



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 04:08 AM UTC

PDB ID : 2PS8 / pdb\_00002ps8  
Title : Y295F Trichodiene Synthase: Complex With Mg and Pyrophosphate  
Authors : Vedula, L.S.; Cane, D.E.; Christianson, D.W.  
Deposited on : 2007-05-04  
Resolution : 2.67 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

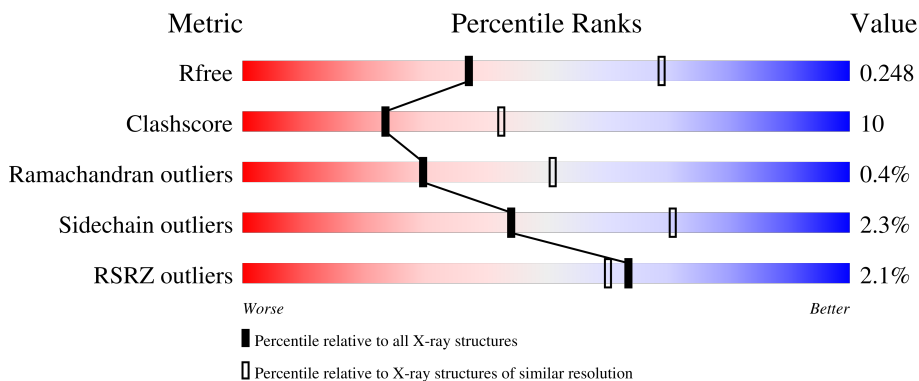
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


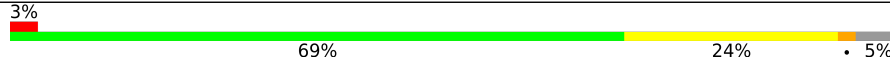
The reported resolution of this entry is 2.67 Å.

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))
$R_{free}$	180053	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	374	 70% 23% • 5%
1	B	374	 69% 24% • 5%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6089 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.

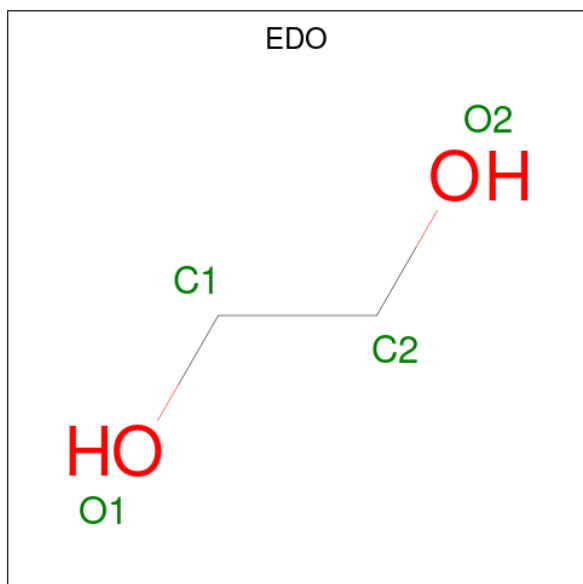
- Molecule 1 is a protein called Trichodiene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2939	1882	493	546	18	0	0	0
1	B	354	2939	1882	493	546	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	295	PHE	TYR	engineered mutation	UNP P13513
B	295	PHE	TYR	engineered mutation	UNP P13513

