



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 06:05 PM GMT

PDB ID : 2HS6  
Title : Crystal structure of the E291K mutant of 12-oxophytodienoate reductase 3 (OPR3) from tomato  
Authors : Breithaupt, C.; Clausen, T.; Huber, R.  
Deposited on : 2006-07-21  
Resolution : 1.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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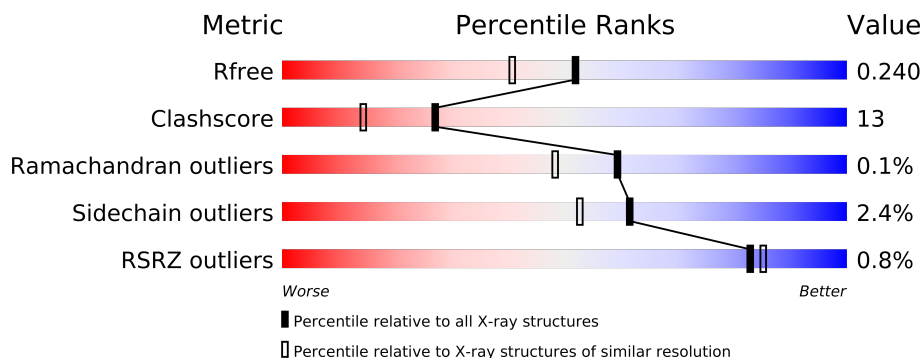
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.90 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))
$R_{free}$	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	402	
1	B	402	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MES	A	3158	-	X
3	MES	B	3158	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6128 atoms, of which 0 are hydrogen and 0 are deuterium.

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 12-oxophytodienoate reductase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2809	1786	500	512	11			
1	B	362	Total	C	N	O	S	0	0	0
			2809	1786	500	512	11			

There are 12 discrepancies between the modelled and reference sequences:

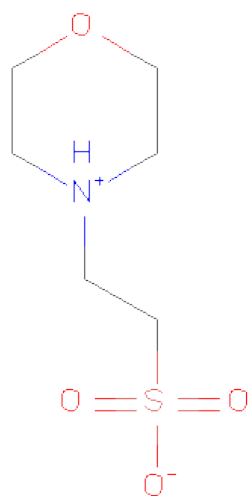
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q9FEW9
A	-4	HIS	-	EXPRESSION TAG	UNP Q9FEW9
A	-3	HIS	-	EXPRESSION TAG	UNP Q9FEW9
A	-2	HIS	-	EXPRESSION TAG	UNP Q9FEW9
A	-1	HIS	-	EXPRESSION TAG	UNP Q9FEW9
A	0	HIS	-	EXPRESSION TAG	UNP Q9FEW9
B	-5	HIS	-	EXPRESSION TAG	UNP Q9FEW9
B	-4	HIS	-	EXPRESSION TAG	UNP Q9FEW9
B	-3	HIS	-	EXPRESSION TAG	UNP Q9FEW9
B	-2	HIS	-	EXPRESSION TAG	UNP Q9FEW9
B	-1	HIS	-	EXPRESSION TAG	UNP Q9FEW9
B	0	HIS	-	EXPRESSION TAG	UNP Q9FEW9

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
2	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		
4	B	192	Total	O	0	0
			192	192		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.18Å 92.24Å 90.09Å 90.00° 99.44° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 16.77 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-1.90) 92.5 (16.77-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.70 (at 1.90Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.205 , 0.235 0.211 , 0.240	Depositor DCC
$R_{free}$ test set	2922 reflections (5.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	19.4	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.45 , 45.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	3 of 57735 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6128	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.33	0/2874	0.59	0/3901
1	B	0.34	0/2874	0.58	0/3901
All	All	0.34	0/5748	0.58	0/7802

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2809	0	2784	82	0
1	B	2809	0	2784	65	0
2	A	31	0	19	2	0
2	B	31	0	19	3	0
3	A	12	0	13	5	0
3	B	12	0	13	2	0
4	A	232	0	0	6	0
4	B	192	0	0	6	0
All	All	6128	0	5632	147	0



Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (147) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:348:ASN:HD21	1:B:362:ASN:H	1.07	1.02
1:A:106:GLN:HE22	2:A:401:FMN:HN3	1.10	0.93
1:A:348:ASN:HD21	1:A:362:ASN:H	1.20	0.88
1:B:106:GLN:HE22	2:B:401:FMN:HN3	1.20	0.87
1:A:211:LEU:HD11	1:A:258:ALA:CB	2.09	0.81
1:B:365:ASN:HB2	4:B:3327:HOH:O	1.82	0.80
1:B:132:PRO:HB3	1:B:151:LYS:HA	1.65	0.79
1:A:211:LEU:HD11	1:A:258:ALA:HB1	1.67	0.76
1:A:159:GLU:HA	1:A:162:GLN:HE21	1.51	0.76
1:A:138:ARG:NH1	1:A:148:ILE:HD12	2.04	0.73
1:B:354:ARG:HH22	1:B:362:ASN:HD21	1.38	0.69
1:A:280:THR:HG21	4:A:3290:HOH:O	1.93	0.67
1:A:20:LYS:HE3	1:A:233:ARG:NH1	2.10	0.67
1:A:10:ASN:C	1:A:10:ASN:HD22	1.98	0.66
1:B:187:ALA:HB1	1:B:239:SER:OG	1.95	0.66
1:A:10:ASN:HD22	1:A:11:PRO:N	1.94	0.65
1:B:169:ARG:HG3	4:B:3236:HOH:O	1.96	0.65
1:A:13:PHE:CZ	1:A:356:LYS:HB2	2.31	0.65
1:B:157:THR:HG21	1:B:206:GLU:OE1	1.96	0.65
1:A:242:ILE:HD11	1:A:280:THR:HG22	1.79	0.63
1:A:187:ALA:HB1	1:A:239:SER:OG	1.99	0.63
1:B:317:ILE:HG12	1:B:338:LEU:HB2	1.80	0.62
1:A:188:HIS:HB3	3:A:3158:MES:H32	1.82	0.61
1:A:11:PRO:HD2	1:A:328:ILE:HG23	1.83	0.61
1:B:348:ASN:ND2	1:B:362:ASN:H	1.91	0.61
1:A:132:PRO:HB3	1:A:151:LYS:HA	1.82	0.60
1:A:10:ASN:ND2	1:A:12:LEU:H	2.00	0.60
1:A:211:LEU:C	1:A:211:LEU:HD13	2.22	0.59
1:B:19:GLY:HA3	4:B:3311:HOH:O	2.02	0.59
1:B:97:HIS:HD2	4:B:3322:HOH:O	1.86	0.58
1:B:14:SER:HB3	1:B:26:ARG:HE	1.68	0.58
1:B:97:HIS:HE1	1:B:180:ASP:OD2	1.87	0.57
1:B:348:ASN:HD21	1:B:362:ASN:N	1.90	0.57
1:A:97:HIS:HE1	1:A:180:ASP:OD2	1.88	0.57
1:A:19:GLY:HA3	4:A:3327:HOH:O	2.05	0.56
1:A:354:ARG:HH22	1:A:362:ASN:HD21	1.53	0.56
1:A:82:THR:OG1	1:A:85:GLN:HG3	2.06	0.56
1:A:135:ASN:HD22	1:A:135:ASN:C	2.09	0.56
1:A:267:GLN:HE21	1:A:274:LEU:H	1.53	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:GLU:HG3	1:A:169:ARG:NH1	2.20	0.55
1:B:160:ILE:O	1:B:164:VAL:HG23	2.07	0.55
1:B:258:ALA:O	1:B:262:ARG:HG2	2.07	0.54
1:A:188:HIS:CG	3:A:3158:MES:H32	2.41	0.54
1:A:20:LYS:HE3	1:A:233:ARG:HH12	1.72	0.53
1:A:244:HIS:CE1	1:A:245:LEU:HG	2.43	0.53
1:A:263:LEU:O	1:A:267:GLN:HG3	2.08	0.53
1:B:319:SER:HB2	1:B:340:SER:OG	2.09	0.53
1:A:183:GLU:OE2	1:A:278:HIS:HD2	1.92	0.53
