



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:15 PM UTC

PDB ID : 1YJ4 / pdb_00001yj4
Title : Y305F Trichodiene Synthase
Authors : Vedula, L.S.; Rynkiewicz, M.J.; Pyun, H.J.; Coates, R.M.; Cane, D.E.; Christianson, D.W.
Deposited on : 2005-01-13
Resolution : 2.30 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

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>.

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)
Xtriage (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

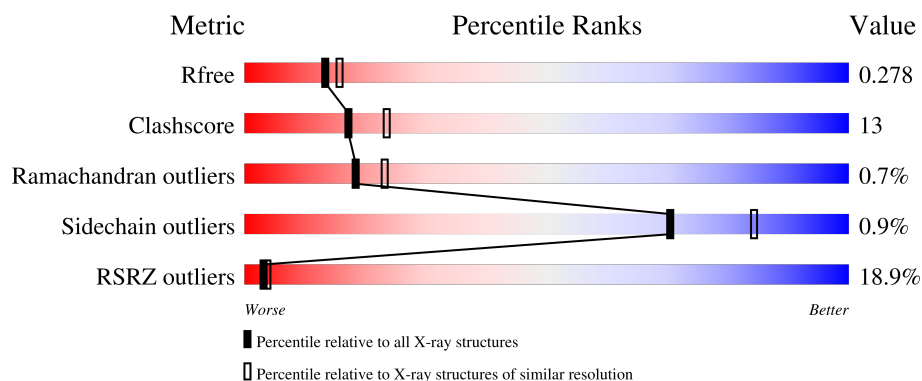
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 ≥ 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	14% 70% 25% 5%
1	B	374	21% 64% 29% 7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6013 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	54	0	0
			2939	1882	493	546	18			
1	B	349	Total	C	N	O	S	167	0	0
			2899	1859	486	537	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	305	PHE	TYR	engineered mutation	UNP P13513
B	305	PHE	TYR	engineered mutation	UNP P13513

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

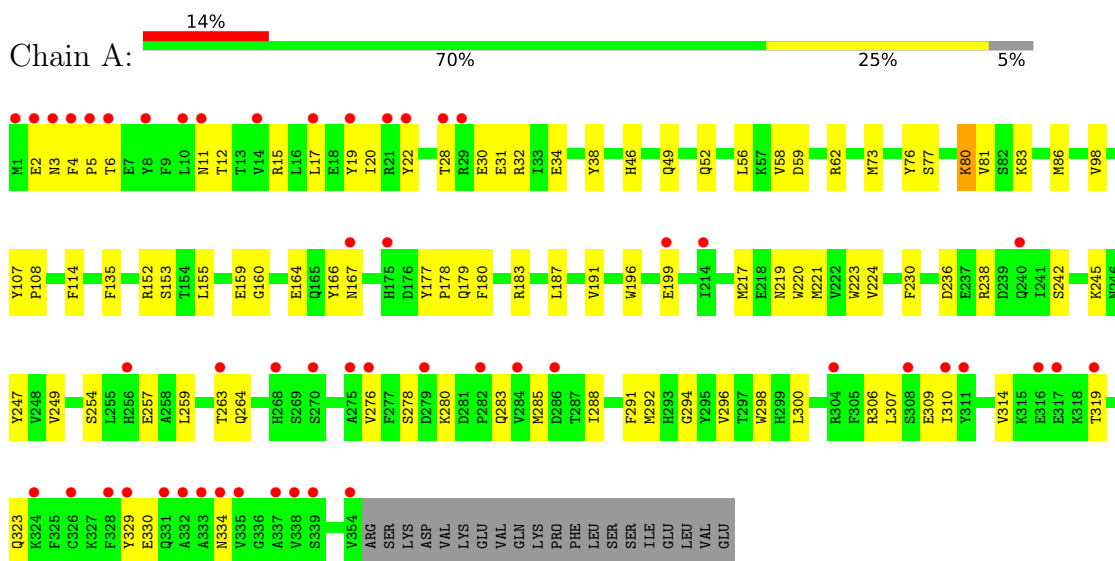
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	82	Total O 82 82	0	0
3	B	77	Total O 77 77	0	0