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

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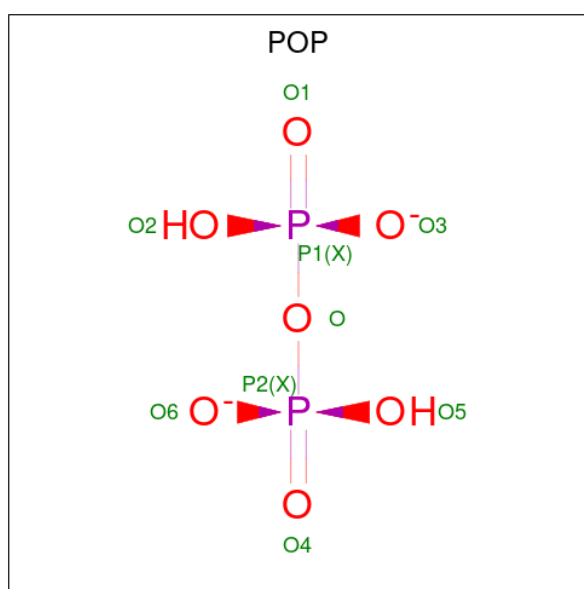
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			9	7	2		

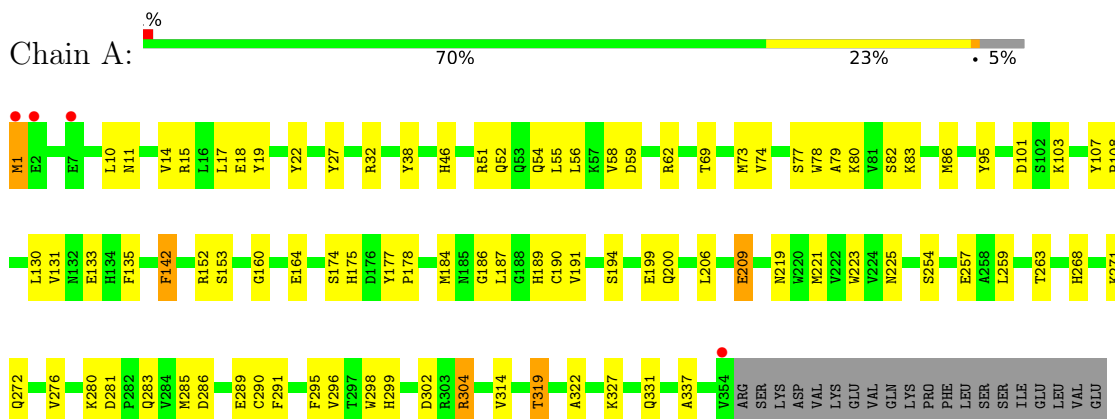
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total	O	0	0
			94	94		
5	B	97	Total	O	0	0
			97	97		

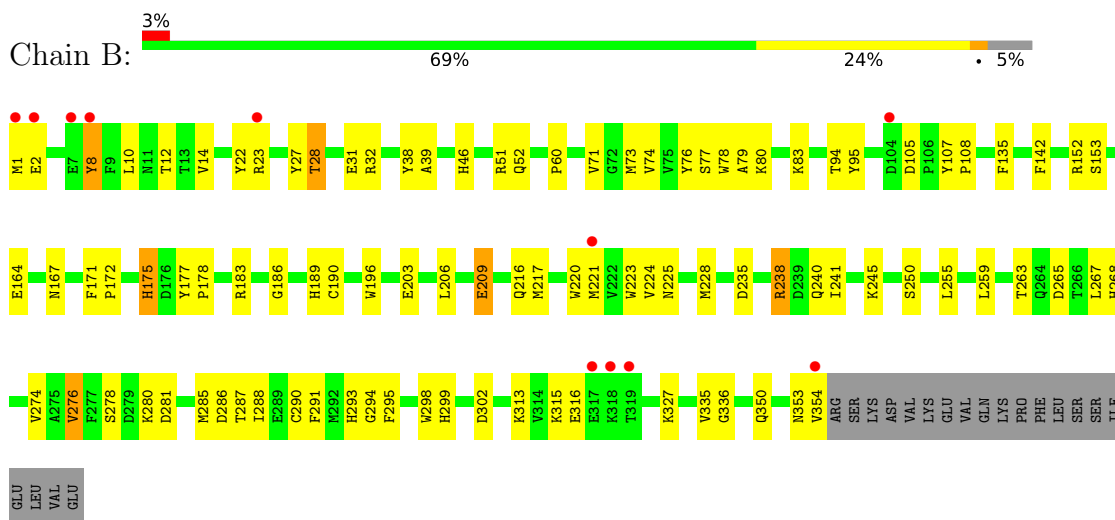
### 3 Residue-property plots [i](#)