1:A:203:ARG:HB2	1:A:208:GLY:HA3	1.91	0.52
1:B:216:LYS:HD3	4:B:3308:HOH:O	2.08	0.52
1:A:244:HIS:ND1	3:A:3158:MES:H31	2.24	0.52
1:A:91:LYS:O	1:A:95:VAL:HG23	2.10	0.52
1:B:267:GLN:HE21	1:B:274:LEU:H	1.57	0.52
1:B:354:ARG:HH22	1:B:362:ASN:ND2	2.06	0.52
1:B:10:ASN:HD22	1:B:10:ASN:C	2.13	0.52
1:A:206:GLU:HG2	4:A:3312:HOH:O	2.09	0.52
1:A:48:GLU:O	1:A:52:GLN:HG3	2.10	0.52
1:A:267:GLN:NE2	1:A:274:LEU:H	2.07	0.51
1:B:212:ALA:HA	1:B:262:ARG:HH21	1.75	0.51
1:B:10:ASN:ND2	1:B:12:LEU:H	2.09	0.51
1:A:265:LYS:HG2	1:A:269:HIS:CD2	2.46	0.51
1:B:71:SER:HB2	1:B:109:HIS:HA	1.93	0.50
1:B:13:PHE:CZ	1:B:356:LYS:HB2	2.47	0.50
1:B:354:ARG:HG2	1:B:384:LEU:HD11	1.93	0.50
1:A:20:LYS:CE	1:A:233:ARG:NH1	2.74	0.50
1:B:115:HIS:CE1	1:B:116:GLU:HG2	2.47	0.50
1:B:183:GLU:OE2	1:B:278:HIS:HD2	1.93	0.50
1:A:211:LEU:O	1:A:211:LEU:HD13	2.11	0.50
1:A:306:ARG:NH1	1:A:335:ASP:OD1	2.44	0.50
1:B:237:ARG:HA	1:B:278:HIS:O	2.12	0.49
1:A:187:ALA:HB2	1:A:238:VAL:HA	1.95	0.49
1:B:244:HIS:ND1	1:B:245:LEU:HG	2.26	0.49
1:B:244:HIS:CE1	1:B:245:LEU:HG	2.48	0.49
1:B:11:PRO:HD2	1:B:328:ILE:HG23	1.94	0.49
1:B:53:ARG:HG3	1:B:53:ARG:HH11	1.78	0.48
1:A:135:ASN:HD22	1:A:136:ARG:N	2.11	0.48
1:A:319:SER:HB2	1:A:340:SER:OG	2.13	0.48
1:B:253:LEU:HD13	1:B:304:LEU:HG	1.94	0.48
1:B:32:MET:HA	2:B:401:FMN:N5	2.28	0.48
1:A:17:LYS:HE3	1:A:22:ASN:OD1	2.14	0.48
1:A:32:MET:HA	2:A:401:FMN:N5	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:ASN:ND2	1:A:10:ASN:C	2.66	0.48
1:B:267:GLN:NE2	1:B:274:LEU:H	2.11	0.47
1:A:237:ARG:HA	1:A:278:HIS:O	2.13	0.47
1:B:239:SER:HB3	1:B:280:THR:OG1	2.14	0.47
1:A:244:HIS:CE1	3:A:3158:MES:H31	2.50	0.47
1:B:188:HIS:CG	3:B:3158:MES:H32	2.50	0.47
1:B:350:ASP:O	1:B:354:ARG:HG3	2.14	0.47
1:A:97:HIS:HD2	4:A:3216:HOH:O	1.97	0.47
1:A:347:SER:HA	1:A:381:TYR:CG	2.50	0.47
1:A:182:ILE:C	1:A:182:ILE:HD12	2.36	0.47
1:A:212:ALA:HA	1:A:262:ARG:NH2	2.29	0.46
1:B:329:GLU:HG3	1:B:333:GLN:CD	2.35	0.46
1:A:275:ALA:O	1:A:276:TYR:HB3	2.15	0.46
1:B:347:SER:HB3	1:B:364:TYR:HB3	1.96	0.46
1:B:275:ALA:O	1:B:276:TYR:HB3	2.16	0.46
1:B:263:LEU:O	1:B:267:GLN:HG3	2.15	0.46
1:A:92:ILE:O	1:A:96:VAL:HG23	2.16	0.46
1:A:366:ARG:HD3	4:A:3372:HOH:O	2.15	0.46
1:A:188:HIS:CB	3:A:3158:MES:H32	2.46	0.45