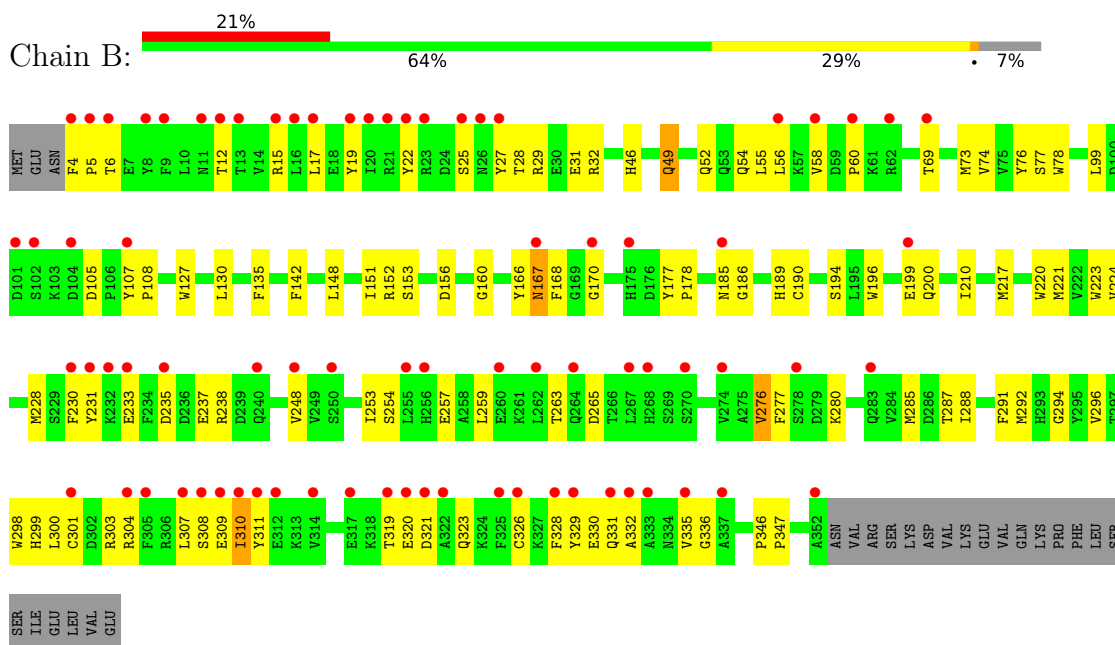
3 Residue-property plots

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, α , β , γ	122.24Å 122.24Å 151.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30 40.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.9 (40.00-2.30) 93.5 (40.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.68 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.275 0.246 , 0.278	Depositor DCC
R_{free} test set	2770 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6013	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.43	0/3024	0.91	11/4104 (0.3%)
1	B	0.41	0/2984	0.87	7/4050 (0.2%)
All	All	0.42	0/6008	0.89	18/8154 (0.2%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	GLN	OE1-CD-NE2	-9.81	112.79	122.60
1	A	283	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	A	264	GLN	OE1-CD-NE2	-9.78	112.82	122.60
1	B	323	GLN	CG-CD-NE2	6.64	126.37	116.40
1	A	283	GLN	CG-CD-NE2	6.63	126.34	116.40
1	A	264	GLN	CG-CD-NE2	6.62	126.33	116.40
1	A	49	GLN	CA-C-N	6.14	125.63	119.24
1	A	49	GLN	C-N-CA	6.14	125.63	119.24
1	A	180	PHE	N-CA-C	-5.85	104.81	111.07
1	A	196	TRP	N-CA-C	5.75	119.43	108.97
1	A	249	VAL	N-CA-C	5.68	116.46	110.72
1	B	277	PHE	N-CA-C	5.39	119.85	113.28
1	A	114	PHE	N-CA-C	5.29	116.73	111.07
1	B	276	VAL	N-CA-C	5.16	115.38	110.53
1	B	49	GLN	CA-C-N	5.12	124.57	119.24
1	B	49	GLN	C-N-CA	5.12	124.57	119.24
1	B	331	GLN	N-CA-C	-5.04	105.78	111.28
1	A	247	TYR	N-CA-C	-5.01	105.71	111.07

