



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:54 PM GMT

PDB ID : 5E9Z  
Title : Cytochrome P450 BM3 mutant M11  
Authors : Capoferri, L.; Leth, R.; ter Haar, E.; Mohanty, A.K.; Grootenhuys, D.J.; Vottero, E.; Commandeur, J.N.M.; Vermeulen, N.P.E.; Jorgensen, F.S.; Olsen, L.; Geerke, D.P.  
Deposited on : 2015-10-15  
Resolution : 2.23 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026982  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : rb-20026982

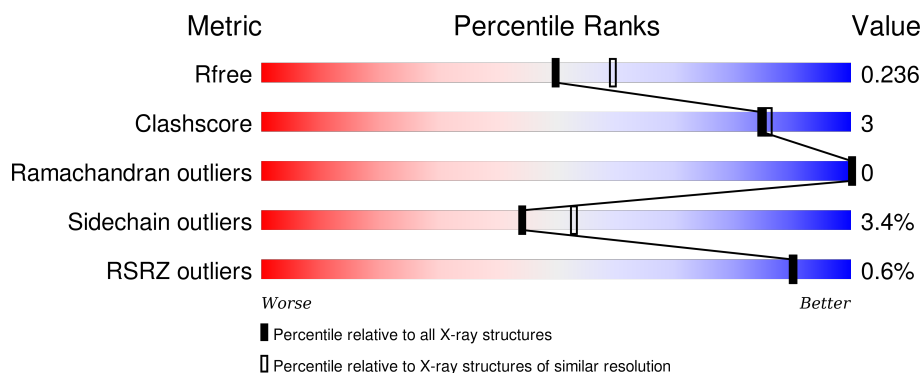
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 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))
$R_{free}$	91344	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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. 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	469	<div> <div>90%</div> <div>6% •</div> </div>
1	B	469	<div> <div>84%</div> <div>11% • •</div> </div>
1	C	469	<div> <div>%</div> <div>88%</div> <div>6% • 5%</div> </div>
1	D	469	<div> <div>%</div> <div>88%</div> <div>5% • 5%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTT	B	501	X	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15704 atoms, of which 133 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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	1	0
			3586	2298	609	661	18			
1	B	451	Total	C	N	O	S	0	1	0
			3574	2287	603	666	18			
1	C	445	Total	C	N	O	S	0	0	0
			3493	2246	586	643	18			
1	D	444	Total	C	N	O	S	0	1	0
			3486	2238	590	641	17			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP P14779
A	47	LEU	ARG	engineered mutation	UNP P14779
A	64	GLY	GLU	engineered mutation	UNP P14779
A	81	ILE	PHE	engineered mutation	UNP P14779
A	87	VAL	PHE	engineered mutation	UNP P14779
A	143	GLY	GLU	engineered mutation	UNP P14779
A	188	GLN	LEU	engineered mutation	UNP P14779
A	198	CYS	TYR	engineered mutation	UNP P14779
A	267	VAL	GLU	engineered mutation	UNP P14779
A	285	TYR	HIS	engineered mutation	UNP P14779
A	415	SER	GLY	engineered mutation	UNP P14779
B	-1	SER	-	expression tag	UNP P14779
B	47	LEU	ARG	engineered mutation	UNP P14779
B	64	GLY	GLU	engineered mutation	UNP P14779
B	81	ILE	PHE	engineered mutation	UNP P14779
B	87	VAL	PHE	engineered mutation	UNP P14779
B	143	GLY	GLU	engineered mutation	UNP P14779
B	188	GLN	LEU	engineered mutation	UNP P14779
B	198	CYS	TYR	engineered mutation	UNP P14779
B	267	VAL	GLU	engineered mutation	UNP P14779
B	285	TYR	HIS	engineered mutation	UNP P14779

