W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2014 – 03:34 AM GMT

PDB ID	:	2HSA
Title	:	Crystal structure of 12-oxophytodienoate reductase 3 (OPR3) from tomato
Authors	:	Breithaupt, C.; Clausen, T.; Huber, R.
Deposited on	:	2006-07-21
Resolution	:	1.50 Å(reported)

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 1.50 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		11
Ramachandran outliers		0.1%
Sidechain outliers		2.7%
RSRZ outliers		8.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
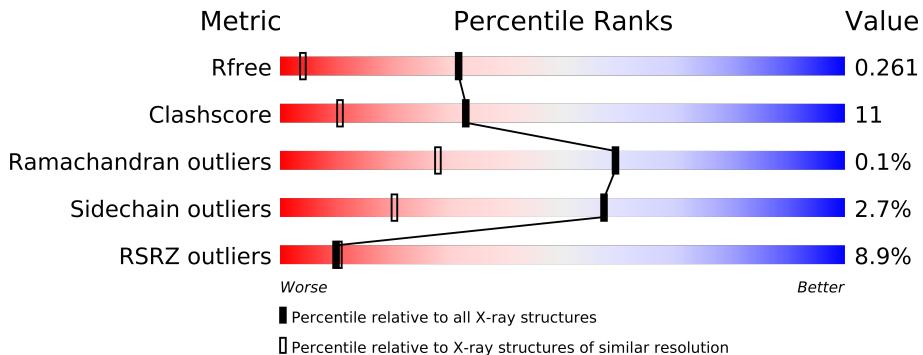
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1513 (1.50-1.50)
Clashscore	79885	1768 (1.50-1.50)
Ramachandran outliers	78287	1720 (1.50-1.50)
Sidechain outliers	78261	1718 (1.50-1.50)
RSRZ outliers	66119	1514 (1.50-1.50)

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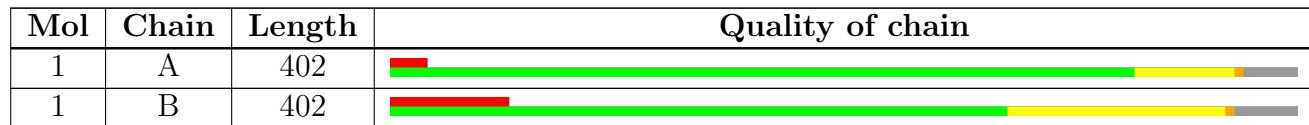
The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	A	603	-	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 6365 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	B	374	Total	C	N	O	S	10	0	0
			2871	1826	506	529	10			
1	A	376	Total	C	N	O	S	7	0	0
			2918	1853	515	539	11			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
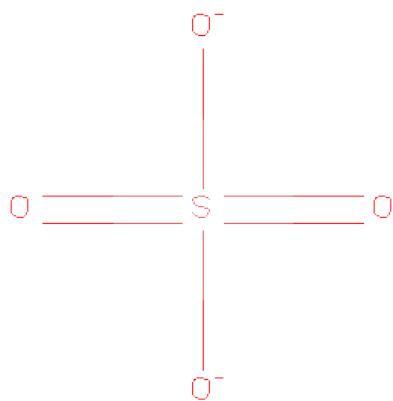
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Cl 1	0	0

- Molecule 4 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).
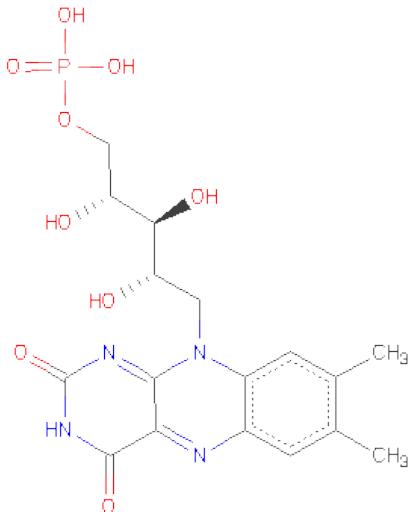
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total 31	C 17	N 4	O 9	P 1	0	0
4	A	1	Total 31	C 17	N 4	O 9	P 1	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	351	Total 351	O 351	0	0
5	B	152	Total 152	O 152	0	0

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: 12-oxophytodienoate reductase 3