1:A:324:ARG:HD3	1:A:358:ASN:OD1	2.15	0.45
1:A:83:LYS:HD3	1:A:83:LYS:HA	1.80	0.45
1:B:329:GLU:O	1:B:333:GLN:HG3	2.16	0.45
1:A:347:SER:HB3	1:A:364:TYR:HB3	1.98	0.44
1:A:216:LYS:HB2	1:A:216:LYS:HE3	1.83	0.44
1:A:31:PRO:HB3	1:A:61:ILE:HG22	1.99	0.44
1:A:160:ILE:O	1:A:164:VAL:HG23	2.18	0.44
1:A:317:ILE:HG12	1:A:338:LEU:HB2	2.00	0.44
1:B:203:ARG:HB2	1:B:208:GLY:HA3	2.00	0.44
1:A:211:LEU:CD1	1:A:258:ALA:HB1	2.44	0.43
1:A:242:ILE:CD1	1:A:280:THR:HG22	2.45	0.43
1:A:20:LYS:NZ	1:A:232:ASP:OD1	2.48	0.43
1:B:116:GLU:H	1:B:116:GLU:CD	2.22	0.43
1:B:139:ILE:HB	1:B:149:TYR:CE2	2.53	0.43
1:B:64:GLY:HA2	1:B:106:GLN:HE21	1.83	0.43
1:B:354:ARG:NH2	1:B:362:ASN:ND2	2.67	0.43
1:B:53:ARG:HG2	1:B:349:PRO:HA	2.01	0.43
1:A:40:ASN:HA	1:A:77:VAL:O	2.19	0.43
1:B:187:ALA:HB2	1:B:238:VAL:HA	2.00	0.43
1:B:148:ILE:HD12	4:B:3197:HOH:O	2.19	0.43
1:B:53:ARG:HG3	1:B:53:ARG:NH1	2.34	0.43
1:A:10:ASN:HD22	1:A:11:PRO:CD	2.32	0.42
1:B:370:TYR:CZ	2:B:401:FMN:HM72	2.53	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:10:ASN:HA	1:A:11:PRO:HD3	1.89	0.42
1:B:198:ASP:OD1	1:B:249:ASP:HA	2.19	0.42
1:A:363:LYS:N	1:A:363:LYS:HD2	2.34	0.42
1:B:188:HIS:HB3	3:B:3158:MES:H32	2.00	0.42
1:B:130:GLU:O	1:B:151:LYS:HG3	2.19	0.42
1:A:384:LEU:O	1:A:385:GLN:C	2.58	0.42
1:B:216:LYS:O	1:B:220:GLN:HG3	2.20	0.42
1:A:366:ARG:HA	1:A:369:PHE:CD1	2.55	0.42
1:B:156:GLY:O	1:B:160:ILE:HG13	2.20	0.41
1:A:21:PHE:CZ	1:A:180:ASP:HB3	2.55	0.41
1:A:304:LEU:HD23	1:A:304:LEU:O	2.20	0.41
1:B:80:ILE:HD11	1:B:174:ALA:HA	2.02	0.41
1:A:62:THR:HG22	1:A:103:ILE:HD11	2.01	0.41
1:B:48:GLU:O	1:B:52:GLN:HG3	2.20	0.41
1:B:325:GLU:CD	1:B:325:GLU:H	2.24	0.41
1:A:216:LYS:O	1:A:220:GLN:HG3	2.21	0.40
1:B:206:GLU:HB2	1:B:216:LYS:NZ	2.36	0.40
1:A:278:HIS:HE1	1:A:319:SER:HB2	1.86	0.40
1:A:71:SER:HB2	1:A:109:HIS:HA	2.03	0.40
1:B:92:ILE:O	1:B:96:VAL:HG23	2.20	0.40
1:A:53:ARG:HG2	1:A:349:PRO:HA	2.03	0.40
1:A:130:GLU:HG3	4:A:3343:HOH:O	2.20	0.40
1:A:258:ALA:O	1:A:262:ARG:HG2	2.21	0.40
1:A:301:GLU:OE1	1:A:301:GLU:HA	2.22	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	358/402 (89%)	347 (97%)	11 (3%)	0	100	100
1	B	358/402 (89%)	348 (97%)	9 (2%)	1 (0%)	50	37
All	All	716/804 (89%)	695 (97%)	20 (3%)	1 (0%)	59	48

