



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 04:36 PM BST

PDB ID : 4HSO  
Title : Crystal structure of S213G variant DAH7PS from *Neisseria meningitidis*  
Authors : Cross, P.J.; Pietersma, A.L.; Allison, T.M.; Wilson-Coutts, S.M.; Cochrane, F.C.; Parker, E.J.  
Deposited on : 2012-10-30  
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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 : 2.14.4.dev1  
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) : 2.14.4.dev1

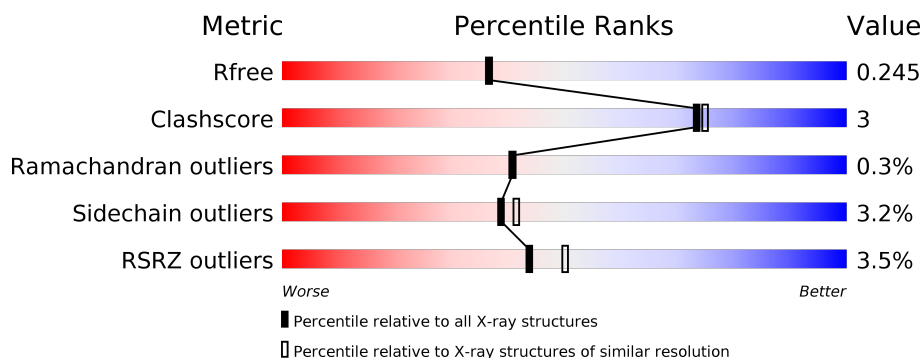
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	351	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>•</div> </div> </div>
1	B	351	<div> <div>4%</div> <div> <div></div> <div>89%</div> <div>9%</div> <div>••</div> </div> </div>
1	C	351	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	D	351	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10871 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.

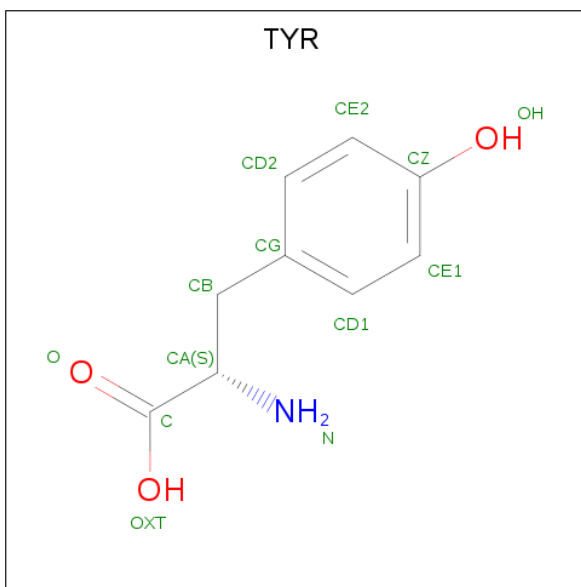
- Molecule 1 is a protein called 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2638	1649	473	502	14			
1	B	343	Total	C	N	O	S	0	1	0
			2597	1625	466	492	14			
1	C	346	Total	C	N	O	S	0	2	0
			2638	1653	472	499	14			
1	D	346	Total	C	N	O	S	0	0	0
			2645	1657	472	502	14			

There are 4 discrepancies between the modelled and reference sequences:

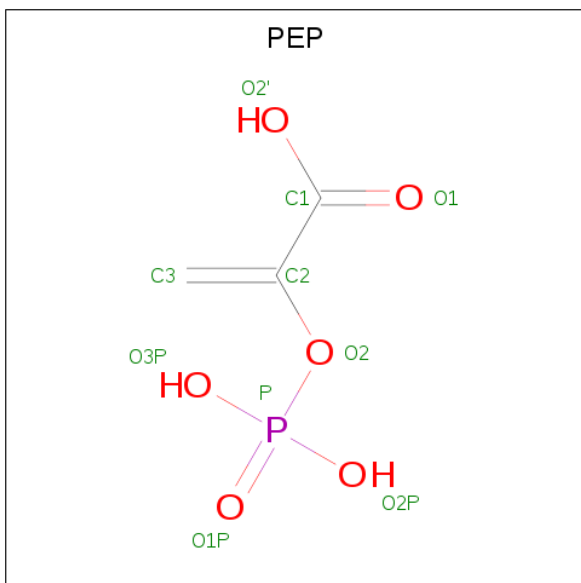
Chain	Residue	Modelled	Actual	Comment	Reference
A	213	GLY	SER	ENGINEERED MUTATION	UNP Q9K169
B	213	GLY	SER	ENGINEERED MUTATION	UNP Q9K169
C	213	GLY	SER	ENGINEERED MUTATION	UNP Q9K169
D	213	GLY	SER	ENGINEERED MUTATION	UNP Q9K169

