



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 02:00 AM EDT

PDB ID : 2PS7  
Title : Y295F trichodiene synthase  
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Deposited on : 2007-05-04  
Resolution : 2.35 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

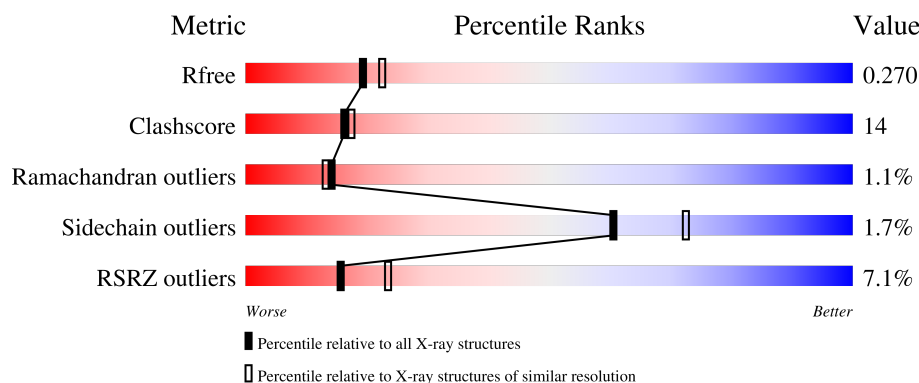
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


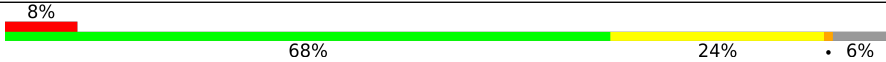
The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	
1	B	374	

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
3	EDO	A	800	-	X	-	-
3	EDO	B	801	-	X	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5961 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
1	A	354	Total	C	N	O	S	0	0	0
			2939	1882	493	546	18			
1	B	350	Total	C	N	O	S	0	0	0
			2903	1859	488	539	17			

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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

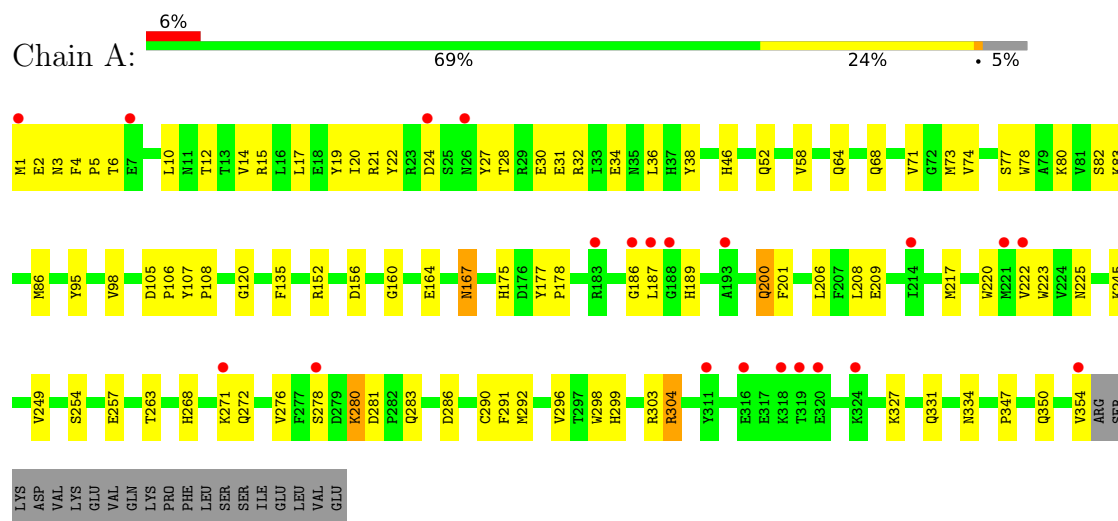
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	47	Total	O	0	0
			47	47		