Chain B:
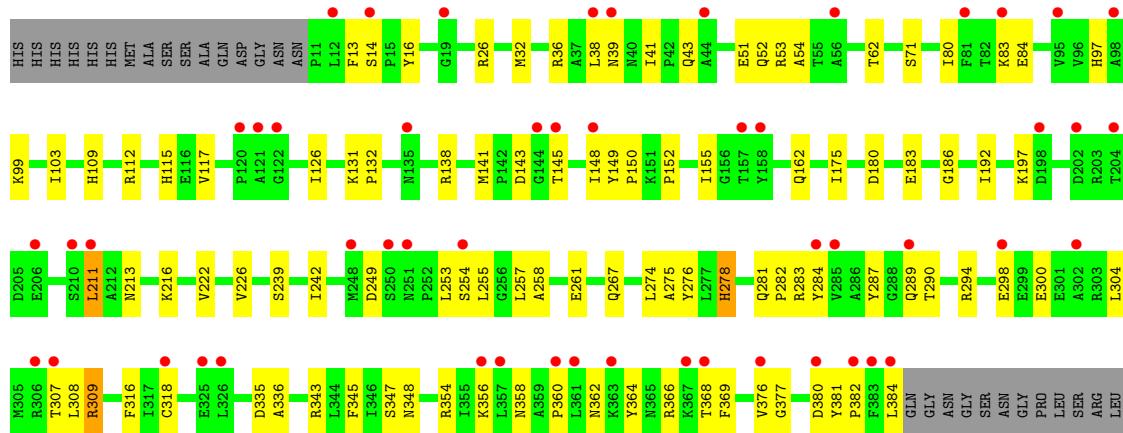
• Molecule 1: 12-oxophytodienoate reductase 3

Chain A:
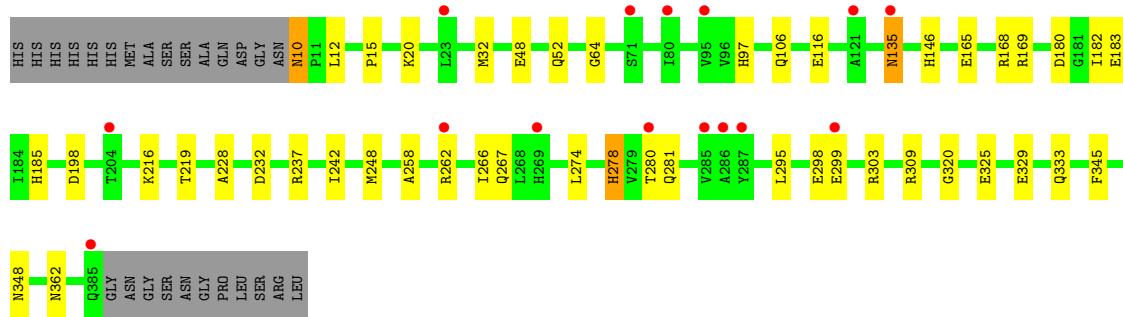
4　Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.90Å　　89.68Å　　81.38Å 90.00°　　109.46°　　90.00°	Depositor
Resolution (Å)	20.00　–　1.50 14.95　–　1.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.50) 91.6 (14.95-1.45)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 1.45Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225　,　0.255 0.233　,　0.261	Depositor DCC
R_{free} test set	5720 reflections (5.02%)	DCC
Wilson B-factor (Å²)	21.5	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.41 , 48.1	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	0 of 126778 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6365	wwPDB-VP
Average B, all atoms (Å²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]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, SO4, CL

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	0.54	0/2986	0.71	1/4054 (0.0%)
1	B	0.35	0/2938	0.61	0/3991
All	All	0.45	0/5924	0.66	1/8045 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	ASP	CB-CG-OD1	5.26	123.03	118.30

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	2918	0	2882	45	0
1	B	2871	0	2820	85	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	4	0
4	A	31	0	19	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	19	1	0
5	A	351	0	0	9	0
5	B	152	0	0	7	0
All	All	6365	0	5740	129	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 11.