- Molecule 2 is TYROSINE (three-letter code: TYR) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			13	9	1	3		
2	B	1	Total	C	N	O	0	0
			13	9	1	3		
2	C	1	Total	C	N	O	0	0
			13	9	1	3		
2	D	1	Total	C	N	O	0	0
			13	9	1	3		

- Molecule 3 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula:  $C_3H_5O_6P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			10	3	6	1		
3	B	1	Total	C	O	P	0	0
			10	3	6	1		
3	C	1	Total	C	O	P	0	0
			10	3	6	1		
3	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

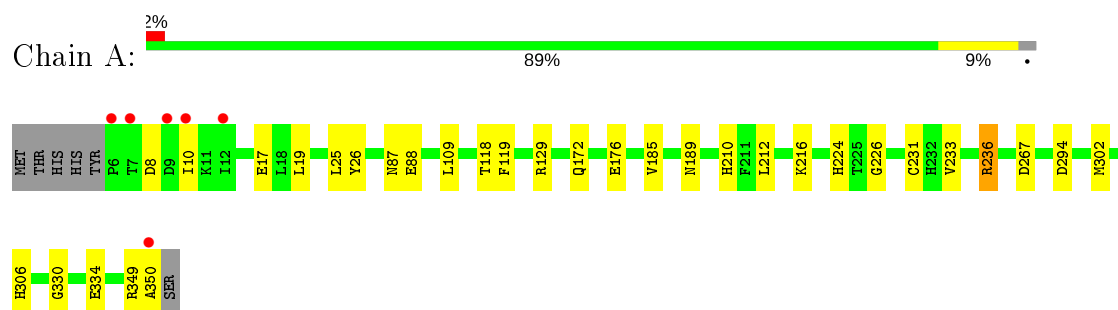
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total	O	0	0
			93	93		
5	B	61	Total	O	0	0
			61	61		
5	C	44	Total	O	0	0
			44	44		
5	D	59	Total	O	0	0
			59	59		

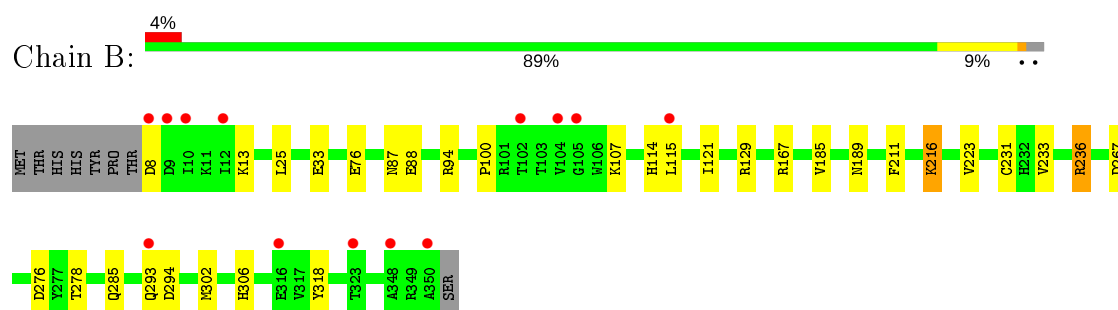
### 3 Residue-property plots [i](#)

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.

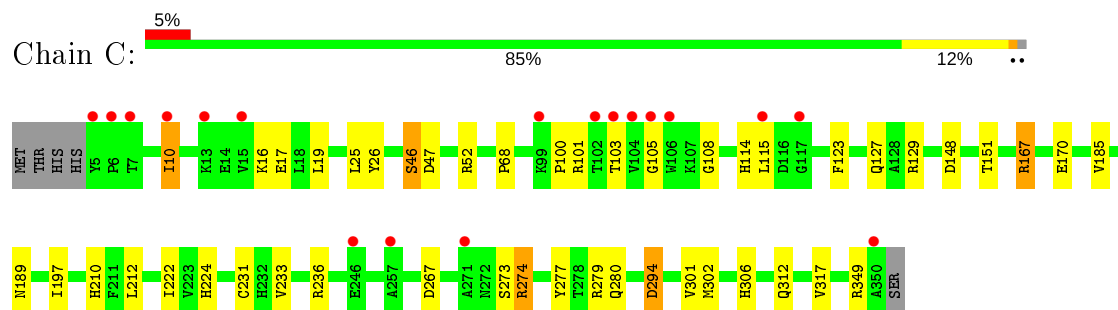
- Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase



- Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase

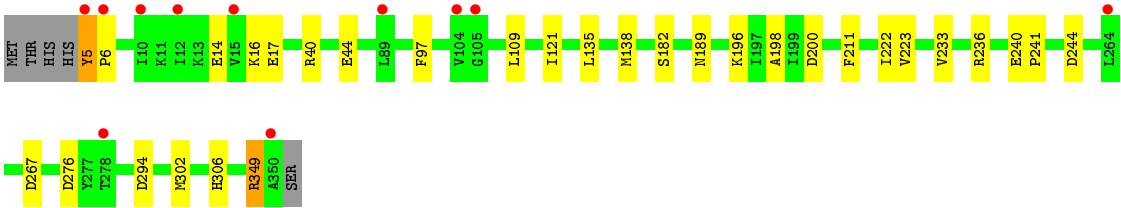


- Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase



- Molecule 1: 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.52Å 137.00Å 76.21Å 90.00° 96.63° 90.00°	Depositor
Resolution (Å)	19.53 – 2.10 19.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.53-2.10) 98.9 (19.52-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.54 (at 2.09Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.204 , 0.242 0.207 , 0.245	Depositor DCC
$R_{free}$ test set	4334 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.047 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10871	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MN, PEP

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	0.85	0/2687	0.82	0/3638
1	B	0.78	0/2645	0.80	2/3584 (0.1%)
1	C	0.83	1/2695 (0.0%)	0.81	0/3653
1	D	0.77	1/2695 (0.0%)	0.79	4/3650 (0.1%)
All	All	0.81	2/10722 (0.0%)	0.80	6/14525 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	241	PRO	N-CD	5.14	1.55	1.47
1	C	46	SER	CB-OG	-5.01	1.35	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	94	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	D	276	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	D	97	PHE	CB-CA-C	-5.22	99.95	110.40
1	D	244	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	240	GLU	C-N-CD	5.08	139.06	128.40
1	B	318	TYR	CA-CB-CG	5.02	122.94	113.40

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	2638	0	2606	17	0
1	B	2597	0	2540	18	0
1	C	2638	0	2591	30	0
1	D	2645	0	2612	16	0
2	A	13	0	8	0	0
2	B	13	0	8	0	0
2	C	13	0	8	0	0
2	D	13	0	8	0	0
3	A	10	0	2	0	0
3	B	10	0	2	0	0
3	C	10	0	2	0	0
3	D	10	0	2	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	93	0	0	0	0
5	B	61	0	0	0	0
5	C	44	0	0	3	0
5	D	59	0	0	0	0
All	All	10871	0	10389	70	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.