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: Trichodiene synthase



- Molecule 1: Trichodiene synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.27Å 122.27Å 150.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.67 50.00 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.67) 99.9 (50.00-2.67)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.69Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.203 , 0.245 0.208 , 0.248	Depositor DCC
$R_{free}$ test set	1867 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtrriage
Anisotropy	0.207	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 34.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6089	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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: EDO, MG, POP

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	0.46	1/3024 (0.0%)	0.87	4/4104 (0.1%)
1	B	0.41	0/3024	0.89	13/4104 (0.3%)
All	All	0.44	1/6048 (0.0%)	0.88	17/8208 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	10.81	2.06	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	VAL	N-CA-C	8.49	118.52	110.53
1	B	28	THR	N-CA-C	-8.08	97.16	110.17
1	B	250	SER	N-CA-C	6.50	118.44	111.36
1	A	103	LYS	N-CA-C	-5.91	105.90	114.12
1	A	79	ALA	N-CA-C	5.72	118.26	111.33
1	A	131	VAL	N-CA-C	5.66	115.85	110.42
1	A	142	PHE	N-CA-C	5.47	117.49	109.24
1	B	302	ASP	N-CA-C	5.39	118.05	110.23
1	B	186	GLY	N-CA-C	5.20	121.11	114.66
1	B	105	ASP	CA-C-N	5.16	124.66	119.19
1	B	105	ASP	C-N-CA	5.16	124.66	119.19
1	B	196	TRP	N-CA-C	5.10	117.91	108.94
1	B	79	ALA	N-CA-C	5.09	118.98	112.87
1	B	142	PHE	N-CA-C	5.07	117.38	109.52
1	B	94	THR	N-CA-C	-5.06	105.47	111.69
1	B	175	HIS	N-CA-C	5.05	118.21	111.75
1	B	315	LYS	N-CA-C	-5.02	106.26	112.38

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2939	0	2793	64	0
1	B	2939	0	2793	59	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
3	B	3	0	0	0	0
4	B	9	0	0	0	0
5	A	94	0	0	0	0
5	B	97	0	0	3	0
All	All	6089	0	5598	117	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 10.

