



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:24 PM UTC

PDB ID : 2PS5 / pdb_00002ps5
Title : N225D Trichodiene Synthase: Complex With Mg and Pyrophosphate
Authors : Vedula, L.S.; Cane, D.E.; Christianson, D.W.
Deposited on : 2007-05-04
Resolution : 2.10 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)
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

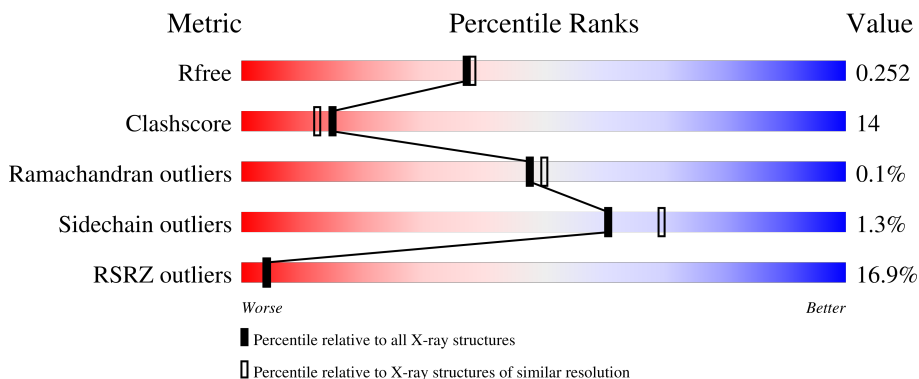
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	 10% 68% 25% • 6%
1	B	374	 22% 67% 26% • 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6251 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.

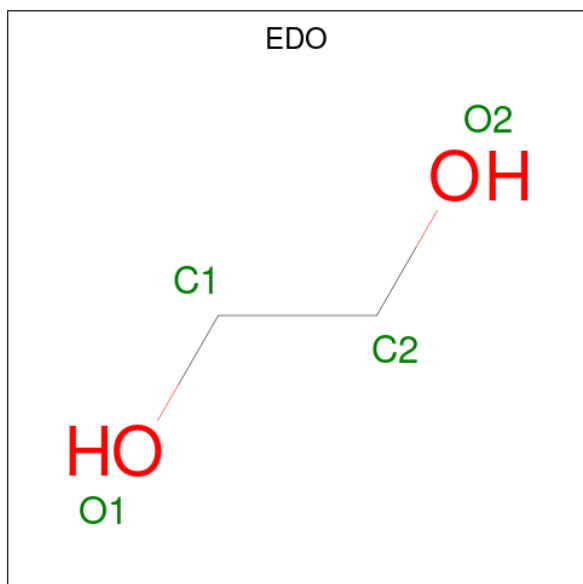
- Molecule 1 is a protein called Trichodiene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	353	2965	1895	498	555	17	0	5	0
1	B	353	2955	1892	494	550	19	0	3	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASP	ASN	engineered mutation	UNP P13513
B	225	ASP	ASN	engineered mutation	UNP P13513

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



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

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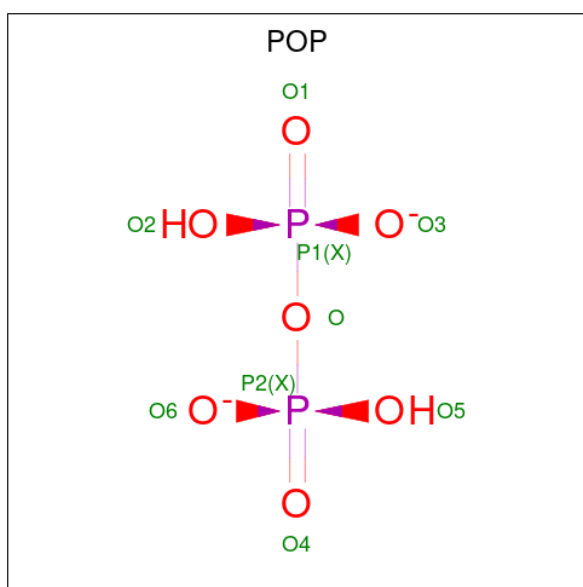
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