All (70) 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:C:101:ARG:O	1:C:167[A]:ARG:NH1	1.91	1.04
1:C:47:ASP:OD1	1:C:52:ARG:NH2	2.06	0.88
1:C:312:GLN:OE1	1:C:317:VAL:HG12	1.86	0.75
1:C:10:ILE:HG22	1:D:182:SER:HA	1.70	0.73
1:C:167[A]:ARG:NH2	5:C:538:HOH:O	2.22	0.72
1:C:101:ARG:HG3	1:C:105:GLY:HA3	1.84	0.58
1:B:87:ASN:HB2	1:B:88:GLU:OE1	2.06	0.56
1:C:100[A]:PRO:HB2	1:C:167[A]:ARG:NH2	2.20	0.56
1:D:5:TYR:HB3	1:D:6:PRO:HD3	1.89	0.55
1:D:349:ARG:CG	1:D:349:ARG:O	2.55	0.54
1:A:87:ASN:HB2	1:A:88:GLU:OE1	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASP:OD2	1:B:278:THR:OG1	2.23	0.54
1:C:274:ARG:HH11	1:C:279:ARG:CB	2.22	0.53
1:C:212:LEU:HD21	1:D:121:ILE:HG21	1.92	0.53
1:B:114:HIS:O	1:B:115:LEU:HB2	2.08	0.52
1:A:210:HIS:CE1	1:A:224:HIS:CD2	2.98	0.52
1:A:216:LYS:HE2	1:B:8:ASP:OD2	2.10	0.52
1:C:101:ARG:HG3	1:C:105:GLY:CA	2.40	0.51
1:D:5:TYR:HB3	1:D:6:PRO:CD	2.41	0.51
1:B:211:PHE:CZ	1:B:223:VAL:CG2	2.94	0.51
1:D:196:LYS:HE3	1:D:200:ASP:OD2	2.10	0.51
1:A:25:LEU:HD23	1:A:129:ARG:CZ	2.41	0.51
1:A:176:GLU:OE2	1:B:107:LYS:NZ	2.34	0.51
1:B:211:PHE:CE2	1:B:223:VAL:CG2	2.94	0.50
1:A:349:ARG:O	1:A:350:ALA:C	2.50	0.49
1:A:8:ASP:OD1	1:B:216:LYS:NZ	2.34	0.49
1:D:267:ASP:HA	1:D:302:MET:HB3	1.95	0.49
1:C:68:PRO:HG3	1:C:127:GLN:HE22	1.78	0.48
1:C:68:PRO:HG3	1:C:127:GLN:NE2	2.29	0.48
1:D:211:PHE:CZ	1:D:223:VAL:HG21	2.48	0.48
1:C:267:ASP:HA	1:C:302:MET:HB3	1.96	0.48
1:C:25:LEU:HD23	1:C:129:ARG:CZ	2.44	0.47
1:A:267:ASP:HA	1:A:302:MET:HB3	1.97	0.47
1:C:16:LYS:HB2	1:D:222:ILE:HB	1.95	0.47
1:B:211:PHE:CE2	1:B:223:VAL:HG21	2.50	0.47
1:C:294:ASP:HA	1:C:349:ARG:NH2	2.29	0.47
1:A:19:LEU:HD11	1:C:26:TYR:CG	2.50	0.46
1:C:170:GLU:HG3	1:C:197:ILE:CG2	2.45	0.46
1:C:108:GLY:C	5:C:543:HOH:O	2.53	0.46
1:A:26:TYR:CG	1:C:19:LEU:HD11	2.51	0.46
1:C:123:PHE:CE1	1:C:127:GLN:HG3	2.50	0.46
1:D:349:ARG:HG3	1:D:349:ARG:O	2.15	0.46
1:C:148:ASP:OD2	1:C:151:THR:HG23	2.16	0.46
1:D:211:PHE:CZ	1:D:223:VAL:CG2	2.98	0.46
1:B:167[A]:ARG:HB2	1:B:167[A]:ARG:HH21	1.81	0.46
1:C:210:HIS:CE1	1:C:224:HIS:CD2	3.05	0.45
1:A:109:LEU:O	1:A:109:LEU:HD23	2.17	0.45
1:A:330:GLY:O	1:A:334:GLU:HG3	2.17	0.45
1:C:273:SER:C	1:C:274:ARG:HG3	2.38	0.44
1:B:267:ASP:HA	1:B:302:MET:HB3	1.99	0.44
1:C:108:GLY:CA	5:C:543:HOH:O	2.66	0.44
1:B:211:PHE:CZ	1:B:223:VAL:HG21	2.54	0.43

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:ARG:HD2	1:D:44:GLU:OE2	2.18	0.43
1:A:212:LEU:HD21	1:B:121:ILE:HG21	2.01	0.43
1:D:211:PHE:CE1	1:D:223:VAL:HG23	2.53	0.42
1:B:185:VAL:O	1:B:231:CYS:HA	2.19	0.42
1:C:185:VAL:O	1:C:231:CYS:HA	2.19	0.42
1:C:114:HIS:O	1:C:115:LEU:HB2	2.19	0.42
1:B:100:PRO:HB2	1:B:167[A]:ARG:CZ	2.49	0.42
1:A:185:VAL:O	1:A:231:CYS:HA	2.20	0.41
1:A:236:ARG:HD3	1:A:236:ARG:C	2.41	0.41
1:A:118:THR:O	1:A:119:PHE:C	2.60	0.41
1:A:226:GLY:HA2	1:B:13:LYS:HE2	2.03	0.41
1:C:222:ILE:HB	1:D:16:LYS:HB2	2.02	0.41
1:B:236:ARG:HD3	1:B:236:ARG:C	2.42	0.41
1:B:25:LEU:HD23	1:B:129:ARG:CZ	2.51	0.41
1:D:135:LEU:O	1:D:138:MET:HG2	2.21	0.40
1:C:277:TYR:O	1:C:280:GLN:HG3	2.21	0.40
1:C:170:GLU:HG3	1:C:197:ILE:HB	2.04	0.40
1:D:198:ALA:HB1	1:D:233:VAL:HG22	2.03	0.40