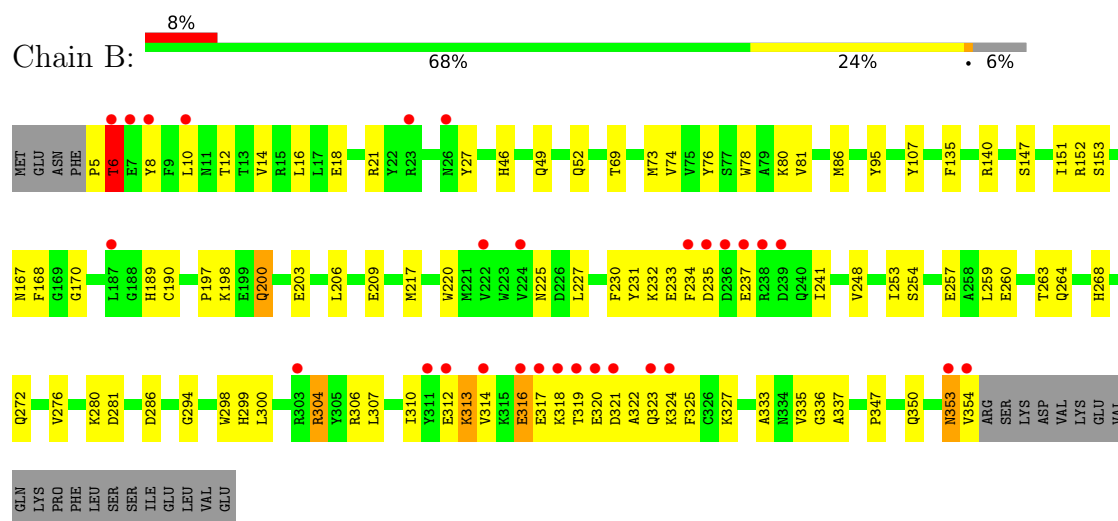
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	122.43Å 122.43Å 151.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.35 38.92 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.35) 97.7 (38.92-2.35)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.34Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.233 , 0.258 0.250 , 0.270	Depositor DCC
$R_{free}$ test set	2177 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.9	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 36.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	5961	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

### 5.1 Standard geometry

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

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	0.39	0/3024	0.54	0/4104
1	B	0.36	0/2987	0.56	0/4054
All	All	0.38	0/6011	0.55	0/8158

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

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	75	0
1	B	2903	0	2761	92	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
4	A	62	0	0	2	0
4	B	47	0	0	1	0
All	All	5961	0	5566	164	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 14.