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

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

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



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

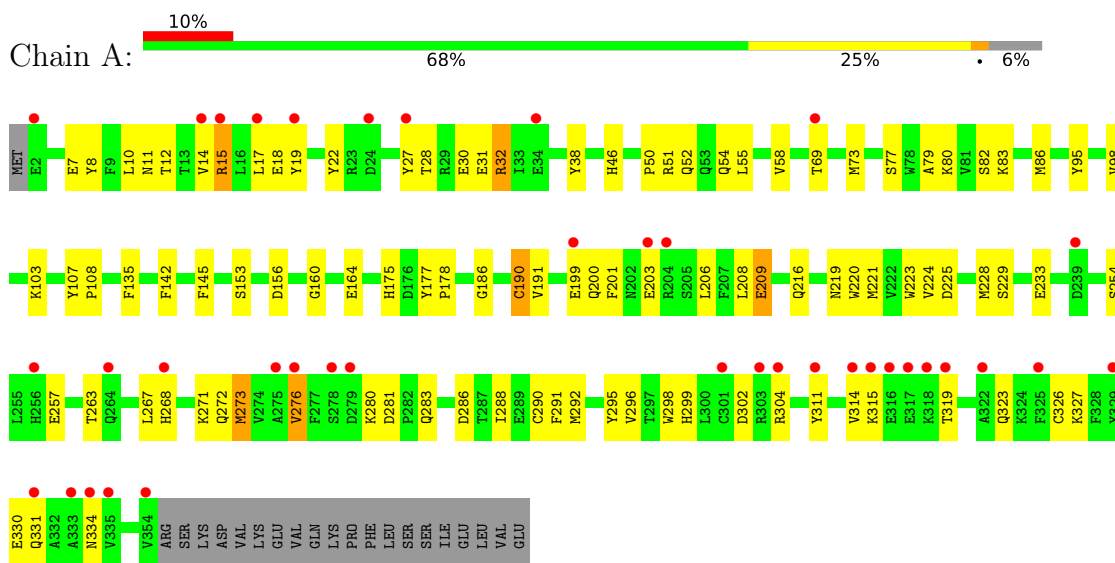
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	169	Total O 169 169	0	0
5	B	138	Total O 138 138	0	0

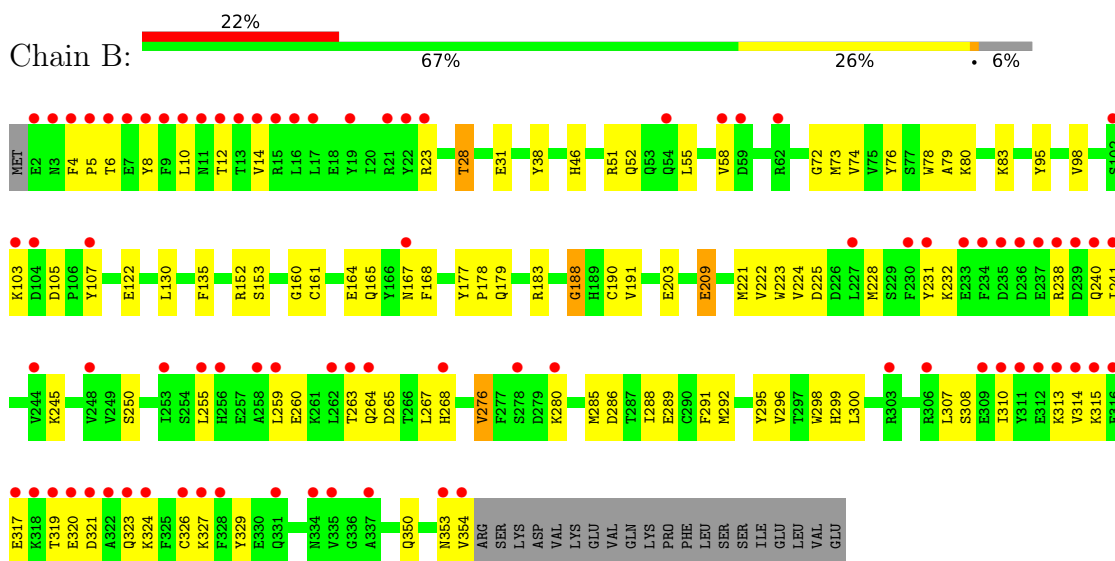
3 Residue-property plots [i](#)

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 i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.23Å 122.23Å 151.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.10) 99.5 (50.00-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.10Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.248 0.232 , 0.252	Depositor DCC
R_{free} test set	1910 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtrriage
Anisotropy	0.120	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.020 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6251	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: POP, EDO, MG