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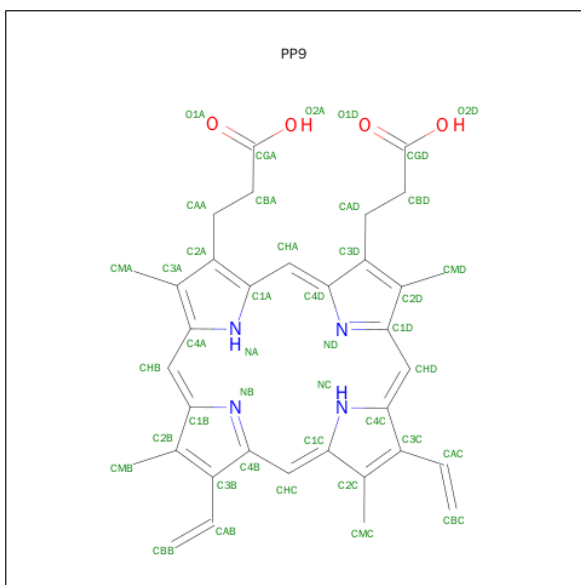
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Chain	Residue	Modelled	Actual	Comment	Reference
B	415	SER	GLY	engineered mutation	UNP P14779
C	-1	SER	-	expression tag	UNP P14779
C	47	LEU	ARG	engineered mutation	UNP P14779
C	64	GLY	GLU	engineered mutation	UNP P14779
C	81	ILE	PHE	engineered mutation	UNP P14779
C	87	VAL	PHE	engineered mutation	UNP P14779
C	143	GLY	GLU	engineered mutation	UNP P14779
C	188	GLN	LEU	engineered mutation	UNP P14779
C	198	CYS	TYR	engineered mutation	UNP P14779
C	267	VAL	GLU	engineered mutation	UNP P14779
C	285	TYR	HIS	engineered mutation	UNP P14779
C	415	SER	GLY	engineered mutation	UNP P14779
D	-1	SER	-	expression tag	UNP P14779
D	47	LEU	ARG	engineered mutation	UNP P14779
D	64	GLY	GLU	engineered mutation	UNP P14779
D	81	ILE	PHE	engineered mutation	UNP P14779
D	87	VAL	PHE	engineered mutation	UNP P14779
D	143	GLY	GLU	engineered mutation	UNP P14779
D	188	GLN	LEU	engineered mutation	UNP P14779
D	198	CYS	TYR	engineered mutation	UNP P14779
D	267	VAL	GLU	engineered mutation	UNP P14779
D	285	TYR	HIS	engineered mutation	UNP P14779
D	415	SER	GLY	engineered mutation	UNP P14779

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

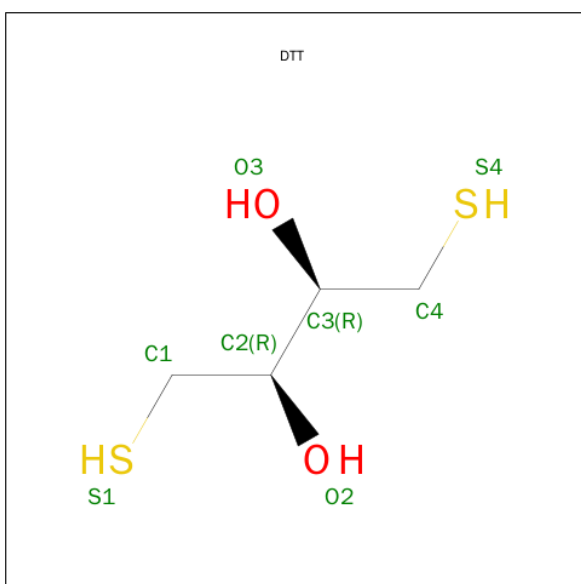
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0

- Molecule 3 is PROTOPORPHYRIN IX (three-letter code: PP9) (formula: C<sub>34</sub>H<sub>34</sub>N<sub>4</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			74	34	32	4	4		
3	B	1	Total	C	H	N	O	0	0
			74	34	32	4	4		
3	C	1	Total	C	H	N	O	0	0
			74	34	32	4	4		
3	D	1	Total	C	H	N	O	0	0
			74	34	32	4	4		

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula:  $C_4H_{10}O_2S_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	H	O	S	0	0
			10	3	5	1	1		

