



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:17 PM UTC

PDB ID : 2PS7 / pdb_00002ps7
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

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

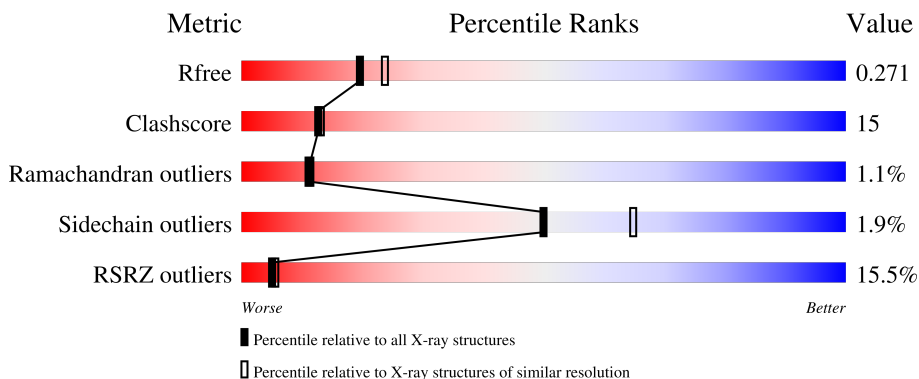
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 ≥ 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
			Total	C	N	O	S			
1	A	354	2939	1882	493	546	18	0	0	0
1	B	350	2903	1859	488	539	17	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 MAGNESIUM ION (CCD ID: 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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

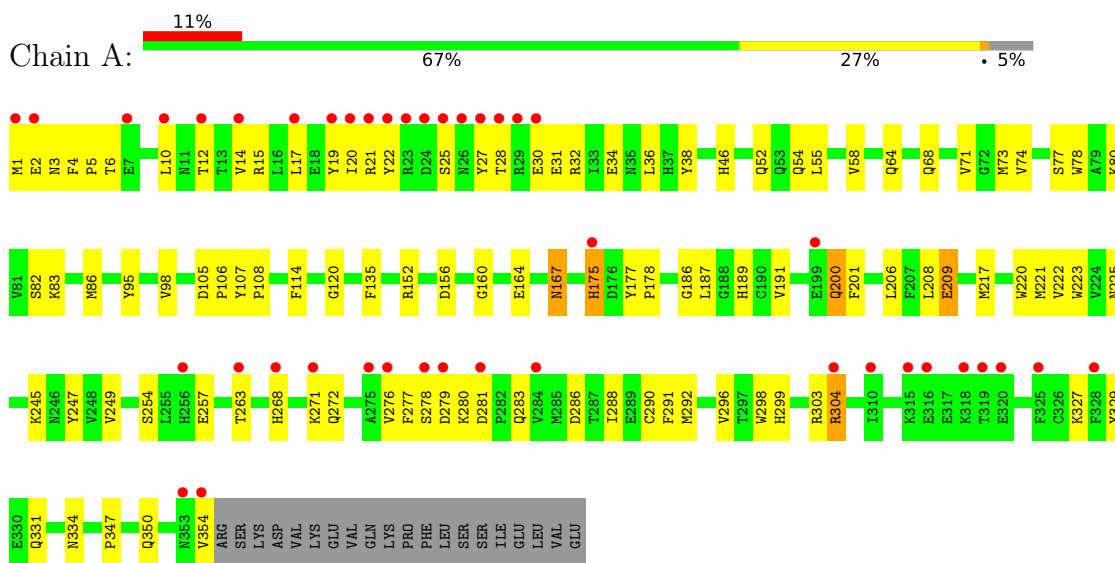
- Molecule 4 is water.