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	0.41	0/3050	0.84	5/4141 (0.1%)
1	B	0.38	0/3040	0.86	8/4126 (0.2%)
All	All	0.40	0/6090	0.85	13/8267 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	THR	N-CA-C	-8.95	97.28	110.52
1	A	186	GLY	N-CA-C	6.42	122.62	114.66
1	B	276	VAL	N-CA-C	6.07	116.71	110.82
1	A	142	PHE	N-CA-C	6.06	118.91	109.52
1	A	276	VAL	N-CA-C	5.57	116.35	110.72
1	A	190	CYS	N-CA-C	-5.53	105.17	111.14
1	B	188	GLY	N-CA-C	5.29	118.63	112.50
1	B	105	ASP	CA-C-N	5.28	124.61	118.85
1	B	105	ASP	C-N-CA	5.28	124.61	118.85
1	B	79	ALA	N-CA-C	5.24	118.78	112.38
1	B	55	LEU	N-CA-C	5.20	117.85	111.82
1	A	79	ALA	N-CA-C	5.08	118.25	111.75
1	B	250	SER	N-CA-C	5.02	116.44	111.07

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	2965	0	2793	76	0
1	B	2955	0	2803	86	0
2	A	8	0	12	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	169	0	0	4	0
5	B	138	0	0	3	0
All	All	6251	0	5614	159	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 (159) 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	1.35	1.08
1:B:288:ILE:HG22	1:B:292:MET:HE2	1.47	0.93
1:A:228:MET:HE1	1:A:296:VAL:HA	1.49	0.91
1:A:326:CYS:O	1:A:330:GLU:HG3	1.83	0.77
1:B:188:GLY:HA2	1:B:221[A]:MET:HE1	1.67	0.77
1:B:324:LYS:HA	1:B:327:LYS:HZ2	1.48	0.76
1:B:260:GLU:HG3	1:B:264:GLN:HE21	1.49	0.74
1:B:221[B]:MET:HE2	1:B:222:VAL:HA	1.69	0.73
1:A:254:SER:OG	1:A:257:GLU:HG3	1.91	0.71
1:A:107:TYR:HB3	1:A:108:PRO:HD3	1.73	0.71
1:B:285:MET:HE2	1:B:289:GLU:HG3	1.76	0.68
1:B:51:ARG:NH1	1:B:130:LEU:HD23	2.10	0.67
1:A:304[A]:ARG:HB2	1:A:304[A]:ARG:NH1	2.10	0.67
1:A:19:TYR:CE2	1:A:271:LYS:HE3	2.30	0.67
1:B:350:GLN:O	1:B:354:VAL:HG23	1.96	0.65
1:A:216:GLN:HB3	1:A:273:MET:HE2	1.77	0.65
1:B:153:SER:HB3	1:B:190:CYS:HB2	1.80	0.63
1:A:175:HIS:HD2	1:B:268:HIS:NE2	1.96	0.63
1:A:80:LYS:HE2	1:A:290:CYS:SG	2.38	0.63
1:A:216:GLN:CB	1:A:273:MET:HE2	2.29	0.62
1:A:54:GLN:HG3	1:A:55:LEU:HD23	1.80	0.62
1:B:80:LYS:HE3	1:B:286:ASP:OD2	1.99	0.62
1:B:221[B]:MET:HE3	1:B:295:TYR:OH	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:GLU:HB2	5:A:867:HOH:O	2.01	0.61
1:A:69[A]:THR:HG23	1:A:302:ASP:OD2	2.01	0.60
