wwPDB X-ray Structure Validation Summary Report (i)

Dec 8, 2023 – 03:20 am GMT

PDB ID	:	1OG0
Title	:	CRYSTAL STRUCTURE OF THE MUTANT G226S OF THE TYROSINE-REGULATED 3-DEOXY-D-ARABINO-HEPTULOSONATE-7-PHOSPHATE SYNTHASE FROM SACCHAROMYCES CEREVISIAE COMPLEXED WITH PHENYLALANINE AND MANGANESE
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Deposited on	:	2003-04-22
Resolution	:	2.70 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 (i)) were used in the production of this report:

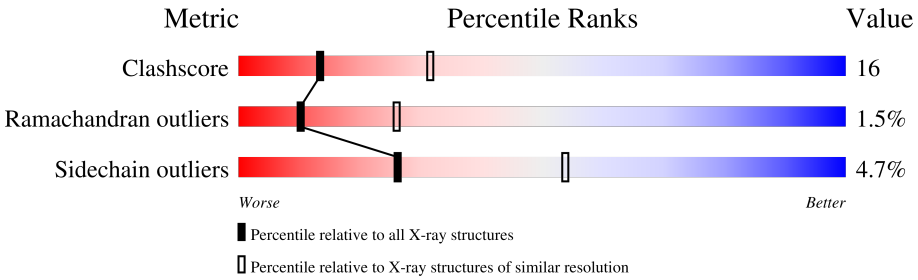
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	370	63% 28% • 7%
1	B	370	63% 28% • 6%
1	C	370	65% 26% • 6%
1	D	370	66% 26% • 5%
1	E	370	59% 29% • 9%
1	F	370	66% 24% • • 6%
1	G	370	59% 31% • 7%
1	H	370	59% 31% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20830 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 Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	1
			2583	1606	464	503	10			
1	B	347	Total	C	N	O	S	0	0	1
			2606	1620	467	509	10			
1	C	347	Total	C	N	O	S	0	0	1
			2602	1617	468	507	10			
1	D	350	Total	C	N	O	S	0	0	1
			2608	1621	468	509	10			
1	E	336	Total	C	N	O	S	0	0	1
			2516	1561	451	494	10			
1	F	346	Total	C	N	O	S	0	0	1
			2591	1611	466	504	10			
1	G	343	Total	C	N	O	S	0	0	1
			2573	1601	461	501	10			
1	H	344	Total	C	N	O	S	0	0	1
			2561	1591	457	503	10			

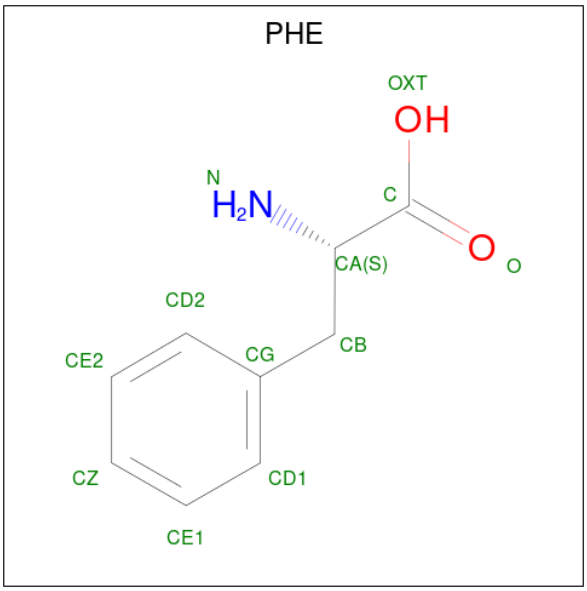
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	SER	GLY	engineered mutation	UNP P32449
B	226	SER	GLY	engineered mutation	UNP P32449
C	226	SER	GLY	engineered mutation	UNP P32449
D	226	SER	GLY	engineered mutation	UNP P32449
E	226	SER	GLY	engineered mutation	UNP P32449
F	226	SER	GLY	engineered mutation	UNP P32449
G	226	SER	GLY	engineered mutation	UNP P32449
H	226	SER	GLY	engineered mutation	UNP P32449