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	80	ILE

### 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	294/328 (90%)	287 (98%)	7 (2%)	61	53
1	B	294/328 (90%)	287 (98%)	7 (2%)	61	53
All	All	588/656 (90%)	574 (98%)	14 (2%)	61	53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	51	GLU
1	A	135	ASN
1	A	278	HIS
1	A	309	ARG
1	A	345	PHE
1	A	363	LYS
1	B	10	ASN
1	B	22	ASN
1	B	48	GLU
1	B	261	GLU
1	B	278	HIS
1	B	309	ARG
1	B	345	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	43	GLN
1	A	97	HIS
1	A	106	GLN

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Mol	Chain	Res	Type
1	A	135	ASN
1	A	146	HIS
1	A	162	GLN
1	A	267	GLN
1	A	278	HIS
1	A	348	ASN
1	A	362	ASN
1	B	10	ASN
1	B	43	GLN
1	B	97	HIS
1	B	106	GLN
1	B	162	GLN
1	B	251	ASN
1	B	267	GLN
1	B	269	HIS
1	B	278	HIS
1	B	348	ASN
1	B	362	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MES	A	3158	-	12,12,12	2.34	6 (50%)	16,16,16	3.93	9 (56%)
2	FMN	A	401	-	33,33,33	1.83	7 (21%)	46,50,50	1.97	7 (15%)
3	MES	B	3158	-	12,12,12	2.46	5 (41%)	16,16,16	4.35	11 (68%)
2	FMN	B	401	-	33,33,33	1.77	7 (21%)	46,50,50	1.92	9 (19%)

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	MES	A	3158	-	-	0/6/14/14	0/1/1/1
2	FMN	A	401	-	-	0/18/18/18	0/0/3/3
3	MES	B	3158	-	-	0/6/14/14	0/1/1/1
2	FMN	B	401	-	-	0/18/18/18	0/0/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	3158	MES	O2S-S	6.08	1.59	1.45
3	A	3158	MES	O2S-S	5.66	1.58	1.45
2	B	401	FMN	C4A-C10	4.89	1.49	1.40
2	A	401	FMN	C4A-C10	4.83	1.49	1.40
2	A	401	FMN	C6-C5A	4.50	1.47	1.41
2	B	401	FMN	C6-C5A	4.01	1.46	1.41
2	B	401	FMN	C4-C4A	3.82	1.47	1.41
2	A	401	FMN	C4-C4A	3.65	1.47	1.41
2	A	401	FMN	C2-N3	3.54	1.44	1.37
2	B	401	FMN	C2-N3	3.24	1.43	1.37
3	B	3158	MES	C8-S	3.12	1.83	1.78
2	A	401	FMN	C9A-N10	2.89	1.43	1.38
2	A	401	FMN	C1'-C2'	2.80	1.54	1.51
3	A	3158	MES	C3-C2	2.65	1.57	1.51
3	A	3158	MES	C8-S	2.49	1.82	1.78
2	A	401	FMN	C8-C7	2.46	1.48	1.40
3	B	3158	MES	C3-C2	2.43	1.56	1.51
2	B	401	FMN	C8-C7	2.43	1.47	1.40
2	B	401	FMN	C9A-N10	2.38	1.42	1.38
3	A	3158	MES	O3S-S	-2.37	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3158	MES	O1S-S	2.29	1.50	1.45
3	B	3158	MES	O3S-S	-2.22	1.40	1.45
3	B	3158	MES	O1S-S	2.09	1.50	1.45
2	B	401	FMN	C1'-C2'	2.07	1.53	1.51
3	A	3158	MES	C3-N4	2.02	1.54	1.49