All (164) 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:B:320:GLU:O	1:B:324:LYS:HG3	1.40	1.19
1:A:304:ARG:HH11	1:A:304:ARG:HB2	1.27	0.99
1:B:320:GLU:HA	1:B:324:LYS:CE	1.92	0.98
1:B:225:ASN:HD22	1:B:299:HIS:HE1	1.11	0.95
1:B:320:GLU:HA	1:B:324:LYS:HE3	1.53	0.90
1:B:319:THR:HG23	1:B:321:ASP:H	1.38	0.88
1:A:217:MET:HA	1:A:217:MET:HE3	1.56	0.88
1:B:320:GLU:O	1:B:324:LYS:CG	2.24	0.85
1:A:17:LEU:HD21	1:A:296:VAL:HG11	1.58	0.85
1:B:46:HIS:HA	1:B:49:GLN:HE21	1.40	0.85
1:B:12:THR:HB	1:B:263:THR:HG21	1.59	0.82
1:B:320:GLU:C	1:B:324:LYS:HG3	2.00	0.81
1:B:217:MET:HE3	1:B:220:TRP:HB3	1.64	0.80
1:A:64:GLN:HE21	1:A:68:GLN:HE21	1.31	0.78
1:B:225:ASN:HD22	1:B:299:HIS:CE1	2.01	0.77
1:B:259:LEU:O	1:B:263:THR:HG23	1.86	0.75
1:B:317:GLU:O	1:B:323:GLN:OE1	2.02	0.75
1:B:320:GLU:HA	1:B:324:LYS:HE2	1.66	0.75
1:A:304:ARG:HB2	1:A:304:ARG:NH1	2.00	0.75
1:B:320:GLU:C	1:B:324:LYS:CG	2.55	0.74
1:B:317:GLU:O	1:B:323:GLN:CD	2.26	0.73
1:B:318:LYS:HA	1:B:323:GLN:HG2	1.73	0.71
1:B:225:ASN:ND2	1:B:299:HIS:HE1	1.89	0.69
1:A:217:MET:CE	1:A:220:TRP:HB3	2.22	0.69
1:B:217:MET:CE	1:B:220:TRP:HB3	2.23	0.68
1:A:268:HIS:O	1:A:272:GLN:HG2	1.94	0.66
1:B:312:GLU:O	1:B:313:LYS:HB2	1.95	0.64
1:B:319:THR:HG23	1:B:320:GLU:H	1.60	0.64
1:A:12:THR:HG21	1:A:263:THR:HG21	1.80	0.64
1:B:237:GLU:HG3	1:B:237:GLU:O	2.00	0.61
1:B:276:VAL:O	1:B:280:LYS:HD3	2.00	0.61
1:B:350:GLN:O	1:B:354:VAL:HG23	2.01	0.61
1:B:10:LEU:O	1:B:14:VAL:HG23	2.01	0.60
1:B:12:THR:CB	1:B:263:THR:HG21	2.29	0.59
1:B:80:LYS:HE3	1:B:286:ASP:OD2	2.03	0.59
1:B:217:MET:O	1:B:217:MET:HE2	2.03	0.59
1:A:254:SER:OG	1:A:257:GLU:HG3	2.04	0.58
1:A:80:LYS:HE2	1:A:290:CYS:SG	2.44	0.57
1:B:206:LEU:HD22	1:B:209:GLU:HG3	1.86	0.57
1:A:32:ARG:HH11	1:A:32:ARG:HG3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:O	1:A:34:GLU:HG3	2.04	0.57
1:B:319:THR:HG23	1:B:320:GLU:N	2.19	0.57
1:B:320:GLU:C	1:B:324:LYS:HG2	2.26	0.56
1:A:276:VAL:O	1:A:280:LYS:HD3	2.05	0.56
1:B:6:THR:OG1	1:B:8:TYR:HB3	2.07	0.55
1:A:217:MET:HE3	1:A:220:TRP:HB3	1.89	0.55
1:A:175:HIS:HD2	1:B:268:HIS:NE2	2.05	0.55
1:B:5:PRO:N	1:B:234:PHE:CE2	2.75	0.54
1:B:300:LEU:HA	1:B:307:LEU:HD12	1.88	0.54
1:B:12:THR:HB	1:B:263:THR:CG2	2.33	0.53
1:A:80:LYS:HE3	1:A:286:ASP:OD2	2.09	0.53
1:B:217:MET:CE	1:B:220:TRP:HE3	2.21	0.53
1:A:46:HIS:O	1:A:52:GLN:HG3	2.07	0.53
1:A:217:MET:HE3	1:A:217:MET:CA	2.35	0.53
1:B:167:ASN:HA	1:B:241:ILE:HD13	1.91	0.53