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0
2	G	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 9 1 2	0	0
3	C	1	Total C N O 12 9 1 2	0	0
3	D	1	Total C N O 12 9 1 2	0	0
3	E	1	Total C N O 12 9 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C N O 12 9 1 2	0	0
3	G	1	Total C N O 12 9 1 2	0	0
3	H	1	Total C N O 12 9 1 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	17	Total O 17 17	0	0
4	B	15	Total O 15 15	0	0
4	C	14	Total O 14 14	0	0
4	D	17	Total O 17 17	0	0
4	E	7	Total O 7 7	0	0
4	F	11	Total O 11 11	0	0
4	G	6	Total O 6 6	0	0
4	H	11	Total O 11 11	0	0

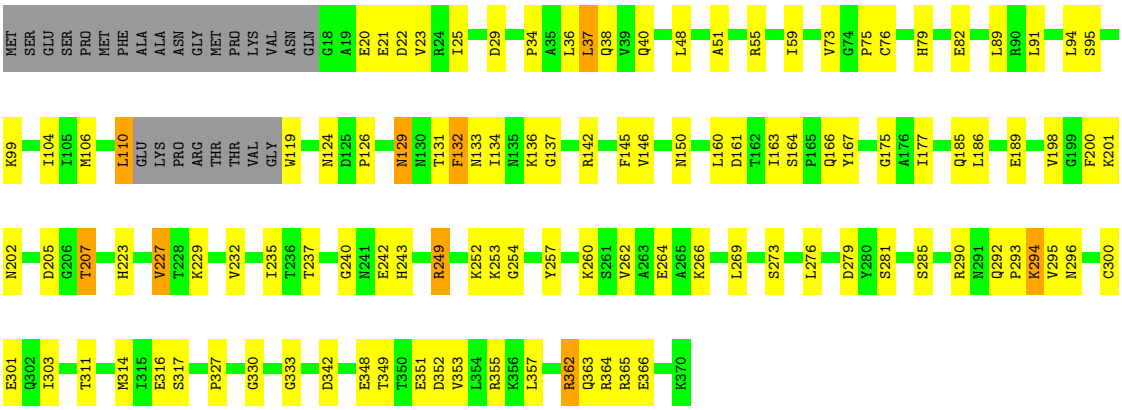
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

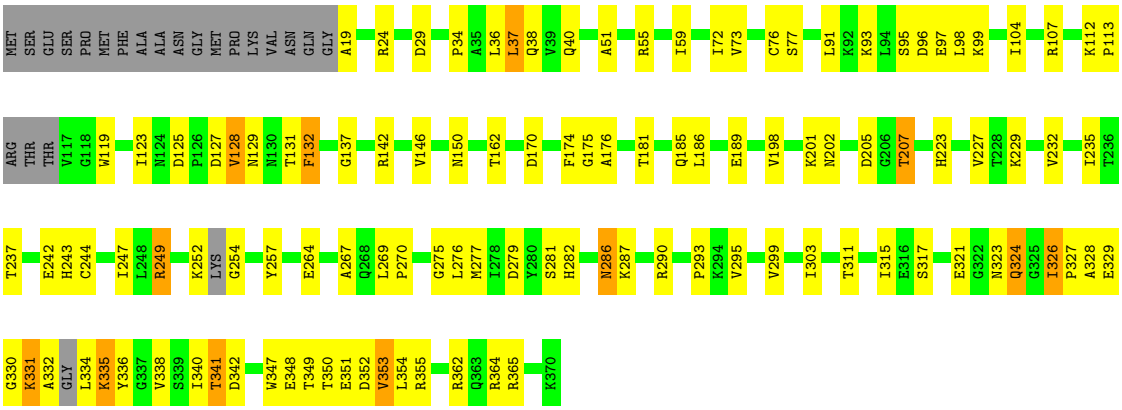
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain A:



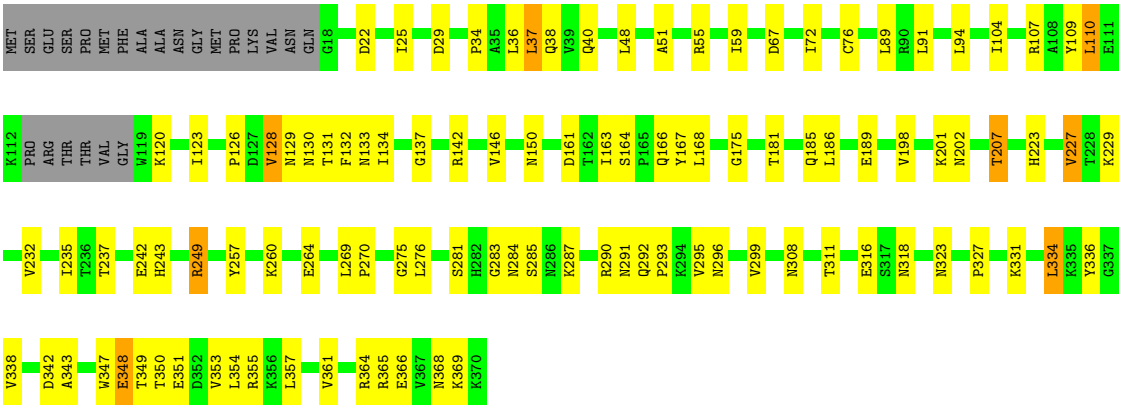
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain B:



• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain C:

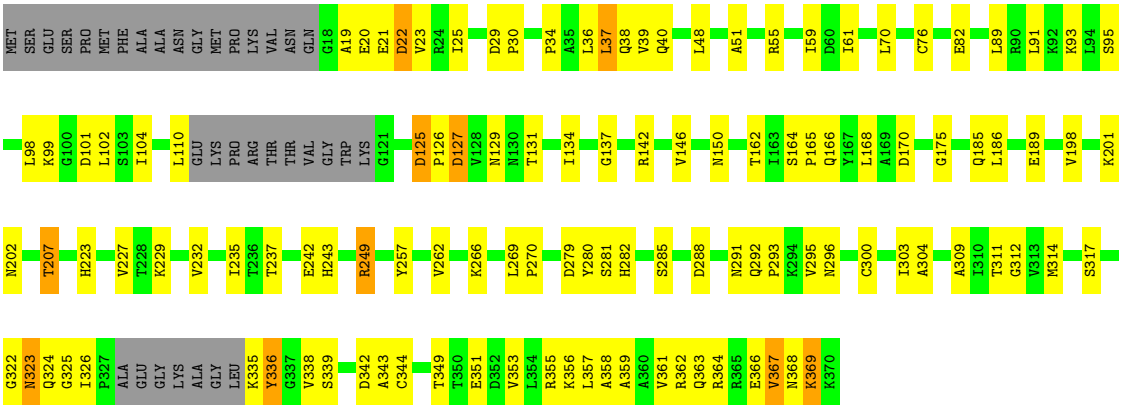


• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain D:

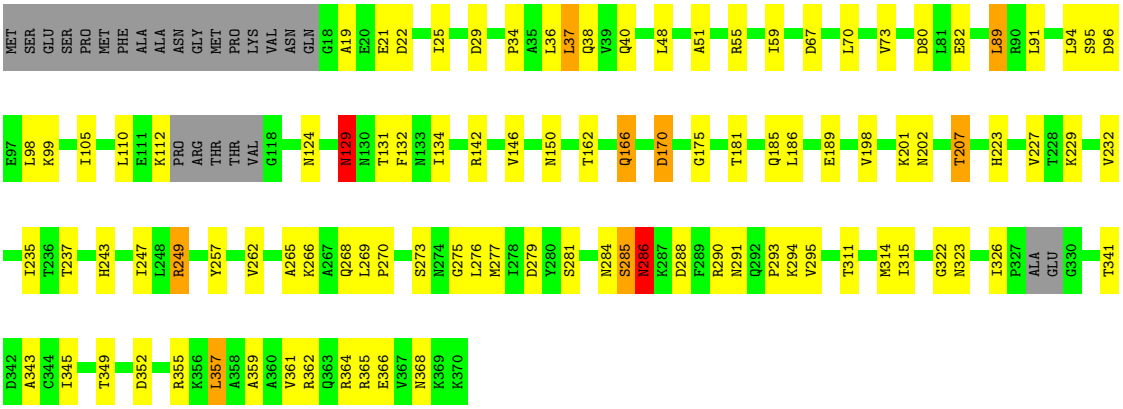
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain E:



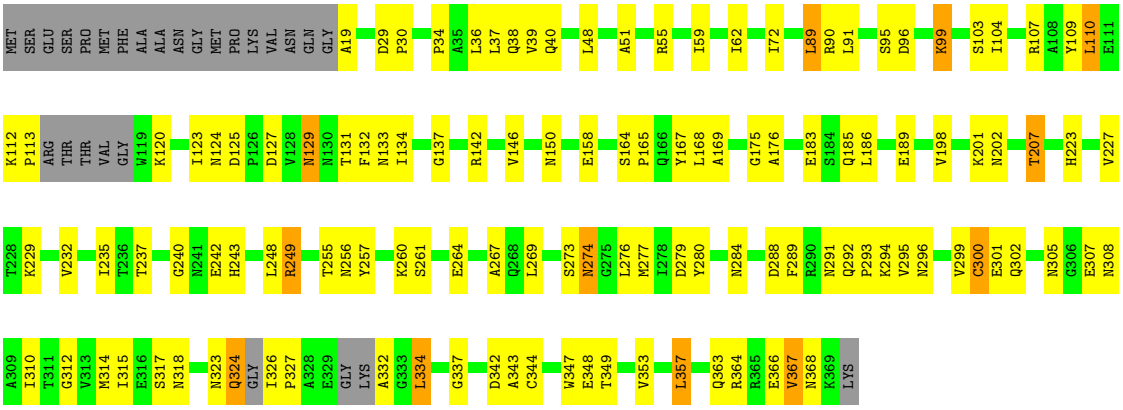
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain F:



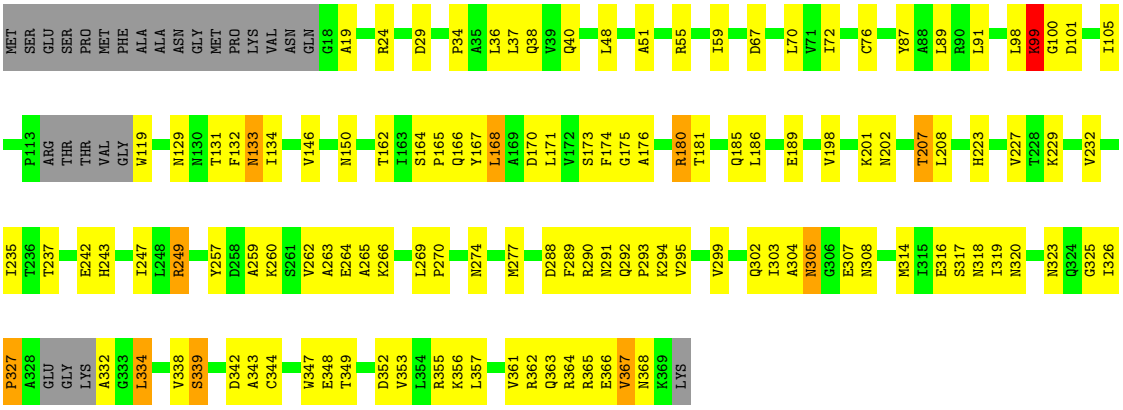
• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain G:



• Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase, tyrosine-inhibited

Chain H:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.15Å 93.97Å 104.84Å 65.39° 85.77° 75.52°	Depositor
Resolution (Å)	29.83 – 2.70	Depositor
% Data completeness (in resolution range)	96.0 (29.83-2.70)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.213 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	20830	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.39	0/2620	0.60	0/3549
1	B	0.41	0/2642	0.62	0/3575
1	C	0.40	0/2639	0.61	0/3572
1	D	0.41	0/2646	0.63	0/3584
1	E	0.37	0/2549	0.60	0/3451
1	F	0.38	0/2627	0.63	0/3555
1	G	0.38	0/2609	0.61	0/3534
1	H	0.38	0/2598	0.60	0/3525
All	All	0.39	0/20930	0.61	0/28345

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

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	2583	0	2571	80	0
1	B	2606	0	2593	86	0
1	C	2602	0	2592	80	0
1	D	2608	0	2585	72	0
1	E	2516	0	2509	107	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2591	0	2581	79	0
1	G	2573	0	2555	114	0
1	H	2561	0	2516	107	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	12	0	8	0	0
3	C	12	0	8	0	0
3	D	12	0	8	0	0
3	E	12	0	8	0	0
3	F	12	0	8	0	0
3	G	12	0	8	1	0
3	H	12	0	8	0	0
4	A	17	0	0	2	0
4	B	15	0	0	2	0
4	C	14	0	0	0	0
4	D	17	0	0	4	0
4	E	7	0	0	2	0
4	F	11	0	0	0	0
4	G	6	0	0	0	0
4	H	11	0	0	3	0
All	All	20830	0	20558	666	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 16.

