wwPDB X-ray Structure Validation Summary Report (i)

Sep 19, 2023 – 11:25 AM EDT

PDB ID	:	5EU9
Title	:	Structure of Human Enolase 2 in complex with ((3S,5S)-1,5-dihydroxy-3-methyl-2-oxopyrrolidin-3-yl)phosphonic acid
Authors	:	Leonard, P.G.; Muller, F.L.
Deposited on	:	2015-11-18
Resolution	:	2.05 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:

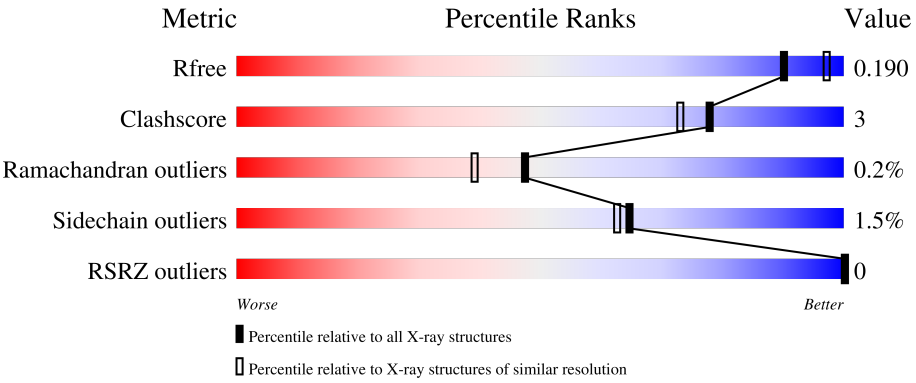
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	440	91% 7% •
1	B	440	92% 6% •
1	C	440	90% 8% ••
1	D	440	93% 5% •
1	E	440	90% 8% •

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Mol	Chain	Length	Quality of chain
1	F	440	91% 8%
1	G	440	90% 8%
1	H	440	90% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 29111 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 Gamma-enolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	433	Total	C	N	O	S	0	3	0
			3338	2098	573	654	13			
1	B	433	Total	C	N	O	S	0	1	0
			3317	2086	568	649	14			
1	C	436	Total	C	N	O	S	0	2	0
			3355	2108	579	654	14			
1	D	433	Total	C	N	O	S	0	2	0
			3326	2091	569	652	14			
1	E	433	Total	C	N	O	S	0	6	0
			3357	2110	576	657	14			
1	F	434	Total	C	N	O	S	0	3	0
			3354	2108	580	653	13			
1	G	433	Total	C	N	O	S	0	2	0
			3329	2095	571	650	13			
1	H	433	Total	C	N	O	S	0	1	0
			3317	2086	568	649	14			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P09104
A	436	HIS	-	expression tag	UNP P09104
A	437	HIS	-	expression tag	UNP P09104
A	438	HIS	-	expression tag	UNP P09104
A	439	HIS	-	expression tag	UNP P09104
A	440	HIS	-	expression tag	UNP P09104
B	435	HIS	-	expression tag	UNP P09104
B	436	HIS	-	expression tag	UNP P09104
B	437	HIS	-	expression tag	UNP P09104
B	438	HIS	-	expression tag	UNP P09104
B	439	HIS	-	expression tag	UNP P09104
B	440	HIS	-	expression tag	UNP P09104
C	435	HIS	-	expression tag	UNP P09104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	436	HIS	-	expression tag	UNP P09104
C	437	HIS	-	expression tag	UNP P09104
C	438	HIS	-	expression tag	UNP P09104
C	439	HIS	-	expression tag	UNP P09104
C	440	HIS	-	expression tag	UNP P09104
D	435	HIS	-	expression tag	UNP P09104
D	436	HIS	-	expression tag	UNP P09104
D	437	HIS	-	expression tag	UNP P09104
D	438	HIS	-	expression tag	UNP P09104
D	439	HIS	-	expression tag	UNP P09104
D	440	HIS	-	expression tag	UNP P09104
E	435	HIS	-	expression tag	UNP P09104
E	436	HIS	-	expression tag	UNP P09104
E	437	HIS	-	expression tag	UNP P09104
E	438	HIS	-	expression tag	UNP P09104
E	439	HIS	-	expression tag	UNP P09104
E	440	HIS	-	expression tag	UNP P09104
F	435	HIS	-	expression tag	UNP P09104
F	436	HIS	-	expression tag	UNP P09104
F	437	HIS	-	expression tag	UNP P09104
F	438	HIS	-	expression tag	UNP P09104
F	439	HIS	-	expression tag	UNP P09104
F	440	HIS	-	expression tag	UNP P09104
G	435	HIS	-	expression tag	UNP P09104
G	436	HIS	-	expression tag	UNP P09104
G	437	HIS	-	expression tag	UNP P09104
G	438	HIS	-	expression tag	UNP P09104
G	439	HIS	-	expression tag	UNP P09104
G	440	HIS	-	expression tag	UNP P09104
H	435	HIS	-	expression tag	UNP P09104
H	436	HIS	-	expression tag	UNP P09104
H	437	HIS	-	expression tag	UNP P09104
H	438	HIS	-	expression tag	UNP P09104
H	439	HIS	-	expression tag	UNP P09104
H	440	HIS	-	expression tag	UNP P09104