All (129) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:287:TYR:HA	1:B:289:GLN:HE22	1.18	1.06
1:A:299:GLU:HG2	1:A:303:ARG:HH12	1.25	0.98
1:A:106:GLN:HE22	4:A:401:FMN:HN3	1.15	0.95
1:A:320:GLY:HA3	5:A:834:HOH:O	1.67	0.94
1:A:299:GLU:HG2	1:A:303:ARG:NH1	1.82	0.93
1:A:348:ASN:HD21	1:A:362:ASN:H	1.09	0.93
1:B:239:SER:HB2	1:B:242:ILE:HG13	1.50	0.92
1:A:299:GLU:CG	1:A:303:ARG:HH12	1.86	0.89
1:B:348:ASN:ND2	1:B:362:ASN:H	1.69	0.88
1:B:348:ASN:HD21	1:B:362:ASN:N	1.70	0.88
1:B:348:ASN:HD21	1:B:362:ASN:H	0.91	0.88
1:B:287:TYR:HA	1:B:289:GLN:NE2	1.91	0.85
1:B:368:THR:HG23	5:B:617:HOH:O	1.81	0.80
1:B:39:ASN:ND2	1:B:41:ILE:HD12	1.98	0.79
1:A:242:ILE:HD11	1:A:280:THR:HG22	1.68	0.76
1:B:143:ASP:OD1	1:B:145:THR:HG22	1.87	0.75
1:B:376:VAL:HA	1:B:380:ASP:OD2	1.88	0.74
1:B:239:SER:HB2	1:B:242:ILE:CG1	2.17	0.74
1:A:242:ILE:CD1	1:A:280:THR:HG22	2.19	0.72
1:A:20:LYS:HE3	3:A:603:CL:CL	2.28	0.70
5:B:613:HOH:O	1:A:280:THR:HG21	1.92	0.69
1:B:253:LEU:HD11	1:B:307:THR:HG21	1.73	0.69
1:A:97:HIS:HE1	1:A:180:ASP:OD2	1.76	0.69
1:B:253:LEU:O	1:B:257:LEU:HD13	1.92	0.68
1:B:39:ASN:HB3	5:B:640:HOH:O	1.93	0.68
1:B:39:ASN:HD21	1:B:41:ILE:HD12	1.58	0.67
1:B:38:LEU:HD22	1:B:38:LEU:H	1.61	0.65
1:B:267:GLN:HE21	1:B:274:LEU:H	1.44	0.65
1:A:267:GLN:HE21	1:A:274:LEU:H	1.42	0.64
1:B:97:HIS:HE1	1:B:180:ASP:OD2	1.81	0.63
1:B:141:MET:CE	1:B:141:MET:HA	2.29	0.63
1:B:267:GLN:NE2	1:B:274:LEU:H	1.96	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:257:LEU:HD12	1:B:308:LEU:CD2	2.30	0.62
1:B:211:LEU:HD13	1:B:258:ALA:HB2	1.80	0.61
1:B:16:TYR:HB2	1:B:26:ARG:NE	2.16	0.60
1:A:348:ASN:HD21	1:A:362:ASN:N	1.90	0.60
1:A:20:LYS:CE	3:A:603:CL:CL	2.87	0.59
1:A:20:LYS:NZ	5:A:795:HOH:O	2.36	0.58
1:A:135:ASN:HD22	1:A:135:ASN:N	1.99	0.58
1:B:257:LEU:HD12	1:B:308:LEU:HD23	1.85	0.58
1:A:267:GLN:NE2	1:A:274:LEU:H	2.01	0.57
1:B:211:LEU:HD21	1:B:255:LEU:HA	1.86	0.57
1:A:183:GLU:OE2	1:A:278:HIS:HD2	1.87	0.56
1:A:281:GLN:N	5:A:834:HOH:O	2.37	0.56
1:B:51:GLU:HG3	1:B:99:LYS:HD2	1.87	0.56
1:B:239:SER:CB	1:B:242:ILE:HG13	2.31	0.56
1:B:289:GLN:H	1:B:289:GLN:CD	2.11	0.55
1:B:318:CYS:SG	1:B:336:ALA:HB2	2.47	0.55
1:B:384:LEU:HA	5:B:638:HOH:O	2.07	0.54
1:A:248:MET:HE3	5:A:898:HOH:O	2.07	0.54
1:A:258:ALA:O	1:A:262:ARG:HG2	2.07	0.53
1:B:141:MET:HE2	1:B:141:MET:HA	1.91	0.53
1:A:165:GLU:HG3	1:A:169:ARG:NH2	2.23	0.53
1:B:183:GLU:OE2	1:B:278:HIS:HD2	1.90	0.53
1:B:289:GLN:HE21	1:B:290:THR:HG23	1.73	0.52
1:B:99:LYS:HB3	1:B:99:LYS:NZ	2.25	0.52
1:B:13:PHE:CZ	1:B:356:LYS:HB2	2.45	0.52
1:A:10:ASN:C	1:A:10:ASN:HD22	2.13	0.52
1:B:112:ARG:HB2	1:B:152:PRO:HG3	1.91	0.52
1:B:309:ARG:HG3	1:B:335:ASP:O	2.10	0.52
1:B:294:ARG:NH1	1:B:298:GLU:OE2	2.42	0.51
1:B:126:ILE:HB	1:B:155:ILE:CG2	2.40	0.51
1:B:97:HIS:HD2	5:B:647:HOH:O	1.93	0.51
1:B:52:GLN:HE21	1:B:53:ARG:HH12	1.59	0.51
1:A:237:ARG:HH21	1:A:278:HIS:CE1	2.29	0.50
1:B:138:ARG:HB2	1:A:295:LEU:O	2.12	0.50