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	60	0
1	B	2899	0	2754	81	0
2	A	8	0	12	0	0
2	B	8	0	12	1	0
3	A	82	0	0	1	0
3	B	77	0	0	0	0
All	All	6013	0	5571	138	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 13.

All (138) 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:17:LEU:HD21	1:A:296:VAL:HG11	1.33	1.04
1:B:217:MET:HE1	1:B:220:TRP:CE3	2.07	0.90
1:A:319:THR:O	1:A:323:GLN:HG2	1.76	0.85
1:A:217:MET:HE1	1:A:220:TRP:CE3	2.14	0.83
1:B:217:MET:HE1	1:B:220:TRP:HE3	1.42	0.81
1:A:278:SER:HA	1:A:285:MET:HE2	1.63	0.80
1:B:12:THR:HG23	1:B:263:THR:HG23	1.65	0.79
1:A:59:ASP:HB3	1:A:62:ARG:HG3	1.64	0.78
1:B:288:ILE:HG22	1:B:292:MET:HE2	1.71	0.72
1:A:30:GLU:O	1:A:34:GLU:HG3	1.89	0.72
1:A:217:MET:HE1	1:A:220:TRP:HE3	1.55	0.72
1:B:300:LEU:HA	1:B:307:LEU:HD12	1.73	0.71
1:A:217:MET:HE3	1:A:220:TRP:HB3	1.72	0.71
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.56	0.69
1:B:217:MET:HE3	1:B:220:TRP:HB3	1.73	0.68
1:A:306:ARG:HD2	1:A:309:GLU:OE2	1.93	0.68
1:A:107:TYR:HB3	1:A:108:PRO:HD3	1.78	0.65
1:B:199:GLU:HG3	1:B:200:GLN:NE2	2.13	0.63
1:B:15:ARG:O	1:B:19:TYR:HD1	1.82	0.63
1:B:224:VAL:O	1:B:228:MET:HG2	1.99	0.62
1:A:217:MET:CE	1:A:220:TRP:HB3	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:SER:HA	1:B:329:TYR:OH	2.00	0.61
1:A:160:GLY:O	1:A:164:GLU:HG3	2.01	0.60
1:A:276:VAL:O	1:A:280:LYS:HD3	2.02	0.60
1:A:254:SER:OG	1:A:257:GLU:HG3	2.02	0.59
1:B:276:VAL:O	1:B:280:LYS:HD3	2.02	0.59
1:B:310:ILE:HG22	1:B:310:ILE:O	2.03	0.58
1:B:74:VAL:HA	1:B:78:TRP:CE3	2.39	0.58
1:A:59:ASP:HB3	1:A:62:ARG:CG	2.33	0.58
1:B:332:ALA:O	1:B:336:GLY:N	2.38	0.57
1:B:107:TYR:HB3	1:B:108:PRO:HD3	1.85	0.56
1:B:329:TYR:O	1:B:332:ALA:HB3	2.05	0.56
1:B:46:HIS:O	1:B:52:GLN:HG3	2.06	0.56
1:A:58:VAL:HG21	1:A:98:VAL:HG11	1.87	0.56
1:A:17:LEU:HD22	1:A:22:TYR:CG	2.41	0.55
1:A:191:VAL:HG21	1:A:221:MET:HE2	1.88	0.55
1:A:17:LEU:HD23	1:A:20:ILE:HD11	1.90	0.54
1:B:32:ARG:HG3	1:B:32:ARG:NH1	2.23	0.54
1:B:69:THR:HG22	1:B:298:TRP:HZ2	1.72	0.54
1:B:228:MET:HE3	1:B:299:HIS:HB2	1.89	0.54
1:B:217:MET:CE	1:B:220:TRP:HE3	2.18	0.53
1:B:217:MET:CE	1:B:220:TRP:HB3	2.38	0.53
1:A:217:MET:HE3	1:A:217:MET:HA	1.91	0.53
1:A:38:TYR:CD2	1:A:83:LYS:HB3	2.44	0.53