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0

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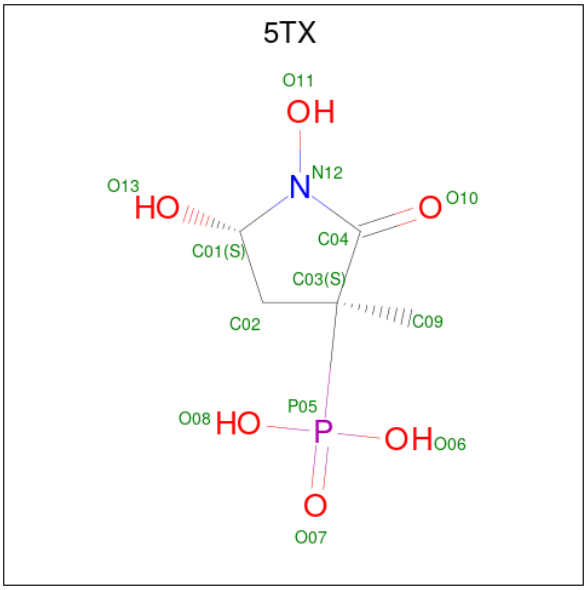
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Mg 2 2	0	0
2	D	2	Total Mg 2 2	0	0
2	E	2	Total Mg 2 2	0	0
2	F	2	Total Mg 2 2	0	0
2	G	2	Total Mg 2 2	0	0
2	H	2	Total Mg 2 2	0	0

- Molecule 3 is ((3S,5S)-1,5-dihydroxy-3-methyl-2-oxopyrrolidin-3-yl)phosphonic acid (three-letter code: 5TX) (formula: $C_5H_{10}NO_6P$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 13 5 1 6 1	0	0
3	B	1	Total C N O P 13 5 1 6 1	0	0
3	C	1	Total C N O P 13 5 1 6 1	0	0
3	D	1	Total C N O P 13 5 1 6 1	0	0
3	E	1	Total C N O P 13 5 1 6 1	0	0