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

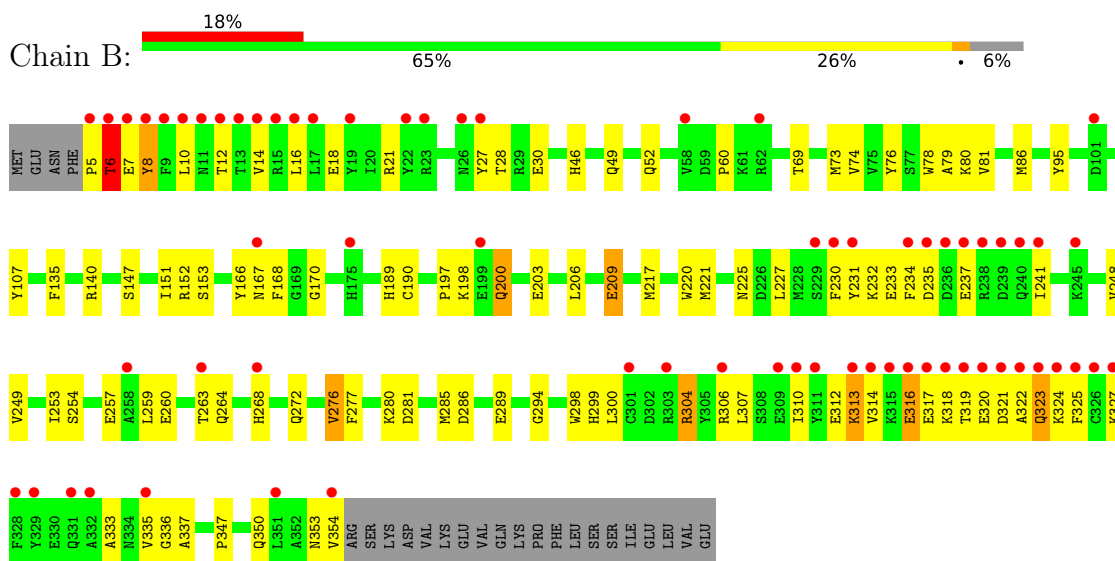
3 Residue-property plots [i](#)

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, α , β , γ	122.43Å 122.43Å 151.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.35 50.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.35) 97.8 (50.00-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.34Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.258 0.251 , 0.271	Depositor DCC
R_{free} test set	2177 reflections (4.03%)	wwPDB-VP
Wilson B-factor (Å ²)	48.9	Xtrriage
Anisotropy	0.197	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 28.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5961	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtrriage'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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.44	0/3024	0.87	4/4104 (0.1%)
1	B	0.40	0/2987	0.89	8/4054 (0.2%)
All	All	0.42	0/6011	0.88	12/8158 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	THR	N-CA-C	-7.05	98.59	109.52
1	B	7	GLU	N-CA-C	-7.01	103.91	113.30
1	B	249	VAL	N-CA-C	5.46	115.67	110.42
1	B	323	GLN	N-CA-C	-5.35	106.75	113.28
1	B	79	ALA	N-CA-C	5.35	118.91	112.38
1	B	276	VAL	N-CA-C	5.29	115.95	110.82
1	B	277	PHE	N-CA-C	5.27	119.71	113.28
1	B	8	TYR	N-CA-C	-5.26	106.13	112.54
1	A	114	PHE	N-CA-C	5.10	116.52	111.07
1	A	247	TYR	N-CA-C	-5.09	105.63	111.07
1	A	54	GLN	N-CA-C	5.04	117.55	111.40
1	A	175	HIS	N-CA-C	5.03	117.49	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	78	0
1	B	2903	0	2761	98	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	173	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 15.

