	501	8HS	C05-O06-P07-O09
2	F	501	8HS	C05-O06-P07-O10
2	F	501	8HS	C04-C05-O06-P07

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 8HS F 501
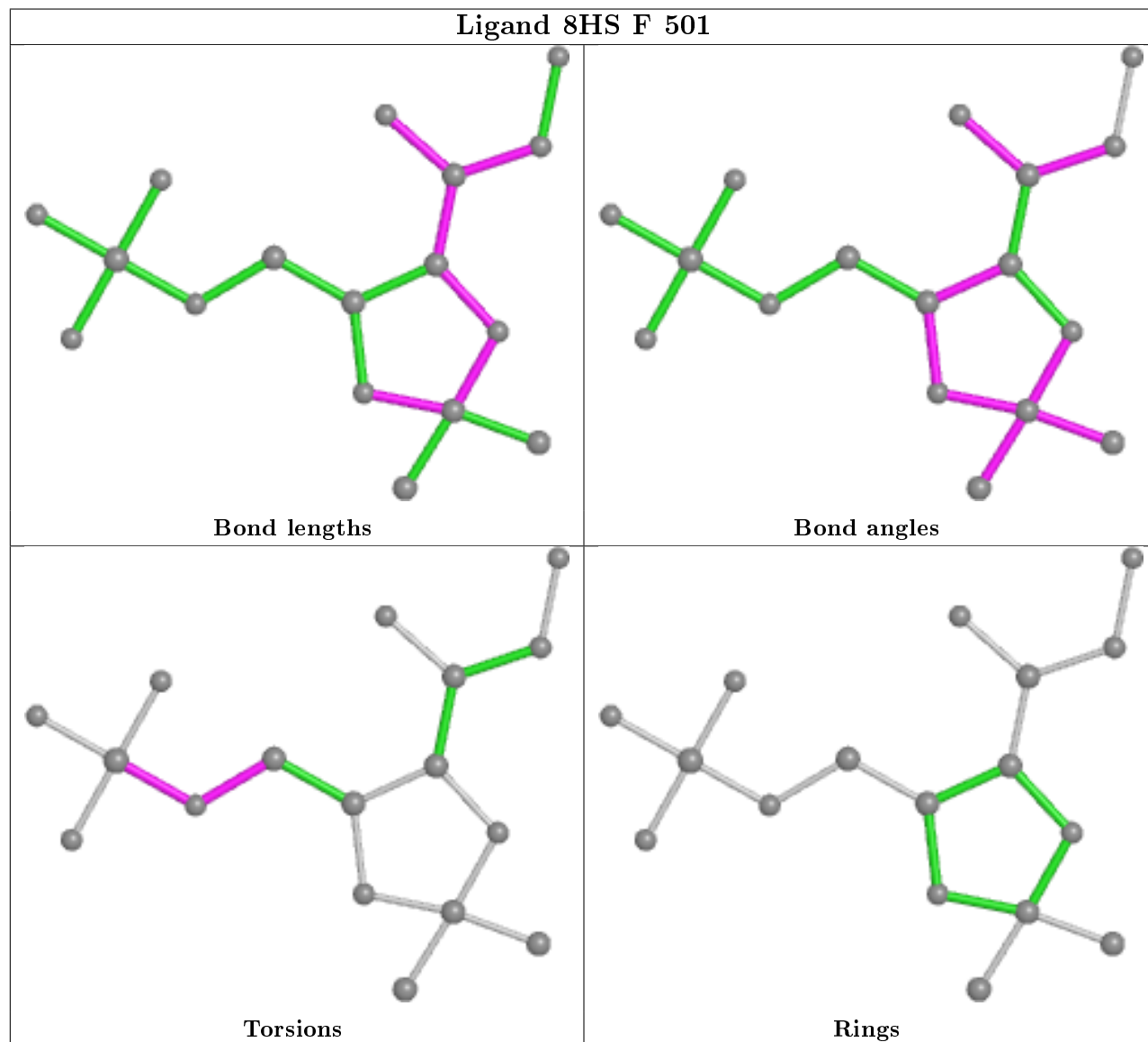
5.7 Other polymers (i)

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	469/489 (95%)	-0.41	2 (0%)	92	79	24, 52, 84, 96	0
1	B	470/489 (96%)	-0.37	5 (1%)	80	56	25, 51, 80, 109	0
1	C	469/489 (95%)	-0.33	1 (0%)	95	87	27, 54, 86, 106	0
1	D	469/489 (95%)	-0.48	0	100	100	25, 44, 74, 92	0
1	E	468/489 (95%)	-0.40	0	100	100	30, 54, 77, 95	0
1	F	469/489 (95%)	-0.42	2 (0%)	92	79	30, 52, 74, 92	0
1	G	466/489 (95%)	0.02	7 (1%)	73	46	39, 77, 106, 116	0
1	H	466/489 (95%)	-0.02	3 (0%)	89	72	44, 79, 104, 122	0
All	All	3746/3912 (95%)	-0.30	20 (0%)	91	75	24, 57, 95, 122	0

The worst 5 of 20 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	245	THR	4.5
1	B	395	PHE	3.4
1	F	246	ASP	3.3
1	C	133	GLU	2.9
1	H	372	PHE	2.8

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.
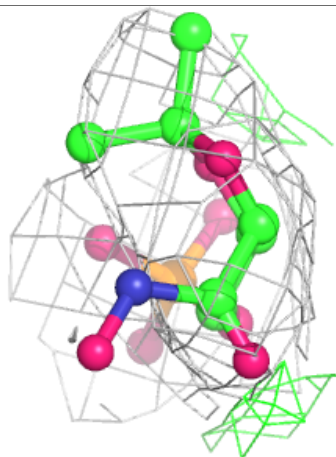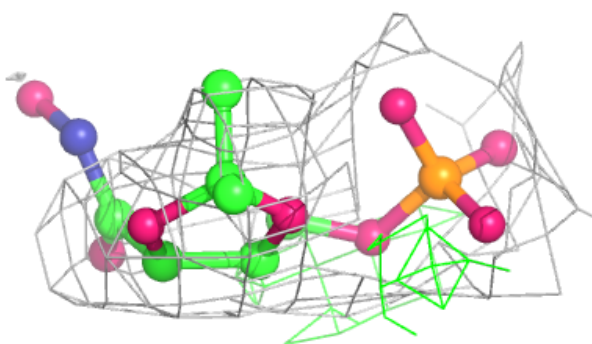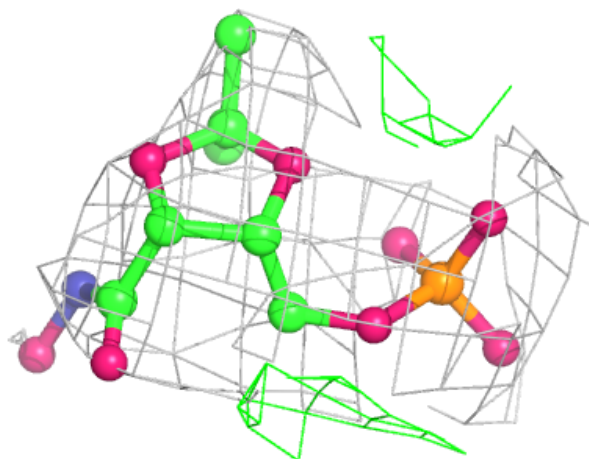
6.4 Ligands (i)

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. 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
2	8HS	F	501	17/17	0.87	0.21	68,74,86,87	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 8HS F 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.