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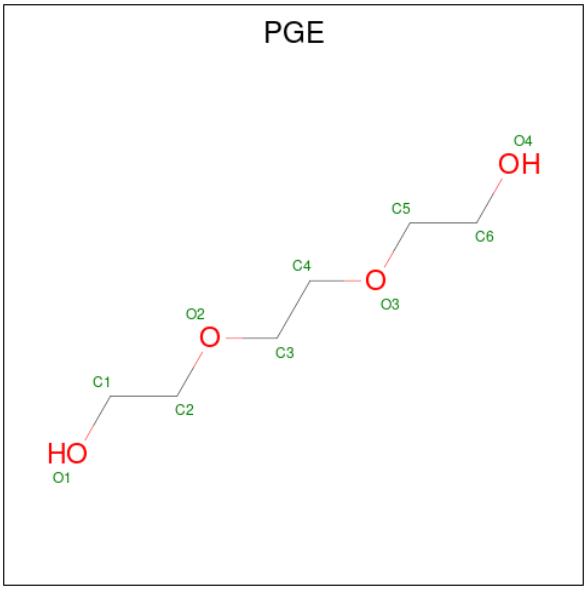
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C N O P 13 5 1 6 1	0	0
3	G	1	Total C N O P 13 5 1 6 1	0	0
3	H	1	Total C N O P 13 5 1 6 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 10 6 4	0	0
4	E	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0
4	G	1	Total C O 10 6 4	0	0
4	H	1	Total C O 10 6 4	0	0

- Molecule 5 is water.

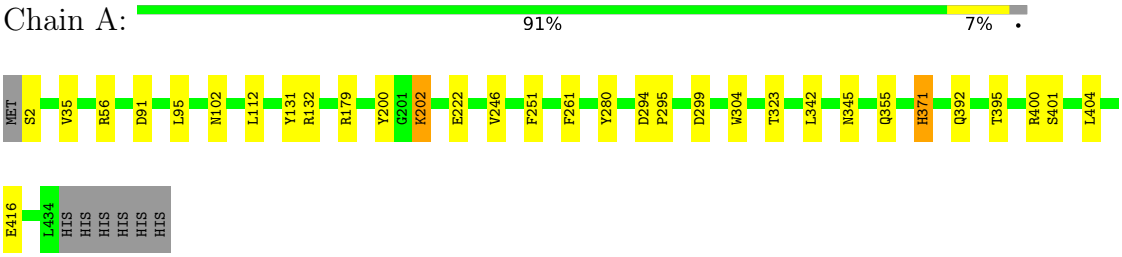
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	283	Total O 283 283	0	0
5	B	294	Total O 294 294	0	0
5	C	274	Total O 274 274	0	0
5	D	275	Total O 275 275	0	0
5	E	283	Total O 283 283	0	0
5	F	274	Total O 274 274	0	0
5	G	268	Total O 268 268	0	0
5	H	287	Total O 287 287	0	0

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.

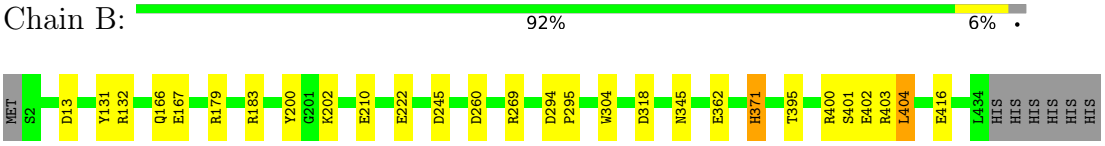
- Molecule 1: Gamma-enolase

Chain A:



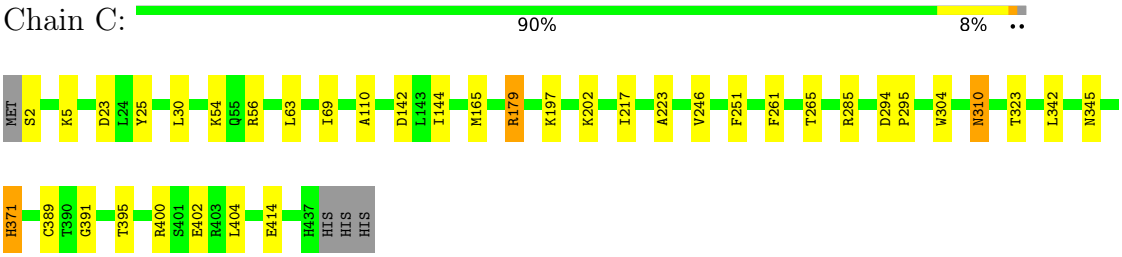
- Molecule 1: Gamma-enolase

Chain B:



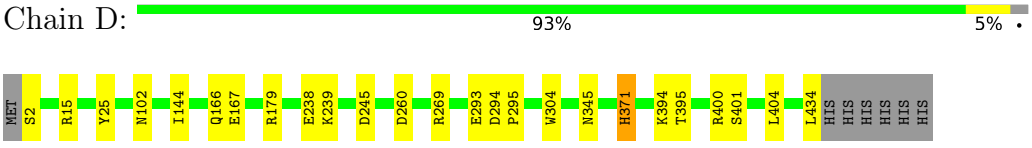
- Molecule 1: Gamma-enolase

Chain C:



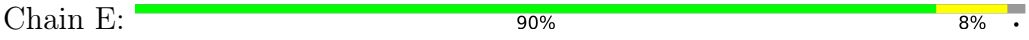
- Molecule 1: Gamma-enolase

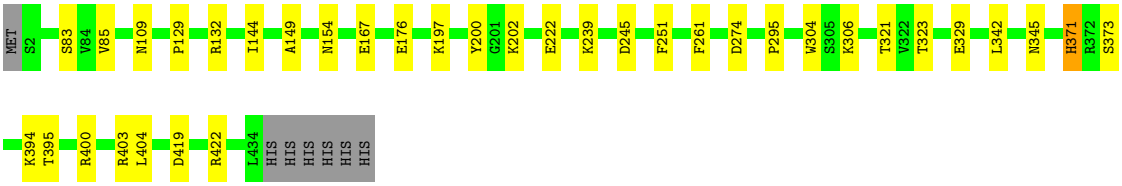
Chain D:



- Molecule 1: Gamma-enolase

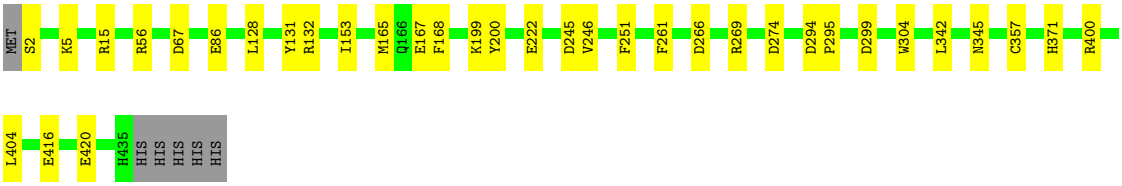
Chain E:





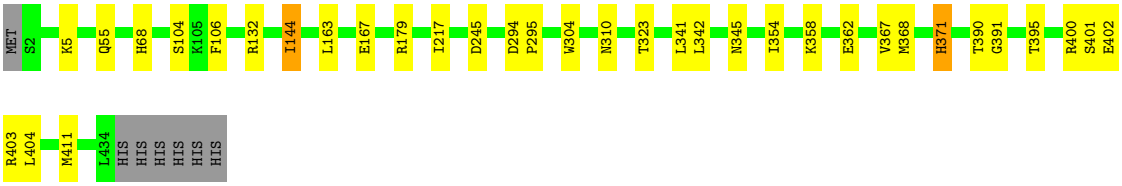
• Molecule 1: Gamma-enolase

Chain F:



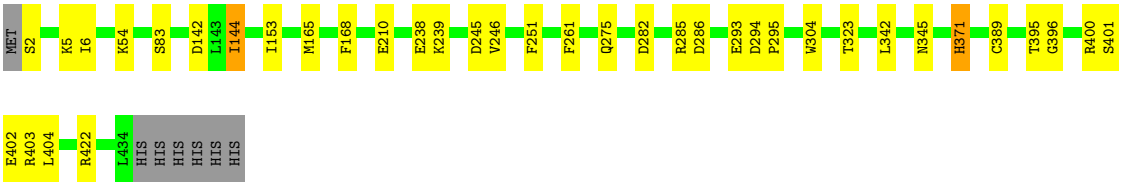
• Molecule 1: Gamma-enolase

Chain G:



• Molecule 1: Gamma-enolase

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.25Å 110.31Å 136.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	89.93 – 2.05 89.93 – 2.05	Depositor EDS
% Data completeness (in resolution range)	97.4 (89.93-2.05) 97.5 (89.93-2.05)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.05Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.154 , 0.192 0.156 , 0.190	Depositor DCC
R_{free} test set	1996 reflections (0.92%)	wwPDB-VP
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.785	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	29111	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 54.17 % 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 3.7956e-05. 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: 5TX, MG, 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	0.38	0/3397	0.51	0/4596
1	B	0.39	0/3375	0.53	1/4566 (0.0%)
1	C	0.38	0/3416	0.53	0/4622
1	D	0.38	0/3384	0.52	0/4578
1	E	0.38	0/3421	0.52	0/4626
1	F	0.37	0/3411	0.52	0/4613
1	G	0.37	0/3387	0.52	0/4580
1	H	0.38	0/3375	0.52	0/4566
All	All	0.38	0/27166	0.52	1/36747 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	13	ASP	CB-CG-OD1	5.04	122.84	118.30

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	3338	0	3303	20	0
1	B	3317	0	3291	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3355	0	3317	24	0
1	D	3326	0	3296	16	0
1	E	3357	0	3332	18	0
1	F	3354	0	3323	19	0
1	G	3329	0	3311	26	0
1	H	3317	0	3291	21	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	13	0	0	0	0
3	B	13	0	0	0	0
3	C	13	0	0	0	0
3	D	13	0	0	0	0
3	E	13	0	0	0	0
3	F	13	0	0	0	0
3	G	13	0	0	0	0
3	H	13	0	0	0	0
4	C	10	0	14	2	0
4	D	10	0	14	0	0
4	E	10	0	14	0	0
4	F	10	0	14	1	0
4	G	10	0	14	2	0
4	H	10	0	14	0	0
5	A	283	0	0	8	0
5	B	294	0	0	3	0
5	C	274	0	0	4	0
5	D	275	0	0	4	0
5	E	283	0	0	0	0
5	F	274	0	0	7	0
5	G	268	0	0	5	0
5	H	287	0	0	2	0
All	All	29111	0	26548	156	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 3.

The worst 5 of 156 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:D:102:ASN:ND2	5:D:601:HOH:O	2.16	0.78
1:A:102[B]:ASN:ND2	5:A:604:HOH:O	2.20	0.74
1:B:371:HIS:HD2	1:B:403:ARG:HH11	1.38	0.72
1:A:2:SER:N	5:A:605:HOH:O	2.23	0.70
1:E:371:HIS:HD2	1:E:403:ARG:HH11	1.40	0.69

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	434/440 (99%)	421 (97%)	12 (3%)	1 (0%)	47	39
1	B	432/440 (98%)	422 (98%)	9 (2%)	1 (0%)	47	39
1	C	436/440 (99%)	427 (98%)	8 (2%)	1 (0%)	47	39
1	D	433/440 (98%)	421 (97%)	11 (2%)	1 (0%)	47	39
1	E	437/440 (99%)	426 (98%)	10 (2%)	1 (0%)	47	39
1	F	435/440 (99%)	423 (97%)	11 (2%)	1 (0%)	47	39
1	G	433/440 (98%)	423 (98%)	9 (2%)	1 (0%)	47	39
1	H	432/440 (98%)	419 (97%)	12 (3%)	1 (0%)	47	39
All	All	3472/3520 (99%)	3382 (97%)	82 (2%)	8 (0%)	47	39

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	400	ARG
1	C	400	ARG
1	D	400	ARG
1	E	400	ARG
1	F	400	ARG