All (117) 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:1:MET:CE	1:A:1:MET:SD	2.06	1.43
1:A:184:MET:HE1	1:B:152:ARG:NH2	1.68	1.08
1:B:278:SER:HA	1:B:285:MET:HE2	1.32	1.07
1:A:17:LEU:HD21	1:A:296:VAL:HG11	1.47	0.95
1:A:69:THR:HG22	1:A:298:TRP:HZ2	1.48	0.79
1:A:285:MET:HE3	1:A:289:GLU:HB2	1.65	0.79
1:A:304:ARG:HH11	1:A:304:ARG:HB2	1.49	0.77
1:A:107:TYR:HB3	1:A:108:PRO:HD3	1.69	0.75
1:A:27:TYR:HB3	1:A:32:ARG:NH1	2.02	0.74
1:A:319:THR:HG23	1:A:322:ALA:HB3	1.68	0.73
1:B:23:ARG:H	1:B:293:HIS:HD2	1.38	0.72
1:B:240:GLN:OE1	1:B:245:LYS:HE2	1.88	0.72
1:A:54:GLN:HG3	1:A:55:LEU:HD23	1.73	0.70
1:A:225:ASN:HD22	1:A:299:HIS:HE1	1.41	0.68
1:B:80:LYS:HE3	1:B:286:ASP:OD2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:HB	1:B:263:THR:HG21	1.78	0.66
1:A:184:MET:HE1	1:B:152:ARG:HH22	1.59	0.65
1:A:285:MET:CE	1:A:289:GLU:HB2	2.28	0.64
1:A:268:HIS:NE2	1:B:175:HIS:HD2	1.96	0.63
1:A:10:LEU:HD11	1:A:314:VAL:HG11	1.79	0.63
1:B:278:SER:CA	1:B:285:MET:HE2	2.19	0.62
1:B:1:MET:HE2	1:B:235:ASP:OD1	2.00	0.62
1:B:263:THR:O	1:B:267:LEU:HG	2.00	0.61
1:A:276:VAL:O	1:A:280:LYS:HD3	2.00	0.61
1:A:153:SER:HB3	1:A:190:CYS:HB2	1.84	0.59
1:B:164:GLU:OE1	1:B:238:ARG:NH2	2.34	0.59
1:A:80:LYS:HE2	1:A:290:CYS:SG	2.43	0.58
1:A:14:VAL:O	1:A:18:GLU:HG3	2.03	0.58
1:A:69:THR:HG23	1:A:302:ASP:OD2	2.04	0.58
1:A:69:THR:HG22	1:A:298:TRP:CZ2	2.36	0.57
1:B:10:LEU:O	1:B:14:VAL:HG23	2.04	0.57
1:B:107:TYR:HB3	1:B:108:PRO:CD	2.35	0.57
1:B:153:SER:HB3	1:B:190:CYS:HB2	1.87	0.56
1:B:12:THR:CG2	1:B:263:THR:HG21	2.35	0.56
1:B:276:VAL:O	1:B:280:LYS:HD3	2.06	0.56
1:B:74:VAL:HA	1:B:78:TRP:CE3	2.41	0.56
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.87	0.55
1:A:319:THR:HG23	1:A:322:ALA:CB	2.35	0.55
1:B:28:THR:OG1	1:B:31:GLU:HG3	2.07	0.55
1:B:225:ASN:HD22	1:B:299:HIS:HE1	1.54	0.55
1:B:350:GLN:O	1:B:354:VAL:HG23	2.08	0.54
1:B:12:THR:CB	1:B:263:THR:HG21	2.37	0.53
1:B:223:TRP:CZ3	1:B:265:ASP:HB3	2.43	0.53
1:A:17:LEU:HD22	1:A:22:TYR:CG	2.44	0.53
1:B:39:ALA:HB3	1:B:71:VAL:HG13	1.91	0.52
1:A:177:TYR:HB3	1:A:178:PRO:HD3	1.91	0.52
1:A:186:GLY:O	1:A:187:LEU:HB2	2.10	0.51
1:B:274:VAL:O	1:B:278:SER:HB2	2.11	0.51
1:B:228:MET:HE3	1:B:299:HIS:HB2	1.93	0.51
1:A:46:HIS:O	1:A:52:GLN:HG3	2.11	0.51
1:A:175:HIS:HD2	1:B:268:HIS:NE2	2.08	0.51
1:A:199:GLU:HB3	1:A:200:GLN:NE2	2.25	0.50
1:B:206:LEU:HD22	1:B:209:GLU:HG3	1.93	0.50
1:A:38:TYR:CD2	1:A:83:LYS:HB3	2.45	0.50
1:A:82:SER:O	1:A:86:MET:HG3	2.12	0.50
1:A:142:PHE:CE2	1:A:194:SER:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:MET:HE1	1:B:288:ILE:HG23	1.93	0.49
1:A:51:ARG:NH1	1:A:133:GLU:OE1	2.46	0.49
1:A:73:MET:HB2	1:A:298:TRP:CE2	2.48	0.49
1:B:73:MET:HB2	1:B:298:TRP:CE2	2.48	0.49