1:B:188:GLY:HA2	1:B:221[A]:MET:CE	2.31	0.60
1:A:224:VAL:CG1	1:A:228:MET:HE2	2.30	0.60
1:B:255:LEU:O	1:B:259:LEU:HD23	2.02	0.60
1:B:28:THR:OG1	1:B:31:GLU:HG3	2.01	0.60
1:B:320:GLU:O	1:B:324:LYS:HG2	2.01	0.60
1:A:156:ASP:OD1	1:B:152:ARG:HD2	2.01	0.59
1:B:167:ASN:HA	1:B:241:ILE:HG13	1.84	0.59
1:A:263[A]:THR:HG21	5:A:906:HOH:O	2.02	0.59
1:B:165:GLN:NE2	1:B:238:ARG:HH12	2.01	0.59
1:A:304[A]:ARG:HB2	1:A:304[A]:ARG:HH11	1.68	0.58
1:A:153:SER:HB3	1:A:190:CYS:HB2	1.85	0.58
1:B:324:LYS:HA	1:B:327:LYS:NZ	2.18	0.58
1:A:82:SER:O	1:A:86:MET:HG3	2.04	0.58
1:B:23:ARG:O	1:B:23:ARG:HG3	2.04	0.57
1:B:319:THR:HG22	1:B:321:ASP:H	1.69	0.57
1:B:183:ARG:NH1	5:B:809:HOH:O	2.32	0.57
1:A:268:HIS:CD2	1:A:272:GLN:HG2	2.40	0.57
1:A:69[A]:THR:HG22	1:A:298:TRP:HZ2	1.71	0.56
1:B:259:LEU:O	1:B:263:THR:HG23	2.05	0.55
1:B:285:MET:CE	1:B:289:GLU:HG3	2.37	0.54
1:A:199:GLU:HB3	1:A:200:GLN:NE2	2.23	0.54
1:B:353:ASN:O	1:B:354:VAL:C	2.50	0.54
1:B:225:ASP:OD2	1:B:299:HIS:HE1	1.91	0.53
1:B:12:THR:HB	1:B:263:THR:HG21	1.90	0.53
1:A:28:THR:OG1	1:A:31:GLU:HG3	2.09	0.53
1:B:203:GLU:HB2	5:B:882:HOH:O	2.09	0.53
1:B:58[A]:VAL:HG21	1:B:98:VAL:CG1	2.38	0.53
1:A:177:TYR:HB3	1:A:178:PRO:HD3	1.90	0.52
1:B:228:MET:HE1	1:B:296:VAL:HG13	1.90	0.52
1:B:285:MET:HG3	1:B:289:GLU:OE2	2.09	0.52
1:A:14:VAL:O	1:A:18:GLU:HG3	2.10	0.52
1:A:52:GLN:OE1	1:A:95:TYR:OH	2.28	0.52
1:B:285:MET:HE2	1:B:289:GLU:CG	2.39	0.52
1:B:240:GLN:OE1	1:B:245:LYS:HE2	2.10	0.51
1:A:27:TYR:HB3	1:A:32:ARG:NH1	2.26	0.51
1:B:10:LEU:O	1:B:14:VAL:HG23	2.10	0.51
1:A:191:VAL:HG21	1:A:221:MET:HE2	1.91	0.51
1:A:12:THR:HG23	1:A:263[B]:THR:HG23	1.93	0.51
1:B:74:VAL:HA	1:B:78:TRP:CE3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:HG3	1:A:8:TYR:N	2.26	0.51
1:B:103:LYS:O	1:B:103:LYS:HG3	2.11	0.50
1:B:263:THR:O	1:B:267:LEU:HG	2.11	0.50
1:A:229:SER:HB3	1:A:233:GLU:OE2	2.11	0.50
1:B:276:VAL:O	1:B:280:LYS:HD3	2.10	0.50
1:B:46:HIS:HE1	1:B:95:TYR:OH	1.94	0.50
1:B:160:GLY:O	1:B:164:GLU:HG3	2.12	0.50
1:A:12:THR:CG2	1:A:263[B]:THR:HG23	2.42	0.50
1:B:224:VAL:HG13	1:B:228:MET:HE3	1.93	0.50