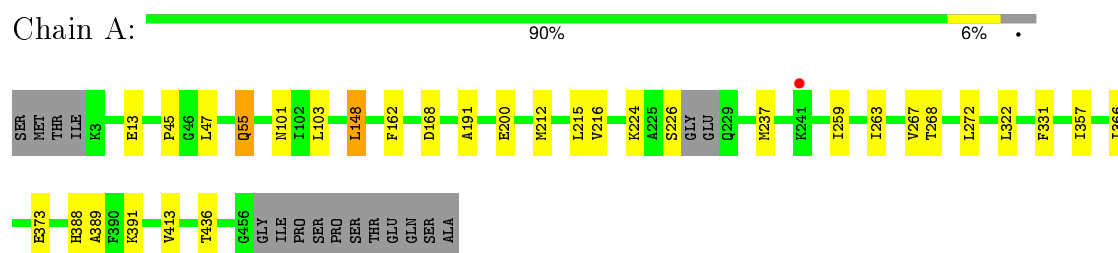
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	367	Total	O	0	0
			367	367		
5	B	326	Total	O	0	0
			326	326		
5	C	281	Total	O	0	0
			281	281		
5	D	281	Total	O	0	0
			281	281		

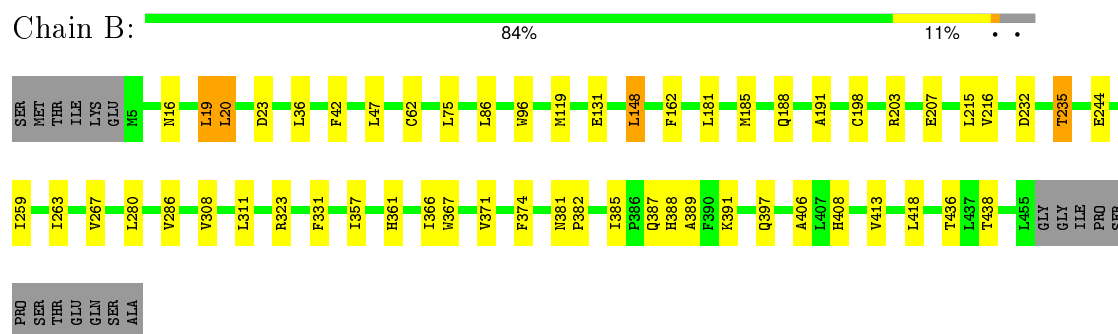
### 3 Residue-property plots

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

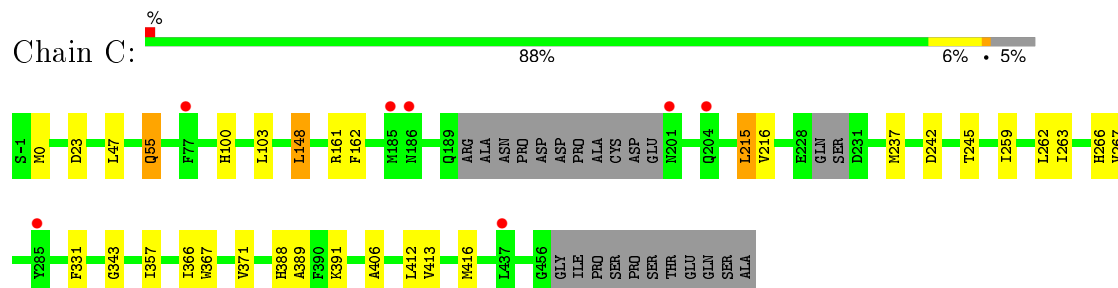
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



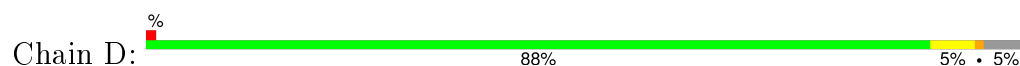
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