1:A:80:LYS:HE3	1:A:80:LYS:HA	1.90	0.53
1:A:217:MET:HE2	1:A:221:MET:HB2	1.91	0.52
1:B:29:ARG:HG3	1:B:29:ARG:HH11	1.74	0.52
1:B:28:THR:OG1	1:B:31:GLU:HG3	2.10	0.52
1:A:58:VAL:HG21	1:A:98:VAL:CG1	2.40	0.51
1:A:179:GLN:O	1:A:183:ARG:HB2	2.09	0.51
1:B:231:TYR:CE1	1:B:310:ILE:HD11	2.46	0.51
1:A:288:ILE:HG22	1:A:292:MET:HE2	1.93	0.51
1:A:32:ARG:HH11	1:A:32:ARG:HG3	1.76	0.50
1:B:76:TYR:O	1:B:294:GLY:HA3	2.11	0.50
1:B:301:CYS:SG	1:B:336:GLY:HA3	2.52	0.50
1:A:15:ARG:O	1:A:19:TYR:CD1	2.64	0.50
1:A:155:LEU:HG	1:B:152:ARG:HG2	1.93	0.50
1:B:29:ARG:HG3	1:B:29:ARG:NH1	2.27	0.50
1:B:27:TYR:O	1:B:32:ARG:NH1	2.46	0.49
1:B:309:GLU:C	1:B:311:TYR:H	2.19	0.49
1:B:166:TYR:O	1:B:167:ASN:C	2.54	0.49
1:A:12:THR:HG23	1:A:263:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG13	1:B:253:ILE:O	2.13	0.49
1:B:300:LEU:HD23	1:B:307:LEU:HD13	1.95	0.49
1:A:76:TYR:O	1:A:294:GLY:HA3	2.13	0.48
1:B:168:PHE:CE2	1:B:170:GLY:HA2	2.48	0.48
1:B:107:TYR:CD1	1:B:107:TYR:C	2.91	0.48
1:B:186:GLY:O	1:B:221:MET:HE1	2.14	0.48
1:B:319:THR:HG22	1:B:320:GLU:N	2.28	0.48
1:B:326:CYS:O	1:B:330:GLU:HG3	2.13	0.48
1:B:223:TRP:CZ3	1:B:265:ASP:HB3	2.48	0.48
1:B:4:PHE:O	1:B:6:THR:N	2.46	0.47
1:B:17:LEU:CD2	1:B:296:VAL:HG11	2.44	0.47
1:A:73:MET:HB2	1:A:298:TRP:CE2	2.49	0.47
1:B:153:SER:HB3	1:B:190:CYS:HB2	1.96	0.47
1:A:56:LEU:HG	1:A:58:VAL:HG23	1.96	0.47
1:A:219:ASN:HB3	1:A:223:TRP:CZ3	2.49	0.47
1:A:199:GLU:HG3	3:A:783:HOH:O	2.15	0.47
1:A:152:ARG:HD2	1:B:156:ASP:OD1	2.15	0.46
1:B:54:GLN:HG2	1:B:55:LEU:HD23	1.97	0.46
1:A:217:MET:CE	1:A:220:TRP:HE3	2.25	0.46
1:A:81:VAL:O	1:A:86:MET:HE3	2.15	0.46
1:B:152:ARG:NH2	1:B:189:HIS:ND1	2.59	0.46
1:A:242:SER:OG	1:A:245:LYS:HG3	2.16	0.46
1:B:230:PHE:CE2	1:B:259:LEU:HD22	2.52	0.45
1:B:231:TYR:C	1:B:233:GLU:H	2.24	0.45
1:A:17:LEU:HD22	1:A:22:TYR:HB2	1.98	0.45
1:B:17:LEU:HB3	1:B:22:TYR:HB2	1.98	0.45
1:A:278:SER:CA	1:A:285:MET:HE2	2.42	0.44
1:B:160:GLY:HA3	1:B:185:ASN:HB3	1.99	0.44
1:B:25:SER:C	1:B:27:TYR:H	2.24	0.44
1:B:17:LEU:HD21	1:B:296:VAL:HG11	1.99	0.44
1:B:32:ARG:HD2	1:B:335:VAL:HG22	1.98	0.44
1:B:99:LEU:HB2	1:B:127:TRP:NE1	2.33	0.44
1:B:17:LEU:HB3	1:B:22:TYR:CB	2.48	0.44
1:B:77:SER:HB3	1:B:291:PHE:CD1	2.53	0.44