1:B:260:GLU:HG3	1:B:264:GLN:NE2	2.24	0.50
1:A:304[A]:ARG:HH11	1:A:304[A]:ARG:CB	2.24	0.49
1:B:51:ARG:HH12	1:B:130:LEU:HD23	1.77	0.49
1:A:331:GLN:O	1:A:334:ASN:HB3	2.11	0.49
1:B:223:TRP:CZ3	1:B:265:ASP:HB3	2.47	0.49
1:A:80:LYS:CE	1:A:290:CYS:SG	3.00	0.49
1:A:206:LEU:HA	1:A:209:GLU:OE2	2.11	0.49
1:B:12:THR:CG2	1:B:263:THR:HG21	2.42	0.49
1:B:191:VAL:HG11	1:B:221[A]:MET:SD	2.53	0.49
1:B:58[A]:VAL:HG21	1:B:98:VAL:HG11	1.95	0.49
1:A:38:TYR:CD2	1:A:83:LYS:HB3	2.48	0.48
1:A:160:GLY:O	1:A:164:GLU:HG3	2.13	0.48
1:A:268:HIS:HD2	1:A:272:GLN:HG2	1.78	0.48
1:B:300:LEU:HA	1:B:307:LEU:HD12	1.95	0.48
1:A:145:PHE:HB3	1:A:203:GLU:CD	2.39	0.48
1:B:291:PHE:O	1:B:295:TYR:HB2	2.12	0.48
1:A:58:VAL:HG21	1:A:98:VAL:HG11	1.95	0.48
1:A:201:PHE:CE2	1:A:283:GLN:HG2	2.48	0.48
1:B:300:LEU:HD23	1:B:307:LEU:CD1	2.43	0.48
1:B:353:ASN:C	1:B:353:ASN:HD22	2.22	0.48
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.95	0.47
1:A:276:VAL:O	1:A:280:LYS:HD3	2.14	0.47
1:B:191:VAL:HB	1:B:221[A]:MET:SD	2.55	0.47
1:B:8:TYR:OH	1:B:260:GLU:OE1	2.32	0.47
1:A:73:MET:HB2	1:A:298:TRP:CE2	2.49	0.47
1:A:295:TYR:O	1:A:299:HIS:HD2	1.98	0.47
1:A:50:PRO:HG2	5:A:851:HOH:O	2.15	0.46
1:A:288:ILE:HG22	1:A:292:MET:HE2	1.97	0.46
1:A:10:LEU:HD11	1:A:314:VAL:HG11	1.96	0.46
1:A:46:HIS:HE1	1:A:95:TYR:OH	1.98	0.46
1:B:292:MET:O	1:B:296:VAL:HG23	2.16	0.46
1:A:15:ARG:NH1	1:A:267:LEU:HD13	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:MET:HB2	1:B:298:TRP:CE2	2.51	0.46
1:B:228:MET:HE1	1:B:296:VAL:HG22	1.98	0.46
1:B:323:GLN:O	1:B:327:LYS:HG3	2.16	0.45
1:A:58:VAL:HG21	1:A:98:VAL:CG1	2.46	0.45
1:B:260:GLU:O	1:B:264:GLN:HG3	2.16	0.45
1:B:353:ASN:C	1:B:353:ASN:ND2	2.73	0.45
1:A:11:ASN:HD21	1:A:15:ARG:HE	1.64	0.45
1:A:80:LYS:HE3	1:A:286:ASP:OD2	2.16	0.45
1:A:219:ASN:HB3	1:A:223:TRP:CZ3	2.52	0.44
1:B:300:LEU:HD23	1:B:307:LEU:HD12	1.99	0.44
1:A:17:LEU:HD22	1:A:22:TYR:CG	2.52	0.44
1:B:317:GLU:HA	1:B:317:GLU:OE1	2.18	0.44
1:A:292:MET:O	1:A:296:VAL:HG23	2.18	0.44
1:A:319:THR:O	1:A:323:GLN:HG3	2.17	0.44
1:A:302:ASP:OD1	1:A:304[B]:ARG:HB3	2.18	0.43
1:A:209:GLU:H	1:A:209:GLU:CD	2.26	0.43