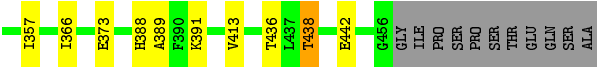
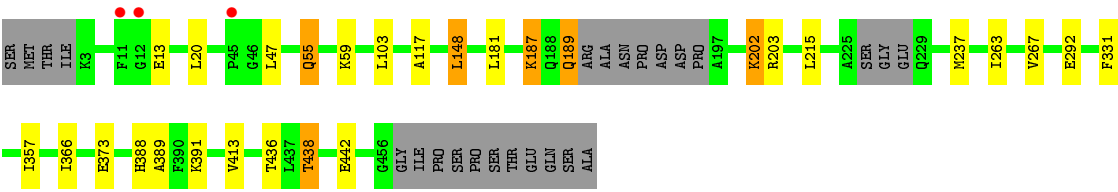
- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	379.12Å 59.72Å 95.59Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	95.12 – 2.23 95.12 – 2.23	Depositor EDS
% Data completeness (in resolution range)	93.3 (95.12-2.23) 93.3 (95.12-2.23)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 2.22Å)	Xtriage
Refinement program	BUSTER-TNT	Depositor
R, $R_{free}$	0.188 , 0.225 0.196 , 0.236	Depositor DCC
$R_{free}$ test set	4824 reflections (5.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.3	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 56.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 97560 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15704	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PP9, FE2, DTT

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	0.47	0/3670	0.64	0/4966
1	B	0.51	0/3659	0.70	0/4958
1	C	0.45	0/3571	0.64	0/4835
1	D	0.46	0/3567	0.65	0/4832
All	All	0.47	0/14467	0.66	0/19591