1:B:329:TYR:C	1:B:329:TYR:CD1	2.96	0.44
1:A:177:TYR:HB3	1:A:178:PRO:HD3	2.00	0.44
1:A:153:SER:OG	1:A:187:LEU:HA	2.18	0.43
1:A:28:THR:OG1	1:A:31:GLU:HG3	2.18	0.43
1:B:307:LEU:O	1:B:329:TYR:HE2	2.01	0.43
1:A:2:GLU:HG2	1:A:3:ASN:N	2.33	0.43
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASP:OD1	1:A:238:ARG:HB3	2.19	0.43
1:A:310:ILE:O	1:A:314:VAL:HG22	2.19	0.43
1:B:105:ASP:OD2	1:B:108:PRO:HD3	2.19	0.43
1:B:73:MET:HB2	1:B:298:TRP:CE2	2.53	0.43
1:B:254:SER:OG	1:B:257:GLU:HG3	2.18	0.43
1:A:4:PHE:O	1:A:6:THR:N	2.50	0.43
1:B:55:LEU:HB2	1:B:130:LEU:HD11	2.00	0.43
1:A:300:LEU:HA	1:A:307:LEU:HD12	2.01	0.43
1:A:166:TYR:O	1:A:167:ASN:C	2.62	0.43
1:B:319:THR:HG22	1:B:321:ASP:H	1.84	0.43
1:A:230:PHE:CE2	1:A:259:LEU:HD22	2.54	0.43
1:B:168:PHE:CZ	1:B:170:GLY:HA2	2.54	0.43
1:B:142:PHE:CE2	1:B:194:SER:HA	2.54	0.42
1:B:27:TYR:HA	1:B:31:GLU:OE1	2.19	0.42
1:A:11:ASN:O	1:A:15:ARG:HG3	2.20	0.42
1:A:220:TRP:O	1:A:224:VAL:HG23	2.20	0.42
1:B:56:LEU:HG	1:B:58:VAL:HG23	2.00	0.42
1:B:231:TYR:C	1:B:233:GLU:N	2.79	0.41
1:B:49:GLN:HB2	1:B:52:GLN:HG2	2.02	0.41
1:A:77:SER:HB3	1:A:291:PHE:CD1	2.55	0.41
1:B:285:MET:O	1:B:285:MET:HE3	2.21	0.41
1:B:346:PRO:HB2	1:B:347:PRO:HD2	2.02	0.41
1:B:151:ILE:HG23	2:B:701:EDO:H22	2.03	0.41
1:B:196:TRP:CD1	1:B:210:ILE:HG23	2.56	0.41
1:B:303:ARG:O	1:B:304:ARG:C	2.64	0.41
1:A:46:HIS:O	1:A:52:GLN:HG3	2.21	0.41
1:B:32:ARG:NH1	1:B:32:ARG:CG	2.84	0.41
1:B:320:GLU:HG2	1:B:320:GLU:O	2.20	0.41
1:A:329:TYR:C	1:A:329:TYR:CD1	2.99	0.41
1:B:217:MET:HE2	1:B:221:MET:HB2	2.03	0.40
1:A:4:PHE:HA	1:A:5:PRO:HD3	1.91	0.40
1:A:17:LEU:HD23	1:A:17:LEU:HA	1.87	0.40
1:A:159:GLU:HB2	1:B:148:LEU:HD21	2.03	0.40
1:A:330:GLU:O	1:A:334:ASN:ND2	2.55	0.40
1:B:17:LEU:HD12	1:B:328:PHE:CG	2.57	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	352/374 (94%)	339 (96%)	13 (4%)	0	100	100
1	B	347/374 (93%)	320 (92%)	22 (6%)	5 (1%)	9	9
All	All	699/748 (93%)	659 (94%)	35 (5%)	5 (1%)	18	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	ARG
1	B	237	GLU
1	B	5	PRO
1	B	235	ASP
1	B	310	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	320/340 (94%)	318 (99%)	2 (1%)	78	89
1	B	315/340 (93%)	311 (99%)	4 (1%)	61	77
All	All	635/680 (93%)	629 (99%)	6 (1%)	70	84