1:A:311:TYR:O	1:A:315:LYS:HB2	2.17	0.43
1:B:4:PHE:CE1	1:B:231:TYR:HA	2.53	0.43
1:B:5:PRO:O	1:B:6:THR:C	2.61	0.43
1:B:161:CYS:O	1:B:165:GLN:HG2	2.18	0.43
1:A:225:ASP:OD1	1:A:299:HIS:HE1	2.02	0.43
1:A:103:LYS:O	1:A:103:LYS:HG2	2.19	0.43
1:A:327:LYS:O	1:A:331:GLN:HG3	2.19	0.43
1:B:232:LYS:HD2	1:B:232:LYS:C	2.45	0.42
1:A:30:GLU:CD	1:A:30:GLU:H	2.28	0.42
1:A:69[A]:THR:HG22	1:A:298:TRP:CZ2	2.54	0.42
1:A:77:SER:HB3	1:A:291:PHE:CD1	2.54	0.42
1:A:220:TRP:CH2	1:A:292:MET:HA	2.55	0.42
1:B:46:HIS:O	1:B:52:GLN:HG3	2.19	0.42
1:A:208:LEU:HD22	1:B:168:PHE:CG	2.55	0.42
1:A:281:ASP:OD1	1:A:283:GLN:N	2.53	0.42
1:B:231:TYR:CD1	1:B:310:ILE:HD11	2.55	0.42
1:B:288:ILE:CG2	1:B:292:MET:HE2	2.35	0.42
1:B:72:GLY:O	1:B:76:TYR:HB2	2.19	0.41
1:B:308:SER:HB3	1:B:329:TYR:OH	2.19	0.41
1:B:51:ARG:NH2	1:B:122:GLU:OE2	2.53	0.41
1:B:188:GLY:CA	1:B:221[A]:MET:HE1	2.46	0.41
1:B:329:TYR:C	1:B:329:TYR:CD1	2.98	0.41
1:A:46:HIS:O	1:A:52:GLN:HG3	2.21	0.41
1:A:69[B]:THR:HG23	5:A:922:HOH:O	2.19	0.41
1:B:315:LYS:HA	1:B:326:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:12:THR:CB	1:B:263:THR:HG21	2.51	0.41
1:B:73:MET:HB2	1:B:298:TRP:CZ2	2.56	0.41
1:B:38:TYR:CD2	1:B:83:LYS:HB3	2.56	0.41
1:B:221[B]:MET:HG2	1:B:295:TYR:CZ	2.56	0.41
1:B:107:TYR:CD1	1:B:107:TYR:C	2.99	0.41
1:B:51:ARG:NH1	1:B:130:LEU:CD2	2.82	0.40
1:B:179:GLN:HG2	5:B:888:HOH:O	2.21	0.40
1:B:314:VAL:HA	1:B:317:GLU:HG2	2.02	0.40
1:A:201:PHE:CZ	1:A:283:GLN:HG2	2.56	0.40
1:A:206:LEU:O	1:A:209:GLU:HG2	2.21	0.40
1:A:281:ASP:OD1	1:A:281:ASP:C	2.65	0.40
1:B:209:GLU:CD	1:B:209:GLU:H	2.28	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	355/374 (95%)	347 (98%)	8 (2%)	0	100	100
1	B	354/374 (95%)	337 (95%)	16 (4%)	1 (0%)	36	36
All	All	709/748 (95%)	684 (96%)	24 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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	323/340 (95%)	317 (98%)	6 (2%)	50	58
1	B	322/340 (95%)	320 (99%)	2 (1%)	78	86
All	All	645/680 (95%)	637 (99%)	8 (1%)	61	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ARG
1	A	32	ARG
1	A	51	ARG
1	A	135	PHE
1	A	209	GLU
1	A	273	MET
1	B	135	PHE
1	B	209	GLU