1:A:146:HIS:HE1	5:A:905:HOH:O	1.94	0.50
1:B:54:ALA:HB3	1:B:99:LYS:HD3	1.93	0.50
1:B:162:GLN:HG3	5:B:627:HOH:O	2.10	0.50
1:B:213:ASN:HA	1:B:216:LYS:HD3	1.93	0.50
1:B:281:GLN:HG2	1:B:283:ARG:CZ	2.43	0.49
1:A:135:ASN:H	1:A:135:ASN:ND2	2.10	0.49
1:B:115:HIS:CE1	1:B:117:VAL:HG13	2.48	0.49
1:B:99:LYS:HB3	1:B:99:LYS:HZ3	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:300:GLU:OE1	1:B:300:GLU:HA	2.13	0.48
1:A:135:ASN:ND2	1:A:135:ASN:N	2.61	0.48
1:B:316:PHE:HE2	1:B:318:CYS:HG	1.60	0.48
1:A:10:ASN:ND2	1:A:12:LEU:H	2.12	0.48
1:A:216:LYS:HB2	1:A:216:LYS:HE3	1.73	0.47
1:A:64:GLY:HA2	1:A:106:GLN:HE21	1.80	0.47
1:B:138:ARG:CD	1:B:148:ILE:HD13	2.44	0.47
1:B:36:ARG:O	1:B:38:LEU:HD22	2.15	0.47
1:A:15:PRO:HG3	5:A:941:HOH:O	2.13	0.47
1:A:280:THR:HG23	5:A:834:HOH:O	2.13	0.47
1:B:38:LEU:HD22	1:B:43:GLN:HG3	1.97	0.46
1:A:20:LYS:NZ	3:A:603:CL:CL	2.85	0.46
1:B:304:LEU:C	1:B:304:LEU:HD13	2.36	0.46
1:B:138:ARG:HD2	1:B:148:ILE:HD13	1.98	0.46
1:B:32:MET:HA	4:B:401:FMN:N5	2.31	0.46
1:B:38:LEU:O	1:B:39:ASN:CG	2.55	0.45
1:B:377:GLY:N	1:B:380:ASP:OD2	2.42	0.45
1:B:71:SER:HB2	1:B:109:HIS:HA	1.98	0.45
1:B:62:THR:HG22	1:B:103:ILE:HD11	1.99	0.45
1:A:116:GLU:CD	1:A:116:GLU:H	2.19	0.45
1:B:366:ARG:HA	1:B:369:PHE:CD1	2.52	0.45
1:A:299:GLU:CD	1:A:303:ARG:HH12	2.20	0.45
1:A:329:GLU:O	1:A:333:GLN:HG3	2.17	0.44
1:B:316:PHE:HE2	1:B:318:CYS:SG	2.41	0.44
1:B:41:ILE:HD13	1:B:84:GLU:OE1	2.17	0.44
1:A:48:GLU:O	1:A:52:GLN:HG3	2.18	0.44
1:B:347:SER:HA	1:B:381:TYR:CG	2.53	0.43
1:B:131:LYS:HA	1:B:132:PRO:HD3	1.78	0.43
1:B:186:GLY:HA2	1:B:192:ILE:HB	2.00	0.43
1:B:242:ILE:HD13	1:B:282:PRO:HA	1.99	0.43
1:B:222:VAL:O	1:B:226:VAL:HG23	2.18	0.43
1:A:32:MET:HA	4:A:401:FMN:N5	2.34	0.43
1:A:97:HIS:HD2	5:A:875:HOH:O	2.02	0.43
1:B:281:GLN:HG2	1:B:283:ARG:NE	2.34	0.43
1:A:182:ILE:HD12	1:A:182:ILE:C	2.40	0.43
1:A:280:THR:CG2	5:A:834:HOH:O	2.67	0.43
1:B:253:LEU:HD11	1:B:307:THR:CG2	2.45	0.42
1:B:149:TYR:HA	1:B:150:PRO:HD3	1.87	0.42
1:A:232:ASP:OD1	3:A:603:CL:CL	2.74	0.42
1:B:354:ARG:NH1	1:B:360:PRO:O	2.50	0.42
1:B:211:LEU:CD1	1:B:258:ALA:HB2	2.48	0.42
1:B:343:ARG:HB3	1:B:364:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:347:SER:HB3	1:B:364:TYR:HB3	2.01	0.42
1:B:175:ILE:HD13	1:B:175:ILE:HA	1.93	0.41
1:B:14:SER:O	1:B:26:ARG:NE	2.47	0.41
1:A:168:ARG:NH1	1:A:228:ALA:HB2	2.35	0.41
1:B:211:LEU:HD11	1:B:254:SER:O	2.21	0.41
1:B:126:ILE:HB	1:B:155:ILE:HG21	2.02	0.41
1:A:219:THR:HG23	1:A:266:ILE:HD11	2.03	0.41
1:B:51:GLU:CG	1:B:99:LYS:HD2	2.50	0.40
1:B:275:ALA:O	1:B:276:TYR:HB3	2.21	0.40
1:B:257:LEU:HD12	1:B:308:LEU:HD21	2.02	0.40
1:B:381:TYR:HA	1:B:382:PRO:HD3	1.81	0.40
1:B:131:LYS:HG3	5:B:749:HOH:O	2.21	0.40
1:B:197:LYS:HD3	1:B:249:ASP:HB2	2.04	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	374/402 (93%)	360 (96%)	14 (4%)	0	100	100
1	B	372/402 (92%)	363 (98%)	8 (2%)	1 (0%)	50	20
All	All	746/804 (93%)	723 (97%)	22 (3%)	1 (0%)	59	28