All (173) 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:B:217:MET:HE1	1:B:220:TRP:CE3	2.09	0.88
1:B:320:GLU:C	1:B:324:LYS:HG3	2.00	0.86
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:217:MET:HE1	1:B:220:TRP:HE3	1.45	0.81
1:A:217:MET:HA	1:A:217:MET:HE3	1.61	0.80
1:B:320:GLU:C	1:B:324:LYS:CG	2.55	0.79
1:A:64:GLN:HE21	1:A:68:GLN:HE21	1.31	0.78
1:B:317:GLU:O	1:B:323:GLN:CD	2.26	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:217:MET:HE3	1:B:220:TRP:HB3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:MET:HE1	1:A:220:TRP:CE3	2.29	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:B:217:MET:HE2	1:B:221:MET:HB2	1.78	0.64
1:B:285:MET:HE2	1:B:289:GLU:HG3	1.80	0.64
1:A:12:THR:HG21	1:A:263:THR:HG21	1.80	0.64
1:B:217:MET:HE3	1:B:217:MET:HA	1.81	0.62
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:320:GLU:C	1:B:324:LYS:HG2	2.26	0.60
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: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
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:A:217:MET:HE3	1:A:220:TRP:HB3	1.86	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:288:ILE:HG22	1:A:292:MET:HE2	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:A:46:HIS:O	1:A:52:GLN:HG3	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:PHE:CE2	1:B:259:LEU:HD22	2.44	0.52
1:B:353:ASN:O	1:B:354:VAL:C	2.53	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:1:MET:C	1:A:3:ASN:H	2.17	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:217:MET:CE	1:B:220:TRP:HE3	2.21	0.49
1:B:237:GLU:O	1:B:237:GLU:CG	2.60	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:81:VAL:O	1:B:86:MET:HE3	2.13	0.49
1:B:107:TYR:CD1	1:B:107:TYR:C	2.90	0.49
1:B:140:ARG:O	1:B:198:LYS:HE2	2.12	0.48
1:A:280:LYS:O	1:A:281:ASP:C	2.56	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:321:ASP:C	1:B:323:GLN:H	2.23	0.47
1:B:5:PRO:N	1:B:234:PHE:HE2	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:280:LYS:O	1:B:281:ASP:C	2.58	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:25:SER:C	1:A:27:TYR:H	2.24	0.46
1:A:177:TYR:HB3	1:A:178:PRO:HD3	1.98	0.46
1:A:191:VAL:HG21	1:A:221:MET:HE2	1.97	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:A:105:ASP:HA	1:A:106:PRO:HD3	1.88	0.44
1:A:107:TYR:C	1:A:107:TYR:CD1	2.95	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: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:B:353:ASN:ND2	1:B:353:ASN:C	2.75	0.43
1:A:201:PHE:CZ	1:A:283:GLN:HG2	2.53	0.43
1:A:74:VAL:O	1:A:78:TRP:HB2	2.18	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:329:TYR:C	1:A:329:TYR:CD1	2.96	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:A:277:PHE:C	1:A:279:ASP:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLU:C	1:B:323:GLN:HB2	2.44	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: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:217:MET:HE1	1:B:220:TRP:HB3	2.02	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:30:GLU:H	1:B:30:GLU:CD	2.28	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:B:5:PRO:C	1:B:6:THR:CG2	2.94	0.41
1:A:20:ILE:O	1:A:21:ARG:HB2	2.21	0.41
1:B:166:TYR:O	1:B:167:ASN:C	2.63	0.40
1:B:232:LYS:O	1:B:232:LYS:HG2	2.21	0.40
1:B:16:LEU:HD22	1:B:227:LEU:HD23	2.03	0.40
1:B:314:VAL:O	1:B:314:VAL:HG12	2.21	0.40
1:A:27:TYR:HB3	1:A:32:ARG:HH12	1.86	0.40
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%)	36	43
1	B	348/374 (93%)	323 (93%)	18 (5%)	7 (2%)	6	4
All	All	700/748 (94%)	659 (94%)	33 (5%)	8 (1%)	11	11

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%)	50	65
1	B	316/340 (93%)	310 (98%)	6 (2%)	50	65
All	All	636/680 (94%)	624 (98%)	12 (2%)	50	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	135	PHE
1	A	167	ASN
1	A	200	GLN
1	A	209	GLU
1	A	304	ARG
1	B	6	THR
1	B	60	PRO