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	3586	0	3555	16	0
1	B	3574	0	3509	32	0
1	C	3493	0	3439	17	0
1	D	3486	0	3417	13	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	42	32	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	42	32	29	4	0
3	C	42	32	27	2	0
3	D	42	32	27	1	0
4	B	5	5	5	1	0
5	A	367	0	0	0	0
5	B	326	0	0	0	0
5	C	281	0	0	2	0
5	D	281	0	0	1	0
All	All	15571	133	14038	83	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 (83) 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:A:55:GLN:HG2	1:A:366:ILE:HD11	1.57	0.87
1:D:55:GLN:HG2	1:D:366:ILE:HD11	1.59	0.82
1:C:55:GLN:HG2	1:C:366:ILE:HD11	1.61	0.81
1:B:119:MET:HE1	1:B:408:HIS:HD2	1.52	0.74
1:A:388:HIS:HA	1:A:391:LYS:HD3	1.71	0.73
1:C:388:HIS:HA	1:C:391:LYS:HD3	1.70	0.73
1:D:388:HIS:HA	1:D:391:LYS:HD3	1.71	0.72
1:B:216:VAL:HG21	1:B:259:ILE:HG13	1.72	0.72
1:C:262:LEU:O	1:C:266:HIS:HD2	1.74	0.70
1:B:119:MET:HE1	1:B:408:HIS:CD2	2.28	0.68
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.76	0.68
1:B:119:MET:CE	1:B:408:HIS:HD2	2.06	0.68
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.75	0.68
1:B:388:HIS:HA	1:B:391:LYS:HD3	1.75	0.66
3:C:501:PP9:HMB1	3:C:501:PP9:HBB1	1.75	0.66
1:C:216:VAL:HG21	1:C:259:ILE:HG13	1.76	0.66
3:D:501:PP9:HMB1	3:D:501:PP9:HBB1	1.77	0.66
3:B:502:PP9:HMB1	3:B:502:PP9:HBB1	1.77	0.65
1:B:198:CYS:SG	4:B:501:DTT:C3	2.85	0.64
1:C:148:LEU:HD21	1:C:413:VAL:HG21	1.78	0.64
1:D:148:LEU:HD21	1:D:413:VAL:HG21	1.80	0.64
1:A:216:VAL:HG21	1:A:259:ILE:HG13	1.78	0.63
1:D:187:LYS:CE	1:D:202:LYS:HE2	2.29	0.62
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.65	0.61
1:B:232:ASP:H	1:B:235:THR:CG2	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:ASP:H	1:B:235:THR:HG23	1.68	0.59
1:B:267:VAL:HG12	1:B:438:THR:HG21	1.86	0.57
1:C:100:HIS:HD2	5:C:602:HOH:O	1.87	0.57
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.40	0.57
3:A:502:PP9:HMC1	3:A:502:PP9:HBC1	1.86	0.57
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.41	0.55
3:A:502:PP9:HBB1	3:A:502:PP9:HMB1	1.89	0.54
1:B:20:LEU:HD22	1:B:42:PHE:CZ	2.41	0.54
1:A:162:PHE:HE1	1:A:215:LEU:HD21	1.74	0.53
1:D:117:ALA:HB3	5:D:606:HOH:O	2.08	0.53
1:B:96:TRP:CH2	1:B:397:GLN:HG2	2.45	0.52
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.91	0.52
1:A:331:PHE:HD2	1:A:357:ILE:HD11	1.76	0.51
1:C:412:LEU:HG	1:C:416:MET:CE	2.41	0.51
1:C:331:PHE:HD2	1:C:357:ILE:HD11	1.76	0.49
1:B:185:MET:O	1:B:188:GLN:HG2	2.12	0.49
1:D:331:PHE:HD2	1:D:357:ILE:HD11	1.77	0.49
3:B:502:PP9:HBC1	3:B:502:PP9:HMC1	1.94	0.49
1:A:162:PHE:HE1	1:A:215:LEU:HD11	1.78	0.48
1:B:367:TRP:HB2	1:B:371:VAL:HG12	1.95	0.48
1:B:96:TRP:HH2	1:B:397:GLN:HG2	1.78	0.48
1:C:103:LEU:HD21	1:C:237:MET:HG3	1.96	0.48
1:D:187:LYS:NZ	1:D:202:LYS:HE2	2.29	0.48
1:A:191:ALA:HB3	1:B:191:ALA:HB3	1.94	0.47
1:B:308:VAL:HA	1:B:311:LEU:HD12	1.96	0.47
1:A:103:LEU:HD21	1:A:237:MET:HG3	1.95	0.47
1:D:103:LEU:HD21	1:D:237:MET:HG3	1.96	0.47
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.97	0.46
1:C:366:ILE:HG21	1:C:389:ALA:HB1	1.97	0.46
1:A:212:MET:CE	1:A:263:ILE:HD11	2.46	0.46
1:C:367:TRP:HB2	1:C:371:VAL:HG12	1.97	0.46
1:B:280:LEU:HD13	1:B:418:LEU:HD21	1.98	0.45
1:B:263:ILE:O	1:B:267:VAL:HG23	2.17	0.45
1:A:55:GLN:HG2	1:A:366:ILE:CD1	2.40	0.45
1:B:331:PHE:HD1	1:B:357:ILE:HD11	1.82	0.44
1:D:55:GLN:HG2	1:D:366:ILE:CD1	2.41	0.44
1:B:86:LEU:HB3	3:B:502:PP9:HMD1	2.00	0.44
1:C:162:PHE:CE1	1:C:215:LEU:HD21	2.52	0.44
1:B:216:VAL:HG21	1:B:259:ILE:CG1	2.44	0.44
1:C:406:ALA:HB2	3:C:501:PP9:HMC2	2.00	0.43
1:D:366:ILE:HG21	1:D:389:ALA:HB1	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ILE:HG21	1:A:389:ALA:HB1	2.01	0.43
1:B:382:PRO:HA	1:B:385:ILE:HD12	2.01	0.43
1:A:263:ILE:O	1:A:267:VAL:HG23	2.19	0.42
1:C:263:ILE:O	1:C:267:VAL:HG23	2.20	0.42
1:C:242:ASP:HB3	1:C:245:THR:HG22	2.01	0.42
1:B:323:ARG:HG2	1:B:361:HIS:HB3	2.02	0.42
1:B:286:VAL:HG11	1:B:374:PHE:HE2	1.85	0.42
1:B:119:MET:CE	1:B:408:HIS:CD2	2.92	0.42
1:C:0:MET:CE	1:C:343:GLY:HA3	2.50	0.42
1:D:263:ILE:O	1:D:267:VAL:HG23	2.20	0.42
1:D:189:GLN:HE21	1:D:189:GLN:HA	1.85	0.41
1:B:16:ASN:O	1:B:19:LEU:HB2	2.21	0.41
1:C:161:ARG:HD3	5:C:679:HOH:O	2.20	0.41
1:D:436:THR:C	1:D:438:THR:H	2.25	0.40
1:B:406:ALA:HB2	3:B:502:PP9:HMC2	2.04	0.40
1:A:331:PHE:CD2	1:A:357:ILE:HD11	2.56	0.40
1:B:62:CYS:SG	1:B:391:LYS:HE2	2.61	0.40