1:B:233:GLU:O	1:B:237:GLU:HB3	2.08	0.53
1:A:331:GLN:HA	1:A:334:ASN:HD22	1.73	0.52
1:B:231:TYR:CD1	1:B:310:ILE:HD11	2.45	0.52
1:B:46:HIS:O	1:B:52:GLN:HG3	2.10	0.52
1:A:38:TYR:CD2	1:A:83:LYS:HB3	2.44	0.52
1:B:230:PHE:CE2	1:B:259:LEU:HD22	2.44	0.52
1:A:347:PRO:HG2	1:A:350:GLN:HB2	1.92	0.52
1:B:197:PRO:HB2	1:B:200:GLN:NE2	2.25	0.52
1:B:319:THR:O	1:B:324:LYS:HE2	2.10	0.52
1:A:58:VAL:HG21	1:A:98:VAL:HG11	1.91	0.52
1:A:304:ARG:HH11	1:A:304:ARG:CB	2.11	0.51
1:A:331:GLN:HA	1:A:334:ASN:ND2	2.26	0.51
1:A:272:GLN:O	1:A:276:VAL:HG23	2.10	0.51
1:B:46:HIS:CA	1:B:49:GLN:HE21	2.19	0.51
1:B:12:THR:CG2	1:B:263:THR:HG21	2.41	0.51
1:A:206:LEU:O	1:A:209:GLU:HG2	2.11	0.50
1:B:248:VAL:HG13	1:B:253:ILE:O	2.12	0.50
1:A:12:THR:HG21	1:A:263:THR:CG2	2.41	0.50
1:B:333:ALA:O	1:B:337:ALA:HB3	2.12	0.50
1:A:64:GLN:HE21	1:A:68:GLN:NE2	2.04	0.50
1:B:237:GLU:O	1:B:237:GLU:CG	2.60	0.49
1:B:217:MET:HE3	1:B:220:TRP:CE3	2.46	0.49
1:B:254:SER:OG	1:B:257:GLU:HG3	2.12	0.49
1:A:19:TYR:CE2	1:A:271:LYS:HB2	2.46	0.49
1:A:82:SER:O	1:A:86:MET:HG3	2.13	0.49
1:B:217:MET:HE1	1:B:220:TRP:HE3	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:MET:HE2	1:A:220:TRP:HE3	1.78	0.48
1:B:140:ARG:O	1:B:198:LYS:HE2	2.12	0.48
1:B:318:LYS:HA	1:B:323:GLN:CG	2.42	0.48
1:A:292:MET:O	1:A:296:VAL:HG23	2.13	0.48
1:B:310:ILE:HG22	1:B:325:PHE:CE2	2.48	0.48
1:B:153:SER:HB3	1:B:190:CYS:HB2	1.96	0.48
1:A:58:VAL:HG21	1:A:98:VAL:CG1	2.44	0.48
1:B:74:VAL:HA	1:B:78:TRP:CE3	2.49	0.48
1:B:46:HIS:HA	1:B:49:GLN:NE2	2.19	0.47
1:A:6:THR:O	1:A:10:LEU:HG	2.14	0.47
1:B:78:TRP:O	1:B:81:VAL:HG22	2.14	0.47
1:B:319:THR:CG2	1:B:320:GLU:H	2.22	0.47
1:A:17:LEU:CD2	1:A:296:VAL:HG11	2.36	0.47
1:A:15:ARG:O	1:A:19:TYR:HD1	1.97	0.47
1:B:46:HIS:HE1	1:B:95:TYR:OH	1.98	0.47
1:B:353:ASN:O	1:B:354:VAL:C	2.53	0.47
1:B:5:PRO:N	1:B:234:PHE:HE2	2.12	0.47
1:B:203:GLU:HG2	4:B:821:HOH:O	2.14	0.46
1:A:225:ASN:HD22	1:A:299:HIS:HE1	1.63	0.46
1:B:12:THR:O	1:B:227:LEU:HD11	2.15	0.46
1:B:300:LEU:HD23	1:B:307:LEU:CD1	2.46	0.46
1:A:2:GLU:O	1:A:2:GLU:HG3	2.15	0.46
1:A:177:TYR:HB3	1:A:178:PRO:HD3	1.98	0.46
1:A:1:MET:C	1:A:3:ASN:H	2.17	0.46
1:B:217:MET:CE	1:B:220:TRP:CE3	2.99	0.45
1:A:120:GLY:HA2	4:A:839:HOH:O	2.17	0.45
1:B:321:ASP:O	1:B:322:ALA:HB3	2.15	0.45
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.46	0.45
1:B:147:SER:O	1:B:151:ILE:HG13	2.17	0.45
1:A:152:ARG:NH2	1:A:189:HIS:ND1	2.61	0.45
1:B:347:PRO:HG2	1:B:350:GLN:HB2	1.99	0.45