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	353/357 (99%)	348 (99%)	5 (1%)	67	65
1	B	351/357 (98%)	346 (99%)	5 (1%)	67	65
1	C	355/357 (99%)	348 (98%)	7 (2%)	55	50
1	D	352/357 (99%)	349 (99%)	3 (1%)	78	79
1	E	356/357 (100%)	348 (98%)	8 (2%)	52	46
1	F	354/357 (99%)	348 (98%)	6 (2%)	60	57
1	G	352/357 (99%)	347 (99%)	5 (1%)	67	65
1	H	351/357 (98%)	346 (99%)	5 (1%)	67	65
All	All	2824/2856 (99%)	2780 (98%)	44 (2%)	65	59

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	56	ARG
1	G	144	ILE
1	F	199	LYS
1	F	371	HIS
1	G	371	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	154	ASN
1	B	371	HIS
1	E	371	HIS
1	G	371	HIS
1	H	426	HIS

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)

Of 30 ligands modelled in this entry, 16 are monoatomic - leaving 14 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	5TX	B	502	2	7,13,13	2.19	5 (71%)	7,22,22	2.32	4 (57%)
3	5TX	E	503	2	7,13,13	2.02	3 (42%)	7,22,22	2.31	3 (42%)
3	5TX	G	503	2	7,13,13	1.89	2 (28%)	7,22,22	2.50	5 (71%)
3	5TX	H	503	2	7,13,13	2.08	3 (42%)	7,22,22	2.56	3 (42%)
4	PGE	D	502	-	9,9,9	0.31	0	8,8,8	0.31	0
4	PGE	G	502	-	9,9,9	0.35	0	8,8,8	0.38	0
3	5TX	D	503	2	7,13,13	2.03	2 (28%)	7,22,22	2.31	4 (57%)
4	PGE	C	502	-	9,9,9	0.33	0	8,8,8	0.34	0
3	5TX	A	502	2	7,13,13	2.10	3 (42%)	7,22,22	2.44	3 (42%)
3	5TX	F	503	2	7,13,13	2.10	2 (28%)	7,22,22	2.83	4 (57%)
3	5TX	C	503	2	7,13,13	2.14	3 (42%)	7,22,22	2.46	3 (42%)
4	PGE	E	502	-	9,9,9	0.36	0	8,8,8	0.35	0
4	PGE	H	502	-	9,9,9	0.35	0	8,8,8	0.25	0
4	PGE	F	502	-	9,9,9	0.37	0	8,8,8	0.31	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	5TX	B	502	2	-	0/0/28/28	0/1/1/1
3	5TX	E	503	2	-	0/0/28/28	0/1/1/1
3	5TX	G	503	2	-	0/0/28/28	0/1/1/1
3	5TX	H	503	2	-	0/0/28/28	0/1/1/1
4	PGE	D	502	-	-	1/7/7/7	-
4	PGE	G	502	-	-	2/7/7/7	-
3	5TX	D	503	2	-	0/0/28/28	0/1/1/1
4	PGE	C	502	-	-	4/7/7/7	-
3	5TX	A	502	2	-	0/0/28/28	0/1/1/1
3	5TX	F	503	2	-	0/0/28/28	0/1/1/1
3	5TX	C	503	2	-	0/0/28/28	0/1/1/1
4	PGE	E	502	-	-	3/7/7/7	-
4	PGE	H	502	-	-	4/7/7/7	-
4	PGE	F	502	-	-	5/7/7/7	-

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	503	5TX	O11-N12	-3.67	1.35	1.40
3	E	503	5TX	P05-O08	-3.39	1.48	1.54
3	H	503	5TX	O11-N12	-3.30	1.36	1.40
3	C	503	5TX	O11-N12	-3.26	1.36	1.40
3	D	503	5TX	O10-C04	3.14	1.27	1.22