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	449/469 (96%)	434 (97%)	15 (3%)	0	100	100
1	B	450/469 (96%)	437 (97%)	13 (3%)	0	100	100
1	C	439/469 (94%)	427 (97%)	12 (3%)	0	100	100
1	D	439/469 (94%)	425 (97%)	14 (3%)	0	100	100
All	All	1777/1876 (95%)	1723 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	383/409 (94%)	370 (97%)	13 (3%)	44	53
1	B	380/409 (93%)	364 (96%)	16 (4%)	36	41
1	C	367/409 (90%)	362 (99%)	5 (1%)	74	84
1	D	365/409 (89%)	349 (96%)	16 (4%)	35	39
All	All	1495/1636 (91%)	1445 (97%)	50 (3%)	44	54

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	45	PRO
1	A	47	LEU
1	A	55	GLN
1	A	101	ASN
1	A	148	LEU
1	A	168	ASP
1	A	200	GLU
1	A	224	LYS
1	A	226	SER
1	A	268	THR
1	A	373	GLU
1	A	436	THR
1	B	19	LEU
1	B	20	LEU
1	B	23	ASP
1	B	36	LEU
1	B	47	LEU
1	B	75	LEU
1	B	131	GLU
1	B	148	LEU
1	B	181	LEU
1	B	203	ARG
1	B	207	GLU

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Mol	Chain	Res	Type
1	B	235	THR
1	B	244	GLU
1	B	381	ASN
1	B	387	GLN
1	B	436	THR
1	C	23	ASP
1	C	47	LEU
1	C	55	GLN
1	C	148	LEU
1	C	215	LEU
1	D	13	GLU
1	D	20	LEU
1	D	47	LEU
1	D	55	GLN
1	D	59	LYS
1	D	148	LEU
1	D	181	LEU
1	D	187	LYS
1	D	189	GLN
1	D	202	LYS
1	D	203	ARG
1	D	215	LEU
1	D	292	GLU
1	D	373	GLU
1	D	438	THR
1	D	442	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	138	HIS
1	A	404	GLN
1	B	169	GLN
1	B	201	ASN
1	C	100	HIS
1	C	188	GLN
1	C	266	HIS
1	C	404	GLN
1	D	189	GLN



### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	PP9	A	502	2	39,46,46	1.73	4 (10%)	41,68,68	0.94	4 (9%)
4	DTT	B	501	-	4,4,7	0.23	0	2,4,8	0.24	0
3	PP9	B	502	2	39,46,46	1.56	4 (10%)	41,68,68	1.23	3 (7%)
3	PP9	C	501	2	39,46,46	1.75	5 (12%)	41,68,68	1.16	3 (7%)
3	PP9	D	501	2	39,46,46	1.65	4 (10%)	41,68,68	1.06	3 (7%)