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	343/351 (98%)	333 (97%)	9 (3%)	1 (0%)	41	41
1	B	342/351 (97%)	334 (98%)	7 (2%)	1 (0%)	41	41
1	C	346/351 (99%)	335 (97%)	10 (3%)	1 (0%)	41	41
1	D	344/351 (98%)	336 (98%)	7 (2%)	1 (0%)	41	41
All	All	1375/1404 (98%)	1338 (97%)	33 (2%)	4 (0%)	41	41

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	B	294	ASP
1	C	294	ASP
1	D	294	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	277/288 (96%)	270 (98%)	7 (2%)	47	52
1	B	267/288 (93%)	258 (97%)	9 (3%)	37	39
1	C	274/288 (95%)	262 (96%)	12 (4%)	28	28
1	D	277/288 (96%)	269 (97%)	8 (3%)	42	46
All	All	1095/1152 (95%)	1059 (97%)	36 (3%)	39	40

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	17	GLU
1	A	172	GLN
1	A	189	ASN
1	A	233	VAL
1	A	236	ARG
1	A	306	HIS
1	B	33	GLU
1	B	76	GLU
1	B	189	ASN
1	B	216	LYS
1	B	233	VAL
1	B	236	ARG
1	B	285	GLN
1	B	293	GLN
1	B	306	HIS
1	C	10	ILE
1	C	17	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	46	SER
1	C	103	THR
1	C	167[A]	ARG
1	C	167[B]	ARG
1	C	189	ASN
1	C	233	VAL
1	C	236	ARG
1	C	274	ARG
1	C	301	VAL
1	C	306	HIS
1	D	5	TYR
1	D	14	GLU
1	D	17	GLU
1	D	109	LEU
1	D	189	ASN
1	D	236	ARG
1	D	306	HIS
1	D	349	ARG

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

Mol	Chain	Res	Type
1	A	224	HIS
1	B	224	HIS
1	C	127	GLN
1	C	224	HIS
1	D	224	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 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	PEP	B	402	-	6,9,9	2.05	2 (33%)	8,13,13	1.24	0
3	PEP	C	402	-	6,9,9	1.48	2 (33%)	8,13,13	2.11	4 (50%)
3	PEP	A	402	-	6,9,9	1.74	2 (33%)	8,13,13	1.69	2 (25%)
2	TYR	C	401	-	10,13,13	1.62	2 (20%)	12,17,17	0.45	0
2	TYR	D	401	-	10,13,13	1.15	1 (10%)	12,17,17	0.34	0
2	TYR	A	401	-	10,13,13	0.98	1 (10%)	12,17,17	0.81	1 (8%)
2	TYR	B	401	-	10,13,13	1.07	0	12,17,17	0.41	0
3	PEP	D	402	4	6,9,9	2.02	2 (33%)	8,13,13	1.83	3 (37%)