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	305/328 (93%)	297 (97%)	8 (3%)	59	21
1	B	295/328 (90%)	287 (97%)	8 (3%)	57	20
All	All	600/656 (92%)	584 (97%)	16 (3%)	57	20

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	83	LYS
1	B	211	LEU
1	B	261	GLU
1	B	278	HIS
1	B	284	TYR
1	B	309	ARG
1	B	345	PHE
1	B	358	ASN
1	A	10	ASN
1	A	135	ASN
1	A	185	HIS
1	A	278	HIS
1	A	298	GLU
1	A	309	ARG
1	A	325	GLU
1	A	345	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	39	ASN
1	B	43	GLN
1	B	52	GLN
1	B	97	HIS
1	B	135	ASN
1	B	267	GLN
1	B	278	HIS
1	B	289	GLN
1	B	333	GLN
1	B	348	ASN
1	B	358	ASN
1	A	10	ASN

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Mol	Chain	Res	Type
1	A	40	ASN
1	A	43	GLN
1	A	97	HIS
1	A	106	GLN
1	A	135	ASN
1	A	146	HIS
1	A	162	GLN
1	A	267	GLN
1	A	278	HIS
1	A	333	GLN
1	A	348	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 ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	$\#|Z| > 2$
4	FMN	A	401	-	33,33,33	1.85	6 (18%)	46,50,50	2.01	5 (10%)
2	SO4	A	601	-	4,4,4	0.29	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	FMN	B	401	-	33,33,33	1.77	7 (21%)	46,50,50	2.05	6 (13%)
2	SO4	B	602	-	4,4,4	0.30	0	6,6,6	0.13	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
4	FMN	A	401	-	-	0/18/18/18	0/0/3/3
2	SO4	A	601	-	-	0/0/0/0	0/0/0/0
4	FMN	B	401	-	-	0/18/18/18	0/0/3/3
2	SO4	B	602	-	-	0/0/0/0	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	FMN	C1'-C2'	6.13	1.57	1.51
4	A	401	FMN	C4A-C10	4.49	1.48	1.40
4	B	401	FMN	C4A-C10	4.48	1.48	1.40
4	A	401	FMN	C2-N3	3.86	1.44	1.37
4	B	401	FMN	C6-C5A	3.84	1.46	1.41
4	B	401	FMN	C4-C4A	3.79	1.47	1.41
4	B	401	FMN	C1'-C2'	2.99	1.54	1.51
4	A	401	FMN	C4-C4A	2.94	1.46	1.41
4	B	401	FMN	C2-N3	2.93	1.43	1.37
4	B	401	FMN	C8-C7	2.59	1.48	1.40
4	B	401	FMN	C5A-N5	2.19	1.38	1.35
4	A	401	FMN	C9A-N10	2.12	1.42	1.38
4	A	401	FMN	C6-C5A	2.04	1.44	1.41