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	PP9	A	502	2	-	0/24/62/62	0/0/5/5
4	DTT	B	501	-	1/1/1/2	0/2/2/8	0/0/0/0
3	PP9	B	502	2	-	0/24/62/62	0/0/5/5
3	PP9	C	501	2	-	0/24/62/62	0/0/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PP9	D	501	2	-	0/24/62/62	0/0/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	PP9	C3C-C2C	-4.33	1.34	1.40
3	D	501	PP9	C3C-C2C	-3.33	1.36	1.40
3	C	501	PP9	C3C-C2C	-3.30	1.36	1.40
3	C	501	PP9	CBC-CAC	-2.12	1.12	1.28
3	A	502	PP9	C3C-C2C	-2.10	1.37	1.40
3	B	502	PP9	C3C-C4C	2.22	1.43	1.40
3	A	502	PP9	C3C-C4C	2.76	1.44	1.40
3	D	501	PP9	C3C-C4C	2.83	1.44	1.40
3	C	501	PP9	C3C-C4C	3.56	1.45	1.40
3	B	502	PP9	CHD-C1D	3.65	1.38	1.35
3	A	502	PP9	CHD-C1D	4.75	1.39	1.35
3	D	501	PP9	CHD-C1D	5.75	1.40	1.35
3	C	501	PP9	CHD-C1D	6.07	1.40	1.35
3	D	501	PP9	CHC-C4B	6.53	1.41	1.35
3	C	501	PP9	CHC-C4B	6.80	1.41	1.35
3	B	502	PP9	CHC-C4B	6.99	1.41	1.35
3	A	502	PP9	CHC-C4B	8.48	1.42	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	PP9	CHC-C4B-NB	-2.88	123.62	128.71
3	B	502	PP9	CHC-C4B-NB	-2.85	123.66	128.71
3	B	502	PP9	CHD-C1D-ND	-2.85	123.66	128.71
3	D	501	PP9	CHC-C4B-NB	-2.82	123.71	128.71
3	C	501	PP9	CHD-C1D-ND	-2.72	123.89	128.71
3	D	501	PP9	CHD-C1D-ND	-2.69	123.94	128.71
3	C	501	PP9	CHC-C4B-NB	-2.67	123.98	128.71
3	A	502	PP9	CHD-C1D-ND	-2.29	124.66	128.71
3	A	502	PP9	C3C-CAC-CBC	2.05	130.51	126.40
3	A	502	PP9	CMC-C2C-C3C	2.19	129.37	125.09
3	D	501	PP9	C3C-CAC-CBC	4.04	134.53	126.40
3	C	501	PP9	C3C-CAC-CBC	4.13	134.69	126.40
3	B	502	PP9	C3C-CAC-CBC	5.46	137.37	126.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	501	DTT	C2

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PP9	2	0
4	B	501	DTT	1	0
3	B	502	PP9	4	0
3	C	501	PP9	2	0
3	D	501	PP9	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 ⓘ

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	452/469 (96%)	-0.37	1 (0%) 95 96	13, 30, 56, 84	0
1	B	451/469 (96%)	-0.39	0 100 100	15, 29, 53, 82	0
1	C	445/469 (94%)	-0.20	7 (1%) 74 76	18, 35, 74, 113	0
1	D	444/469 (94%)	-0.21	3 (0%) 89 89	16, 33, 66, 108	0
All	All	1792/1876 (95%)	-0.29	11 (0%) 90 90	13, 32, 62, 113	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	ASN	4.7
1	D	45	PRO	3.3
1	C	285	TYR	2.5
1	C	437	LEU	2.5
1	C	185	MET	2.4
1	D	11	PHE	2.4
1	A	241	LYS	2.3
1	D	12	GLY	2.2
1	C	204	GLN	2.2
1	C	77	PHE	2.0
1	C	186	ASN	2.0

### 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 carbohydrates 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	DTT	B	501	5/8	0.75	0.33	7.90	45,50,68,69	0
3	PP9	C	501	42/42	0.97	0.12	0.32	13,23,29,33	0
3	PP9	B	502	42/42	0.97	0.11	0.22	11,15,21,24	0
3	PP9	D	501	42/42	0.97	0.11	0.00	12,21,27,35	0
3	PP9	A	502	42/42	0.97	0.10	-0.11	10,17,24,29	0
2	FE2	D	502	1/1	1.00	0.13	-	20,20,20,20	0
2	FE2	B	503	1/1	1.00	0.15	-	21,21,21,21	0
2	FE2	A	501	1/1	1.00	0.13	-	16,16,16,16	0
2	FE2	C	502	1/1	1.00	0.13	-	22,22,22,22	0

## 6.5 Other polymers

There are no such residues in this entry.