1:A:327:LYS:O	1:A:331:GLN:HG3	2.12	0.48
1:B:353:ASN:O	1:B:354:VAL:C	2.56	0.48
1:B:167:ASN:HA	1:B:241:ILE:HG13	1.96	0.48
1:A:219:ASN:HB3	1:A:223:TRP:CZ3	2.49	0.48
1:A:152:ARG:NH2	1:A:189:HIS:ND1	2.59	0.47
1:A:160:GLY:O	1:A:164:GLU:HG3	2.13	0.47
1:B:22:TYR:O	1:B:23:ARG:CG	2.62	0.47
1:A:19:TYR:CE2	1:A:271:LYS:HE3	2.50	0.47
1:B:23:ARG:H	1:B:293:HIS:CD2	2.26	0.47
1:A:184:MET:HE1	1:B:152:ARG:CZ	2.39	0.47
1:B:46:HIS:O	1:B:52:GLN:HG3	2.15	0.47
1:B:220:TRP:O	1:B:224:VAL:HG23	2.15	0.47
1:A:11:ASN:HD21	1:A:15:ARG:HE	1.63	0.47
1:B:224:VAL:O	1:B:228:MET:HG2	2.15	0.46
1:B:38:TYR:CD2	1:B:83:LYS:HB3	2.51	0.46
1:B:203:GLU:HB2	5:B:859:HOH:O	2.16	0.46
1:B:27:TYR:HB2	1:B:32:ARG:HG3	1.96	0.46
1:B:12:THR:HG22	1:B:263:THR:HG21	1.98	0.46
1:A:15:ARG:O	1:A:19:TYR:CD1	2.69	0.45
1:B:12:THR:HB	1:B:263:THR:CG2	2.46	0.45
1:A:191:VAL:HG21	1:A:221:MET:HE2	1.98	0.45
1:A:52:GLN:OE1	1:A:95:TYR:OH	2.34	0.45
1:A:62:ARG:NH1	1:A:101:ASP:OD1	2.49	0.44
1:B:46:HIS:HE1	1:B:95:TYR:OH	2.00	0.44
1:A:206:LEU:HD22	1:A:209:GLU:HG3	1.99	0.44
1:B:80:LYS:HE2	1:B:290:CYS:SG	2.58	0.44
1:B:152:ARG:NH2	1:B:189:HIS:ND1	2.62	0.44
1:B:291:PHE:O	1:B:295:PHE:HB2	2.17	0.44
1:A:254:SER:OG	1:A:257:GLU:HG3	2.18	0.44
1:B:76:TYR:O	1:B:294:GLY:HA3	2.18	0.44
1:A:80:LYS:HE3	1:A:286:ASP:OD2	2.18	0.44
1:A:268:HIS:CD2	1:A:272:GLN:HG2	2.53	0.43
1:A:295:PHE:O	1:A:299:HIS:HD2	2.01	0.43
1:B:107:TYR:HB3	1:B:108:PRO:HD3	2.00	0.43
1:A:259:LEU:O	1:A:263:THR:HG23	2.18	0.43
1:A:77:SER:HB3	1:A:291:PHE:CD1	2.54	0.43
1:B:255:LEU:O	1:B:259:LEU:HD23	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG23	1:B:336:GLY:N	2.33	0.43
1:A:27:TYR:HB3	1:A:32:ARG:HH12	1.79	0.43
1:B:171:PHE:O	1:B:172:PRO:C	2.60	0.42
1:A:304:ARG:HB2	1:A:304:ARG:NH1	2.25	0.42
1:A:174:SER:OG	1:B:216:GLN:NE2	2.52	0.42
1:B:183:ARG:NH1	5:B:844:HOH:O	2.51	0.42
1:A:281:ASP:OD1	1:A:283:GLN:N	2.52	0.42
1:B:183:ARG:NH2	5:B:807:HOH:O	2.52	0.42
1:A:74:VAL:HA	1:A:78:TRP:CE3	2.55	0.42
1:A:56:LEU:HG	1:A:58:VAL:HG23	2.01	0.41
1:B:73:MET:HB2	1:B:298:TRP:CZ2	2.55	0.41
1:B:280:LYS:O	1:B:281:ASP:C	2.64	0.41
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.47	0.41
1:A:19:TYR:CD2	1:A:271:LYS:HG3	2.55	0.41
1:A:51:ARG:NH1	1:A:130:LEU:HD23	2.36	0.41
1:A:59:ASP:HB3	1:A:62:ARG:HG3	2.03	0.41
1:B:8:TYR:HD2	1:B:8:TYR:HA	1.76	0.41
1:A:17:LEU:HD22	1:A:22:TYR:CB	2.51	0.41
1:A:73:MET:HB2	1:A:298:TRP:CZ2	2.56	0.40
1:A:281:ASP:OD1	1:A:281:ASP:C	2.64	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	352/374 (94%)	339 (96%)	12 (3%)	1 (0%)	36 57
1	B	352/374 (94%)	338 (96%)	12 (3%)	2 (1%)	21 41
All	All	704/748 (94%)	677 (96%)	24 (3%)	3 (0%)	30 51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	337	ALA
1	B	2	GLU
1	B	313	LYS