The worst 5 of 666 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:112:LYS:HG3	1:G:113:PRO:HD2	1.18	1.12
1:G:288:ASP:HB3	1:G:291:ASN:HD22	1.16	1.04
1:C:281:SER:HA	1:C:285:SER:HB2	1.45	0.98
1:E:19:ALA:HB2	1:F:48:LEU:HD13	1.50	0.91
1:G:112:LYS:CG	1:G:113:PRO:HD2	2.00	0.91

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	341/370 (92%)	307 (90%)	29 (8%)	5 (2%)	10 26
1	B	339/370 (92%)	309 (91%)	24 (7%)	6 (2%)	8 21
1	C	343/370 (93%)	317 (92%)	23 (7%)	3 (1%)	17 40
1	D	346/370 (94%)	323 (93%)	17 (5%)	6 (2%)	9 23
1	E	330/370 (89%)	301 (91%)	24 (7%)	5 (2%)	10 26
1	F	340/370 (92%)	313 (92%)	24 (7%)	3 (1%)	17 40
1	G	335/370 (90%)	300 (90%)	28 (8%)	7 (2%)	7 18
1	H	338/370 (91%)	308 (91%)	23 (7%)	7 (2%)	7 18
All	All	2712/2960 (92%)	2478 (91%)	192 (7%)	42 (2%)	10 26

5 of 42 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	LYS
1	D	331	LYS
1	E	22	ASP
1	G	129	ASN
1	H	133	ASN

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	273/299 (91%)	260 (95%)	13 (5%)	25 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	277/299 (93%)	266 (96%)	11 (4%)	31	60
1	C	275/299 (92%)	264 (96%)	11 (4%)	31	60
1	D	274/299 (92%)	260 (95%)	14 (5%)	24	50
1	E	269/299 (90%)	257 (96%)	12 (4%)	27	55
1	F	274/299 (92%)	258 (94%)	16 (6%)	20	43
1	G	273/299 (91%)	261 (96%)	12 (4%)	28	56
1	H	269/299 (90%)	254 (94%)	15 (6%)	21	45
All	All	2184/2392 (91%)	2080 (95%)	104 (5%)	26	53

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	207	THR
1	F	249	ARG
1	H	269	LEU
1	E	249	ARG
1	F	129	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	324	GLN
1	F	274	ASN
1	H	305	ASN
1	E	363	GLN
1	F	129	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	PHE	H	1012	-	11,12,12	0.77	0	14,15,15	0.52	0
3	PHE	A	1012	-	11,12,12	0.80	0	14,15,15	0.62	0
3	PHE	C	1012	-	11,12,12	0.75	0	14,15,15	0.53	0
3	PHE	G	1012	-	11,12,12	0.72	0	14,15,15	0.55	0
3	PHE	F	1012	-	11,12,12	0.76	0	14,15,15	0.57	0
3	PHE	E	1012	-	11,12,12	0.72	0	14,15,15	0.56	0
3	PHE	D	1012	-	11,12,12	0.80	0	14,15,15	0.49	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	PHE	H	1012	-	-	3/8/8/8	0/1/1/1
3	PHE	A	1012	-	-	0/8/8/8	0/1/1/1
3	PHE	C	1012	-	-	0/8/8/8	0/1/1/1
3	PHE	G	1012	-	-	6/8/8/8	0/1/1/1
3	PHE	F	1012	-	-	0/8/8/8	0/1/1/1
3	PHE	E	1012	-	-	2/8/8/8	0/1/1/1
3	PHE	D	1012	-	-	0/8/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1012	PHE	O-C-CA-N
3	G	1012	PHE	OXT-C-CA-N
3	E	1012	PHE	CA-CB-CG-CD1
3	E	1012	PHE	CA-CB-CG-CD2
3	H	1012	PHE	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1012	PHE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.