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS

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Mol	Chain	Res	Type
1	A	135	PHE
1	B	60	PRO
1	B	135	PHE
1	B	167	ASN
1	B	287	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	219	ASN
1	A	268	HIS
1	A	331	GLN
1	A	350	GLN
1	B	54	GLN
1	B	149	ASN
1	B	179	GLN
1	B	200	GLN
1	B	331	GLN
1	B	350	GLN

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](#)

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	$\# Z > 2$
2	EDO	A	702	-	3,3,3	0.61	0	2,2,2	0.56	0
2	EDO	A	700	-	3,3,3	0.57	0	2,2,2	0.44	0
2	EDO	B	703	-	3,3,3	0.51	0	2,2,2	0.51	0
2	EDO	B	701	-	3,3,3	0.52	0	2,2,2	0.38	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
2	EDO	A	702	-	-	1/1/1/1	-
2	EDO	A	700	-	-	1/1/1/1	-
2	EDO	B	703	-	-	1/1/1/1	-
2	EDO	B	701	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	EDO	O1-C1-C2-O2
2	A	700	EDO	O1-C1-C2-O2
2	B	701	EDO	O1-C1-C2-O2
2	B	703	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	348/374 (93%)	0.92	51 (14%) 6 6	31, 47, 73, 103	0
1	B	331/374 (88%)	1.41	77 (23%) 2 2	2, 50, 102, 116	1 (0%)
All	All	679/748 (90%)	1.16	128 (18%) 3 4	2, 48, 92, 116	1 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	26	ASN	13.5
1	B	4	PHE	9.1
1	B	322	ALA	8.7
1	B	314	VAL	7.6
1	B	328	PHE	6.8
1	B	13	THR	6.6
1	B	8	TYR	6.4
1	B	326	CYS	6.4
1	B	11	ASN	6.4
1	B	9	PHE	6.3
1	B	333	ALA	6.2
1	B	312	GLU	5.9
1	A	354	VAL	5.9
1	B	325	PHE	5.8
1	B	5	PRO	5.7
1	A	326	CYS	5.2
1	B	235	ASP	5.0
1	A	2	GLU	5.0
1	B	25	SER	4.8
1	B	319	THR	4.6
1	B	309	GLU	4.6
1	B	6	THR	4.5
1	B	335	VAL	4.5
1	B	337	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	308	SER	4.4
1	B	233	GLU	4.4
1	B	329	TYR	4.2
1	A	335	VAL	4.2
1	A	319	THR	4.2
1	B	317	GLU	4.2
1	A	317	GLU	4.1
1	B	15	ARG	4.0
1	B	17	LEU	4.0
1	A	8	TYR	3.9
1	B	307	LEU	3.9
1	B	27	TYR	3.8
1	B	22	TYR	3.8
1	A	275	ALA	3.7
1	B	19	TYR	3.7