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Mol	Chain	Res	Type
1	B	135	PHE
1	B	200	GLN
1	B	209	GLU
1	B	316	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) 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	200	GLN
1	A	216	GLN
1	A	256	HIS
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	179	GLN
1	B	200	GLN
1	B	216	GLN
1	B	256	HIS
1	B	264	GLN
1	B	272	GLN
1	B	299	HIS
1	B	334	ASN
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 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	B	801	-	3,3,3	2.26	2 (66%)	2,2,2	0.47	0
3	EDO	A	800	-	3,3,3	2.32	2 (66%)	2,2,2	0.43	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	B	801	-	-	1/1/1/1	-
3	EDO	A	800	-	-	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	3.11	1.57	1.42
3	B	801	EDO	O2-C2	2.97	1.57	1.42
3	B	801	EDO	O1-C1	2.43	1.54	1.42
3	A	800	EDO	O1-C1	2.42	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	B	801	EDO	O1-C1-C2-O2
3	A	800	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, 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	354/374 (94%)	0.75	42 (11%) 9 10	31, 49, 82, 104	0
1	B	350/374 (93%)	1.22	67 (19%) 3 3	32, 53, 98, 131	0
All	All	704/748 (94%)	0.98	109 (15%) 5 5	31, 51, 89, 131	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PRO	12.2
1	B	320	GLU	10.7
1	B	239	ASP	10.4
1	B	236	ASP	9.5
1	B	7	GLU	8.8
1	B	238	ARG	8.1
1	B	23	ARG	7.4
1	B	237	GLU	7.3
1	B	6	THR	6.5
1	A	316	GLU	6.4
1	A	25	SER	6.2
1	B	303	ARG	6.1
1	B	323	GLN	5.8
1	B	10	LEU	5.7
1	B	314	VAL	5.6
1	B	321	ASP	5.5
1	A	354	VAL	5.5
1	A	7	GLU	5.5
1	B	354	VAL	5.4
1	B	318	LYS	5.0
1	A	319	THR	5.0
1	B	324	LYS	4.8
1	B	241	ILE	4.7
1	B	319	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	26	ASN	4.7
1	A	318	LYS	4.7
1	A	1	MET	4.6
1	A	19	TYR	4.2
1	B	315	LYS	4.2
1	A	271	LYS	4.0
1	A	27	TYR	3.9
1	B	317	GLU	3.9
1	B	22	TYR	3.8
1	B	12	THR	3.8
1	A	275	ALA	3.7
1	B	14	VAL	3.6
1	B	316	GLU	3.6
1	B	311	TYR	3.5
1	A	23	ARG	3.5
1	B	234	PHE	3.4
1	B	322	ALA	3.3
1	A	26	ASN	3.3
1	B	231	TYR	3.3
1	A	22	TYR	3.2
1	A	284	VAL	3.2
1	B	8	TYR	3.2
1	B	268	HIS	3.1
1	A	278	SER	3.0
1	B	62	ARG	3.0
1	B	13	THR	2.9
1	B	240	GLN	2.9
1	B	327	LYS	2.9
1	B	27	TYR	2.9
1	B	328	PHE	2.8
1	A	325	PHE	2.8
1	B	335	VAL	2.8
1	B	301	CYS	2.8
1	A	17	LEU	2.8
1	A	328	PHE	2.8
1	B	235	ASP	2.7
1	A	24	ASP	2.7
1	B	199	GLU	2.7
1	A	199	GLU	2.6
1	B	9	PHE	2.6
1	A	20	ILE	2.6
1	A	12	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	21	ARG	2.6
1	B	258	ALA	2.6
1	A	2	GLU	2.5
1	A	276	VAL	2.5
1	A	256	HIS	2.5
1	A	30	GLU	2.5
1	B	351	LEU	2.5
1	B	313	LYS	2.5
1	A	14	VAL	2.4
1	B	167	ASN	2.4
1	B	101	ASP	2.4
1	A	320	GLU	2.4
1	B	230	PHE	2.4
1	A	315	LYS	2.3
1	A	28	THR	2.3
1	B	310	ILE	2.3
1	A	353	ASN	2.3
1	B	19	TYR	2.3
1	B	329	TYR	2.3
1	A	263	THR	2.3
1	A	304	ARG	2.3
1	B	306	ARG	2.3
1	A	268	HIS	2.3
1	B	332	ALA	2.2
1	A	10	LEU	2.2
1	B	16	LEU	2.2
1	B	11	ASN	2.2
1	A	29	ARG	2.2
1	B	17	LEU	2.2
1	B	325	PHE	2.2
1	B	229	SER	2.2
1	B	15	ARG	2.1
1	A	281	ASP	2.1
1	A	310	ILE	2.1
1	B	245	LYS	2.1
1	B	175	HIS	2.1
1	B	58	VAL	2.1
1	B	326	CYS	2.1
1	A	175	HIS	2.1
1	A	279	ASP	2.1
1	B	309	GLU	2.0
1	B	263	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLN	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	MG	B	702	1/1	0.82	0.22	70,70,70,70	0
2	MG	A	701	1/1	0.90	0.12	61,61,61,61	0
3	EDO	A	800	4/4	0.96	0.07	34,40,41,42	0
3	EDO	B	801	4/4	0.96	0.08	34,38,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.