1:A:156:ASP:OD1	1:B:152:ARG:HD2	2.17	0.45
1:B:76:TYR:O	1:B:294:GLY:HA3	2.16	0.45
1:B:152:ARG:NH2	1:B:189:HIS:ND1	2.59	0.45
1:B:272:GLN:NE2	1:B:272:GLN:HA	2.32	0.44
1:B:260:GLU:HG3	1:B:264:GLN:HE21	1.82	0.44
1:A:10:LEU:O	1:A:14:VAL:HG23	2.17	0.44
1:A:28:THR:OG1	1:A:31:GLU:HG3	2.17	0.44
1:A:46:HIS:HE1	1:A:95:TYR:OH	2.00	0.44
1:B:217:MET:HE2	1:B:217:MET:HA	1.99	0.44
1:A:105:ASP:HA	1:A:106:PRO:HD3	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:VAL:O	1:B:86:MET:HE3	2.17	0.44
1:B:107:TYR:CD1	1:B:107:TYR:C	2.90	0.44
1:A:280:LYS:N	1:A:280:LYS:HD2	2.32	0.44
1:A:19:TYR:HE2	1:A:271:LYS:HB2	1.83	0.44
1:A:73:MET:HB2	1:A:298:TRP:CE2	2.52	0.44
1:A:160:GLY:O	1:A:164:GLU:HG3	2.18	0.44
1:A:200:GLN:HG3	4:A:830:HOH:O	2.17	0.44
1:A:280:LYS:O	1:A:281:ASP:C	2.56	0.44
1:A:350:GLN:O	1:A:354:VAL:HG23	2.18	0.43
1:B:323:GLN:O	1:B:327:LYS:HB2	2.18	0.43
1:A:201:PHE:CZ	1:A:283:GLN:HG2	2.53	0.43
1:A:217:MET:HE1	1:A:220:TRP:CE3	2.53	0.43
1:A:74:VAL:O	1:A:78:TRP:HB2	2.18	0.43
1:A:217:MET:CE	1:A:220:TRP:CE3	3.01	0.43
1:A:4:PHE:HA	1:A:5:PRO:HD3	1.91	0.43
1:B:69:THR:HG21	1:B:304:ARG:HD2	2.00	0.43
1:A:58:VAL:CG2	1:A:98:VAL:CG1	2.97	0.43
1:A:167:ASN:HD22	1:A:167:ASN:HA	1.64	0.42
1:B:168:PHE:CE2	1:B:170:GLY:HA2	2.54	0.42
1:A:327:LYS:O	1:A:331:GLN:HG3	2.20	0.42
1:B:321:ASP:C	1:B:323:GLN:H	2.23	0.42
1:B:73:MET:HB2	1:B:298:TRP:CE2	2.54	0.42
1:A:17:LEU:HD22	1:A:22:TYR:CG	2.54	0.42
1:A:303:ARG:NH1	1:A:303:ARG:HG2	2.35	0.42
1:A:208:LEU:HD22	1:B:168:PHE:CG	2.55	0.41
1:B:8:TYR:OH	1:B:260:GLU:OE1	2.38	0.41
1:B:280:LYS:O	1:B:281:ASP:C	2.58	0.41
1:A:32:ARG:HG3	1:A:32:ARG:NH1	2.35	0.41
1:A:36:LEU:HD23	1:A:71:VAL:HG12	2.03	0.41
1:A:186:GLY:O	1:A:187:LEU:HB2	2.20	0.41
1:B:335:VAL:HG23	1:B:336:GLY:N	2.35	0.41
1:A:225:ASN:HD22	1:A:299:HIS:CE1	2.38	0.41
1:B:319:THR:OG1	1:B:320:GLU:N	2.54	0.41
1:A:245:LYS:O	1:A:249:VAL:HG23	2.20	0.41
1:B:18:GLU:O	1:B:21:ARG:HG3	2.21	0.41
1:A:77:SER:HB3	1:A:291:PHE:CD1	2.56	0.41
1:A:20:ILE:O	1:A:21:ARG:HB2	2.21	0.41
1:B:232:LYS:O	1:B:232:LYS:HG2	2.21	0.40
1:B:314:VAL:O	1:B:314:VAL:HG12	2.21	0.40
1:B:16:LEU:HD22	1:B:227:LEU:HD23	2.03	0.40
1:A:27:TYR:HB3	1:A:32:ARG:HH12	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG23	1:A:223:TRP:N	2.36	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%)	336 (96%)	15 (4%)	1 (0%)	41	47
1	B	348/374 (93%)	323 (93%)	18 (5%)	7 (2%)	7	5
All	All	700/748 (94%)	659 (94%)	33 (5%)	8 (1%)	14	13