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	11	ASN
1	A	46	HIS
1	A	137	ASN
1	A	167	ASN
1	A	175	HIS
1	A	200	GLN
1	A	216	GLN
1	A	219	ASN
1	A	268	HIS
1	A	299	HIS
1	A	350	GLN
1	A	353	ASN
1	B	46	HIS
1	B	53	GLN

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Mol	Chain	Res	Type
1	B	137	ASN
1	B	175	HIS
1	B	216	GLN
1	B	264	GLN
1	B	272	GLN
1	B	299	HIS
1	B	350	GLN
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 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	803	-	3,3,3	0.62	0	2,2,2	0.56	0
2	EDO	B	801	-	3,3,3	0.57	0	2,2,2	0.46	0
4	POP	B	700	3	6,8,8	1.55	1 (16%)	12,13,13	1.63	1 (8%)
2	EDO	A	802	-	3,3,3	0.65	0	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
2	EDO	A	803	-	-	0/1/1/1	-
2	EDO	B	801	-	-	1/1/1/1	-
4	POP	B	700	3	-	0/6/6/6	-
2	EDO	A	802	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	700	POP	P2-O6	-2.47	1.45	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	4.72	120.48	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 [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	353/374 (94%)	0.61	38 (10%) 11 11	14, 34, 60, 78	4 (1%)
1	B	353/374 (94%)	1.07	81 (22%) 2 2	20, 39, 71, 85	3 (0%)
All	All	706/748 (94%)	0.84	119 (16%) 4 4	14, 36, 65, 85	7 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	GLU	7.5
1	B	316	GLU	7.1
1	B	3	ASN	7.0
1	B	317	GLU	7.0
1	B	8	TYR	6.9
1	A	354	VAL	5.9
1	B	319	THR	5.3
1	B	23	ARG	4.8
1	B	104	ASP	4.6
1	B	12	THR	4.5
1	B	238	ARG	4.5
1	A	304[A]	ARG	4.5
1	B	314	VAL	4.0
1	A	335	VAL	3.9
1	B	10	LEU	3.9
1	B	318	LYS	3.8
1	B	11	ASN	3.8
1	B	327	LYS	3.8
1	B	315	LYS	3.8
1	B	354	VAL	3.8
1	B	9	PHE	3.8
1	A	334	ASN	3.7
1	B	321	ASP	3.7
1	B	4	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	7	GLU	3.7
1	B	22	TYR	3.7
1	B	326	CYS	3.5
1	B	6	THR	3.5
1	B	231	TYR	3.5
1	B	337	ALA	3.4
1	B	278	SER	3.4
1	B	264	GLN	3.4
1	B	328	PHE	3.4
1	A	303[A]	ARG	3.3
1	B	263	THR	3.3
1	B	5	PRO	3.3
1	A	333	ALA	3.3
1	B	255	LEU	3.3
1	B	236	ASP	3.3
1	A	19	TYR	3.3
1	A	2	GLU	3.3
1	A	314	VAL	3.2
1	B	107	TYR	3.2
1	B	303	ARG	3.2
1	B	235	ASP	3.1
1	B	239	ASP	3.1
1	B	311	TYR	3.1
1	B	268	HIS	3.1
1	B	237	GLU	3.1
1	B	102	SER	3.0
1	B	306	ARG	2.9
1	B	324	LYS	2.9
1	B	62	ARG	2.9
1	B	335	VAL	2.9
1	A	317	GLU	2.9
1	B	13	THR	2.9
1	B	227	LEU	2.8
1	A	319	THR	2.8
1	A	199	GLU	2.8
1	A	275	ALA	2.8
1	B	234	PHE	2.8
1	B	16	LEU	2.8
1	A	69[A]	THR	2.8
1	B	248	VAL	2.8
1	A	315	LYS	2.7
1	A	256	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	14	VAL	2.7
1	A	15	ARG	2.7
1	B	310	ILE	2.7
1	B	241	ILE	2.6
1	A	311	TYR	2.6
1	B	19	TYR	2.6
1	B	259	LEU	2.6
1	B	312	GLU	2.5
1	A	27	TYR	2.5
1	B	353	ASN	2.5
1	A	279	ASP	2.5
1	B	167	ASN	2.5
1	A	316	GLU	2.5
1	B	256	HIS	2.4
1	A	204	ARG	2.4
1	B	320	GLU	2.4
1	A	268	HIS	2.4
1	B	59	ASP	2.4
1	A	318	LYS	2.4
1	B	322	ALA	2.3
1	B	17	LEU	2.3
1	B	15	ARG	2.3
1	B	103	LYS	2.3
1	A	14	VAL	2.3
1	A	239	ASP	2.3
1	A	325	PHE	2.3
1	A	276	VAL	2.3
1	A	24	ASP	2.3
1	B	313	LYS	2.3
1	A	278	SER	2.3
1	B	253	ILE	2.3
1	B	58[A]	VAL	2.3
1	B	244	VAL	2.3
1	B	233	GLU	2.2
1	B	323	GLN	2.2
1	B	331	GLN	2.2
1	A	301	CYS	2.2
1	B	258	ALA	2.2
1	B	54	GLN	2.2
1	B	240	GLN	2.2
1	B	334	ASN	2.2
1	A	329	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	230	PHE	2.1
1	B	309	GLU	2.1
1	A	264	GLN	2.1
1	A	322	ALA	2.1
1	A	331	GLN	2.1
1	A	17	LEU	2.1
1	A	203	GLU	2.0
1	B	21	ARG	2.0
1	A	34	GLU	2.0
1	B	262	LEU	2.0
1	B	280	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 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	A	803	4/4	0.87	0.14	39,44,44,47	0
2	EDO	B	801	4/4	0.93	0.10	29,31,33,34	0
4	POP	B	700	9/9	0.93	0.09	43,46,47,48	0
2	EDO	A	802	4/4	0.94	0.09	29,31,32,33	0
3	MG	B	703	1/1	0.97	0.11	45,45,45,45	0
3	MG	B	701	1/1	0.97	0.07	49,49,49,49	0
3	MG	B	702	1/1	0.99	0.10	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.