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	PEP	B	402	-	-	1/5/9/9	-
3	PEP	C	402	-	-	2/5/9/9	-
3	PEP	A	402	-	-	0/5/9/9	-
2	TYR	C	401	-	-	0/4/8/8	0/1/1/1
2	TYR	D	401	-	-	0/4/8/8	0/1/1/1
2	TYR	A	401	-	-	0/4/8/8	0/1/1/1
2	TYR	B	401	-	-	0/4/8/8	0/1/1/1
3	PEP	D	402	4	-	0/5/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	PEP	P-O2	4.04	1.65	1.59
3	B	402	PEP	P-O2	3.38	1.64	1.59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	PEP	O2-C2	3.28	1.48	1.39
3	A	402	PEP	P-O2	2.77	1.63	1.59
3	D	402	PEP	O2-C2	2.70	1.46	1.39
3	A	402	PEP	O2-C2	2.69	1.46	1.39
2	D	401	TYR	CA-N	2.69	1.53	1.47
2	A	401	TYR	CA-N	2.58	1.52	1.47
3	C	402	PEP	O2-C2	2.53	1.46	1.39
2	C	401	TYR	CB-CG	2.31	1.56	1.51
3	C	402	PEP	P-O2	2.19	1.62	1.59
2	C	401	TYR	CE1-CD1	2.05	1.42	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	PEP	O2-P-O1P	-3.54	96.74	109.32
3	A	402	PEP	O3P-P-O2P	3.42	120.72	107.64
3	D	402	PEP	O3P-P-O2P	3.29	120.21	107.64
3	C	402	PEP	O3P-P-O2	-2.71	97.00	105.25
3	D	402	PEP	O2P-P-O2	-2.68	97.07	105.25
3	C	402	PEP	O3P-P-O1P	2.66	121.11	110.68
2	A	401	TYR	CB-CA-C	-2.52	106.61	110.69
3	C	402	PEP	O3P-P-O2P	2.48	117.10	107.64
3	A	402	PEP	O3P-P-O2	-2.37	98.03	105.25
3	D	402	PEP	O2P-P-O1P	2.31	119.72	110.68

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	PEP	C2-O2-P-O1P
3	B	402	PEP	C2-O2-P-O3P
3	C	402	PEP	C2-O2-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	345/351 (98%)	-0.13	6 (1%) 70 74	23, 32, 48, 69	0
1	B	343/351 (97%)	0.17	13 (3%) 40 46	26, 38, 64, 89	0
1	C	346/351 (98%)	0.16	18 (5%) 27 32	24, 37, 68, 100	0
1	D	346/351 (98%)	0.11	11 (3%) 47 54	27, 39, 54, 84	0
All	All	1380/1404 (98%)	0.08	48 (3%) 44 50	23, 37, 61, 100	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	105	GLY	7.6
1	D	5	TYR	7.1
1	C	5	TYR	6.6
1	B	350	ALA	6.1
1	A	350	ALA	5.9
1	C	350	ALA	5.6
1	B	10	ILE	5.2
1	A	10	ILE	5.2
1	C	10	ILE	4.5
1	C	6	PRO	4.3
1	B	105	GLY	4.3
1	C	103	THR	4.0
1	C	15	VAL	3.9
1	B	12	ILE	3.5
1	D	350	ALA	3.5
1	A	6	PRO	3.4
1	C	102	THR	3.4
1	B	293	GLN	3.3
1	B	102	THR	3.3
1	A	9	ASP	3.1
1	B	104	VAL	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	106	TRP	2.9
1	C	104	VAL	2.8
1	C	271	ALA	2.8
1	D	10	ILE	2.7
1	B	348	ALA	2.7
1	B	316	GLU	2.7
1	C	99	LYS	2.7
1	B	9	ASP	2.7
1	C	257	ALA	2.6
1	D	6	PRO	2.6
1	B	115	LEU	2.6
1	A	12	ILE	2.5
1	D	104	VAL	2.4
1	C	246	GLU	2.4
1	D	264	LEU	2.4
1	C	115	LEU	2.4
1	C	117	GLY	2.3
1	C	7	THR	2.3
1	D	278	THR	2.3
1	B	8	ASP	2.3
1	D	12	ILE	2.3
1	C	13	LYS	2.2
1	A	7	THR	2.2
1	D	105	GLY	2.2
1	D	15	VAL	2.1
1	B	323	THR	2.0
1	D	89	LEU	2.0

## 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 monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	TYR	C	401	13/13	0.87	0.15	42,47,51,53	0
2	TYR	D	401	13/13	0.87	0.14	41,54,58,60	0
2	TYR	A	401	13/13	0.87	0.18	43,51,54,63	0
2	TYR	B	401	13/13	0.87	0.14	43,44,51,52	0
3	PEP	B	402	10/10	0.89	0.22	44,55,65,66	0
3	PEP	C	402	10/10	0.92	0.21	48,64,74,74	0
3	PEP	D	402	10/10	0.94	0.14	35,43,46,51	0
3	PEP	A	402	10/10	0.96	0.14	32,38,42,49	0
4	MN	C	403	1/1	0.96	0.04	45,45,45,45	0
4	MN	B	403	1/1	0.98	0.04	40,40,40,40	0
4	MN	D	403	1/1	0.98	0.06	38,38,38,38	0
4	MN	A	403	1/1	0.99	0.07	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.