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	6	THR
1	B	235	ASP
1	B	313	LYS
1	B	304	ARG
1	B	306	ARG
1	B	27	TYR
1	B	316	GLU
1	A	278	SER

### 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%)	314 (98%)	6 (2%)	57	68
1	B	316/340 (93%)	311 (98%)	5 (2%)	62	75
All	All	636/680 (94%)	625 (98%)	11 (2%)	60	72

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	135	PHE
1	A	167	ASN
1	A	200	GLN
1	A	280	LYS
1	A	304	ARG
1	B	6	THR
1	B	135	PHE
1	B	200	GLN
1	B	316	GLU
1	B	353	ASN

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

Mol	Chain	Res	Type
1	A	46	HIS
1	A	49	GLN
1	A	68	GLN
1	A	137	ASN
1	A	167	ASN
1	A	175	HIS
1	A	216	GLN
1	A	219	ASN
1	A	268	HIS
1	A	299	HIS
1	A	334	ASN
1	B	46	HIS
1	B	49	GLN
1	B	137	ASN
1	B	200	GLN
1	B	216	GLN
1	B	256	HIS
1	B	264	GLN
1	B	272	GLN

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Mol	Chain	Res	Type
1	B	299	HIS
1	B	334	ASN
1	B	353	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	EDO	A	800	-	3,3,3	2.31	2 (66%)	2,2,2	0.44	0
3	EDO	B	801	-	3,3,3	2.24	2 (66%)	2,2,2	0.48	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
3	EDO	A	800	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	801	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	EDO	O2-C2	3.07	1.57	1.42
3	B	801	EDO	O2-C2	2.93	1.57	1.42
3	B	801	EDO	O1-C1	2.41	1.54	1.42
3	A	800	EDO	O1-C1	2.40	1.54	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	800	EDO	O1-C1-C2-O2
3	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 [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	354/374 (94%)	0.36	21 (5%) 22 33	31, 49, 82, 104	0
1	B	350/374 (93%)	0.52	29 (8%) 11 16	32, 53, 98, 131	0
All	All	704/748 (94%)	0.44	50 (7%) 16 23	31, 51, 89, 131	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	318	LYS	7.4
1	B	236	ASP	7.3
1	B	320	GLU	7.1
1	B	238	ARG	7.0
1	B	239	ASP	6.6
1	B	319	THR	6.3
1	A	318	LYS	5.8
1	B	354	VAL	5.4
1	B	23	ARG	5.3
1	A	26	ASN	5.2
1	B	7	GLU	4.9
1	A	316	GLU	4.7
1	B	303	ARG	4.6
1	A	1	MET	4.6
1	B	237	GLU	4.6
1	B	323	GLN	4.3
1	B	8	TYR	4.1
1	A	7	GLU	4.1
1	B	316	GLU	3.7
1	B	10	LEU	3.7
1	A	24	ASP	3.6
1	A	271	LYS	3.5
1	B	235	ASP	3.1
1	B	321	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	353	ASN	2.9
1	B	187	LEU	2.9
1	B	324	LYS	2.8
1	B	314	VAL	2.8
1	A	222	VAL	2.8
1	A	187	LEU	2.8
1	A	319	THR	2.7
1	A	278	SER	2.6
1	B	317	GLU	2.4
1	B	234	PHE	2.3
1	B	312	GLU	2.2
1	A	193	ALA	2.2
1	A	221	MET	2.2
1	A	311	TYR	2.2
1	B	311	TYR	2.2
1	A	186	GLY	2.2
1	A	183	ARG	2.2
1	B	222	VAL	2.2
1	A	188	GLY	2.2
1	A	354	VAL	2.1
1	B	6	THR	2.1
1	B	224	VAL	2.1
1	B	26	ASN	2.1
1	A	214	ILE	2.1
1	A	320	GLU	2.0
1	A	324	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MG	B	702	1/1	0.86	0.33	70,70,70,70	0
2	MG	A	701	1/1	0.96	0.20	61,61,61,61	0
3	EDO	A	800	4/4	0.96	0.17	34,40,41,42	0
3	EDO	B	801	4/4	0.98	0.17	34,38,41,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.