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3158	MES	O3S-S-O1S	8.76	135.01	112.48
3	A	3158	MES	O3S-S-O1S	8.41	134.12	112.48
2	A	401	FMN	C4A-C10-N10	-7.81	116.61	120.51
3	B	3158	MES	O2S-S-C8	-7.16	84.28	106.36
2	B	401	FMN	C4A-C10-N10	-7.04	116.99	120.51
3	A	3158	MES	O2S-S-C8	-6.26	87.06	106.36
3	B	3158	MES	C6-C5-N4	6.17	117.87	109.96
3	A	3158	MES	C7-N4-C5	-5.98	96.01	111.66
3	B	3158	MES	C8-C7-N4	-5.79	102.54	112.44
2	B	401	FMN	C2-N1-C10	5.77	120.79	114.98
3	A	3158	MES	C8-C7-N4	-5.53	102.98	112.44
3	B	3158	MES	C7-N4-C5	-5.40	97.53	111.66
3	A	3158	MES	C5-N4-C3	5.34	120.35	109.75
2	A	401	FMN	C2-N1-C10	5.21	120.23	114.98
2	A	401	FMN	C2'-C1'-N10	-4.53	106.45	112.45
3	B	3158	MES	C7-C8-S	4.09	123.63	112.49
3	A	3158	MES	C6-C5-N4	3.67	114.67	109.96
2	B	401	FMN	P-O5'-C5'	3.59	128.58	118.19
3	B	3158	MES	C5-N4-C3	3.58	116.85	109.75
2	B	401	FMN	C2'-C1'-N10	-3.53	107.77	112.45
3	B	3158	MES	C2-C3-N4	-3.46	105.52	109.96
3	B	3158	MES	O1-C6-C5	3.45	115.45	111.34
3	B	3158	MES	O3S-S-O2S	-2.93	104.94	112.48
2	A	401	FMN	P-O5'-C5'	2.89	126.53	118.19
3	A	3158	MES	C2-C3-N4	-2.80	106.36	109.96
2	A	401	FMN	C1'-C2'-C3'	2.73	117.61	109.82
2	B	401	FMN	C1'-C2'-C3'	2.50	116.97	109.82
2	A	401	FMN	O2'-C2'-C3'	-2.49	102.85	109.05
3	A	3158	MES	C7-C8-S	2.41	119.05	112.49
3	A	3158	MES	O3S-S-O2S	-2.40	106.31	112.48
3	B	3158	MES	O1S-S-C8	-2.27	99.37	106.36
2	A	401	FMN	C4A-N5-C5A	2.24	119.21	116.69
2	B	401	FMN	C5'-C4'-C3'	-2.22	107.88	112.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	FMN	O2'-C2'-C3'	-2.21	103.54	109.05
2	B	401	FMN	C4A-N5-C5A	2.01	118.95	116.69
2	B	401	FMN	C8-C9-C9A	2.00	123.85	119.81

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	362/402 (90%)	-0.04	3 (0%) 83 85	12, 18, 29, 42	0
1	B	362/402 (90%)	-0.01	3 (0%) 83 85	13, 20, 29, 45	0
All	All	724/804 (90%)	-0.03	6 (0%) 83 85	12, 19, 29, 45	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	269	HIS	3.9
1	A	385	GLN	3.8
1	B	385	GLN	3.5
1	B	243	ASP	2.4
1	A	243	ASP	2.3
1	B	202	ASP	2.1

### 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MES	B	3158	12/12	0.25	10.57	52,52,55,56	0
3	MES	A	3158	12/12	0.25	9.31	55,56,57,58	0
2	FMN	A	401	31/31	0.10	0.80	12,14,18,20	0
2	FMN	B	401	31/31	0.10	0.44	12,15,19,21	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.