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	401	FMN	C4A-C10-N10	-7.63	116.70	120.51
4	A	401	FMN	C4A-C10-N10	-7.36	116.84	120.51
4	A	401	FMN	C2'-C1'-N10	-7.17	102.93	112.45
4	B	401	FMN	C2'-C1'-N10	-6.33	104.05	112.45
4	A	401	FMN	C2-N1-C10	5.35	120.37	114.98
4	B	401	FMN	C2-N1-C10	5.10	120.12	114.98
4	B	401	FMN	C1'-C2'-C3'	3.40	119.54	109.82
4	B	401	FMN	O2'-C2'-C3'	-2.93	101.74	109.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	401	FMN	C5'-C4'-C3'	-2.73	106.91	112.06
4	A	401	FMN	C10-C4A-N5	2.35	123.31	120.45
4	A	401	FMN	C1'-C2'-C3'	2.29	116.36	109.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

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, 95th 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	376/402 (93%)	0.17	15 (3%)	36	40	12, 20, 32, 41	9 (2%)
1	B	374/402 (93%)	0.83	52 (13%)	4	3	16, 34, 44, 48	6 (1%)
All	All	750/804 (93%)	0.50	67 (8%)	10	10	12, 26, 41, 48	15 (2%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	CYS	10.3
1	A	23	LEU	9.8
1	A	95	VAL	9.6
1	A	280	THR	8.1
1	A	71	SER	7.2
1	B	284	TYR	6.4
1	B	289	GLN	6.1
1	B	384	LEU	5.9
1	B	383	PHE	5.3
1	B	357	LEU	4.6
1	A	262	ARG	4.6
1	B	285	VAL	4.3
1	A	286	ALA	4.3
1	B	306	ARG	4.3
1	A	285	VAL	4.2
1	B	360	PRO	3.9
1	B	38	LEU	3.9
1	B	376	VAL	3.8
1	B	122	GLY	3.6
1	B	204	THR	3.6
1	B	248	MET	3.5
1	B	98	ALA	3.5
1	B	158	TYR	3.5
1	B	251	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	120	PRO	3.2
1	B	56	ALA	3.2
1	B	361	LEU	3.1
1	B	83	LYS	3.0
1	B	95	VAL	2.9
1	B	298	GLU	2.9
1	B	250	SER	2.8
1	B	121	ALA	2.7
1	B	382	PRO	2.7
1	A	204	THR	2.7
1	B	206	GLU	2.7
1	B	210	SER	2.7
1	B	211	LEU	2.6
1	B	356	LYS	2.6
1	A	287	TYR	2.6
1	B	367	LYS	2.5
1	B	148	ILE	2.5
1	B	39	ASN	2.4
1	B	135	ASN	2.4
1	B	325	GLU	2.3
1	B	198	ASP	2.3
1	A	299	GLU	2.3
1	B	302	ALA	2.3
1	B	19	GLY	2.2
1	B	145	THR	2.2
1	B	44	ALA	2.2
1	A	121	ALA	2.2
1	A	269	HIS	2.2
1	B	363	LYS	2.2
1	B	144	GLY	2.2
1	B	326	LEU	2.2
1	B	12	LEU	2.1
1	B	254	SER	2.1
1	A	135	ASN	2.1
1	A	385	GLN	2.1
1	B	202	ASP	2.0
1	B	380	ASP	2.0
1	A	80	ILE	2.0
1	B	368	THR	2.0
1	B	14	SER	2.0
1	B	157	THR	2.0
1	B	307	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	81	PHE	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 carbohydrates 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. 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, 95th 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(Å^2)	Q<0.9
3	CL	A	603	1/1	0.17	4.02	72,72,72,72	0
2	SO4	B	602	5/5	0.16	0.32	38,40,40,41	0
4	FMN	B	401	31/31	0.09	-0.07	20,24,28,30	0
4	FMN	A	401	31/31	0.07	-0.26	10,12,16,18	0
2	SO4	A	601	5/5	0.08	-0.46	25,25,27,32	0

6.5 Other polymers (i)

There are no such residues in this entry.