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/340 (94%)	316 (99%)	4 (1%)	61	81
1	B	320/340 (94%)	309 (97%)	11 (3%)	32	59
All	All	640/680 (94%)	625 (98%)	15 (2%)	44	71

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	PHE
1	A	209	GLU
1	A	304	ARG
1	A	319	THR
1	B	8	TYR
1	B	51	ARG
1	B	60	PRO
1	B	77	SER
1	B	135	PHE
1	B	209	GLU
1	B	221	MET
1	B	238	ARG
1	B	287	THR
1	B	316	GLU
1	B	327	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN

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Mol	Chain	Res	Type
1	A	46	HIS
1	A	49	GLN
1	A	137	ASN
1	A	167	ASN
1	A	175	HIS
1	A	200	GLN
1	A	216	GLN
1	A	240	GLN
1	A	299	HIS
1	A	334	ASN
1	A	353	ASN
1	B	46	HIS
1	B	137	ASN
1	B	175	HIS
1	B	216	GLN
1	B	246	ASN
1	B	293	HIS
1	B	299	HIS
1	B	353	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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
2	EDO	B	801	-	3,3,3	0.52	0	2,2,2	0.51	0
2	EDO	A	802	-	3,3,3	0.55	0	2,2,2	0.53	0
4	POP	B	700	3	6,8,8	1.61	1 (16%)	12,13,13	1.71	1 (8%)

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
2	EDO	B	801	-	-	1/1/1/1	-
2	EDO	A	802	-	-	0/1/1/1	-
4	POP	B	700	3	-	0/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	POP	P2-O6	-2.69	1.44	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	700	POP	O2-P1-O	5.06	121.61	104.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	354/374 (94%)	-0.12	4 (1%) 78 76	26, 41, 67, 88	0
1	B	354/374 (94%)	0.03	11 (3%) 51 47	27, 45, 72, 106	0
All	All	708/748 (94%)	-0.05	15 (2%) 63 60	26, 42, 69, 106	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	GLU	6.4
1	B	2	GLU	6.1
1	B	23	ARG	6.0
1	A	1	MET	4.7
1	B	1	MET	4.5
1	A	7	GLU	3.7
1	A	354	VAL	3.4
1	B	354	VAL	2.9
1	B	319	THR	2.8
1	B	318	LYS	2.8
1	B	8	TYR	2.6
1	B	7	GLU	2.5
1	B	104	ASP	2.2
1	B	317	GLU	2.1
1	B	221	MET	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 oligosaccharides 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(Å <sup>2</sup> )	Q<0.9
3	MG	B	701	1/1	0.89	0.12	50,50,50,50	0
3	MG	B	703	1/1	0.91	0.15	51,51,51,51	0
4	POP	B	700	9/9	0.94	0.09	47,49,52,52	0
2	EDO	B	801	4/4	0.95	0.12	40,42,46,48	0
2	EDO	A	802	4/4	0.96	0.10	39,41,41,43	0
3	MG	B	702	1/1	0.99	0.03	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.