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	503	5TX	O11-N12-C04	4.39	129.30	121.21
3	F	503	5TX	P05-C03-C09	-4.05	104.00	110.21
3	H	503	5TX	O11-N12-C04	4.05	128.68	121.21
3	A	502	5TX	O08-P05-O06	4.00	119.27	107.99
3	H	503	5TX	P05-C03-C09	-3.95	104.16	110.21

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	502	PGE	O3-C5-C6-O4
4	H	502	PGE	O1-C1-C2-O2
4	C	502	PGE	O2-C3-C4-O3
4	G	502	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
4	C	502	PGE	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	502	PGE	2	0
4	C	502	PGE	2	0
4	F	502	PGE	1	0

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, 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	433/440 (98%)	-0.91	0	100	100	8, 18, 36, 58	0
1	B	433/440 (98%)	-0.92	0	100	100	8, 18, 36, 54	0
1	C	436/440 (99%)	-0.91	0	100	100	9, 18, 37, 56	0
1	D	433/440 (98%)	-0.90	0	100	100	10, 19, 39, 58	0
1	E	433/440 (98%)	-0.93	0	100	100	9, 18, 35, 57	0
1	F	434/440 (98%)	-0.88	0	100	100	8, 18, 38, 64	0
1	G	433/440 (98%)	-0.89	0	100	100	9, 19, 38, 58	0
1	H	433/440 (98%)	-0.90	0	100	100	9, 18, 37, 51	0
All	All	3468/3520 (98%)	-0.90	0	100	100	8, 18, 37, 64	0

There are no RSRZ outliers to report.

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
4	PGE	H	502	10/10	0.85	0.13	40,45,48,49	0
4	PGE	F	502	10/10	0.89	0.10	32,37,43,45	0
4	PGE	C	502	10/10	0.90	0.13	33,42,45,49	0
4	PGE	E	502	10/10	0.90	0.14	37,41,51,54	0
4	PGE	D	502	10/10	0.91	0.12	33,38,46,47	0
4	PGE	G	502	10/10	0.92	0.09	30,38,42,45	0
2	MG	H	501	1/1	0.97	0.05	15,15,15,15	0
2	MG	G	500	1/1	0.98	0.06	15,15,15,15	0
2	MG	F	500	1/1	0.98	0.04	15,15,15,15	0
2	MG	A	500	1/1	0.99	0.04	13,13,13,13	0
2	MG	F	501	1/1	0.99	0.04	15,15,15,15	0
2	MG	A	501	1/1	0.99	0.04	15,15,15,15	0
2	MG	G	501	1/1	0.99	0.04	15,15,15,15	0
2	MG	H	500	1/1	0.99	0.03	16,16,16,16	0
2	MG	B	500	1/1	0.99	0.05	10,10,10,10	0
3	5TX	A	502	13/13	0.99	0.07	10,13,15,17	0
3	5TX	B	502	13/13	0.99	0.09	10,12,15,15	0
3	5TX	C	503	13/13	0.99	0.06	10,13,17,18	0
3	5TX	D	503	13/13	0.99	0.06	10,13,15,16	0
3	5TX	E	503	13/13	0.99	0.07	10,11,14,16	0
3	5TX	F	503	13/13	0.99	0.07	9,14,15,16	0
3	5TX	G	503	13/13	0.99	0.06	11,12,14,15	0
3	5TX	H	503	13/13	0.99	0.07	11,13,17,17	0
2	MG	C	500	1/1	0.99	0.03	15,15,15,15	0
2	MG	C	501	1/1	0.99	0.04	14,14,14,14	0
2	MG	D	500	1/1	0.99	0.06	16,16,16,16	0
2	MG	D	501	1/1	0.99	0.06	12,12,12,12	0
2	MG	E	500	1/1	0.99	0.05	13,13,13,13	0
2	MG	E	501	1/1	0.99	0.03	16,16,16,16	0
2	MG	B	501	1/1	1.00	0.05	13,13,13,13	0

6.5 Other polymers (i)

There are no such residues in this entry.