1	A	199	GLU	3.6
1	A	1	MET	3.5
1	B	270	SER	3.5
1	A	316	GLU	3.4
1	B	352	ALA	3.4
1	B	311	TYR	3.4
1	B	101	ASP	3.4
1	B	104	ASP	3.4
1	B	240	GLN	3.4
1	A	263	THR	3.3
1	A	311	TYR	3.3
1	B	321	ASP	3.3
1	A	14	VAL	3.3
1	B	331	GLN	3.2
1	B	310	ILE	3.2
1	A	282	PRO	3.2
1	A	3	ASN	3.1
1	B	199	GLU	3.1
1	A	6	THR	3.1
1	B	304	ARG	3.1
1	B	320	GLU	3.1
1	A	28	THR	3.0
1	B	12	THR	3.0
1	A	337	ALA	3.0
1	B	256	HIS	3.0
1	B	20	ILE	3.0
1	B	69	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	4	PHE	2.9
1	A	17	LEU	2.9
1	A	256	HIS	2.9
1	B	231	TYR	2.9
1	A	308	SER	2.9
1	A	279	ASP	2.9
1	B	170	GLY	2.9
1	B	21	ARG	2.9
1	B	56	LEU	2.9
1	B	274	VAL	2.9
1	B	264	GLN	2.8
1	A	10	LEU	2.8
1	B	332	ALA	2.8
1	A	268	HIS	2.8
1	B	262	LEU	2.7
1	A	328	PHE	2.7
1	B	305	PHE	2.7
1	B	248	VAL	2.7
1	B	102	SER	2.7
1	B	16	LEU	2.6
1	B	255	LEU	2.6
1	A	339	SER	2.6
1	B	175	HIS	2.6
1	A	324	LYS	2.5
1	B	268	HIS	2.5
1	A	19	TYR	2.5
1	A	276	VAL	2.4
1	A	334	ASN	2.4
1	A	332	ALA	2.4
1	B	232	LYS	2.4
1	B	60	PRO	2.4
1	A	22	TYR	2.4
1	B	23	ARG	2.4
1	B	62	ARG	2.4
1	A	167	ASN	2.4
1	A	5	PRO	2.4
1	B	278	SER	2.4
1	B	260	GLU	2.4
1	A	333	ALA	2.3
1	B	250	SER	2.3
1	A	175	HIS	2.3
1	A	284	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	230	PHE	2.2
1	A	310	ILE	2.2
1	A	240	GLN	2.2
1	A	214	ILE	2.2
1	A	304	ARG	2.2
1	B	185	ASN	2.2
1	B	301	CYS	2.2
1	B	107	TYR	2.1
1	A	11	ASN	2.1
1	B	167	ASN	2.1
1	B	283	GLN	2.1
1	A	21	ARG	2.1
1	B	58	VAL	2.1
1	A	270	SER	2.1
1	A	338	VAL	2.1
1	A	331	GLN	2.1
1	A	329	TYR	2.1
1	A	29	ARG	2.1
1	A	286	ASP	2.0
1	B	267	LEU	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, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	B	703	4/4	0.81	0.18	74,75,76,77	0
2	EDO	A	702	4/4	0.91	0.10	45,46,48,52	0
2	EDO	B	701	4/4	0.93	0.09	36,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	700	4/4	0.96	0.07	34,36,36,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.