



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 06:50 AM GMT

PDB ID : 2PS6
Title : N225D/S229T trichodiene synthase
Authors : Vedula, L.S.; Cane, D.E.; Christianson, D.W.
Deposited on : 2007-05-04
Resolution : 2.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

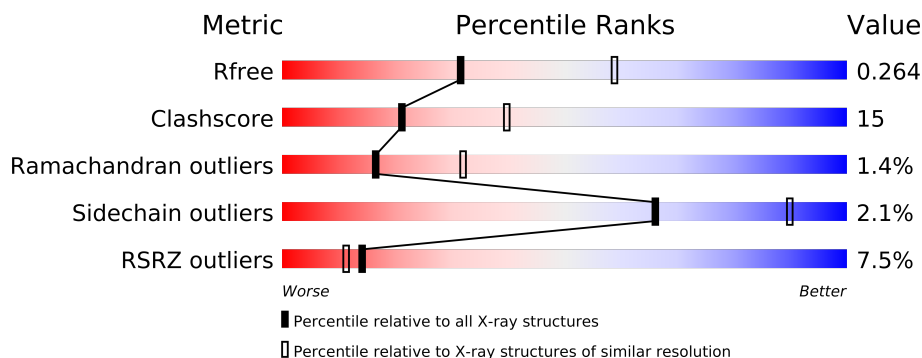
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	374	
1	B	374	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EDO	A	700	-	X
2	EDO	B	701	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5909 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

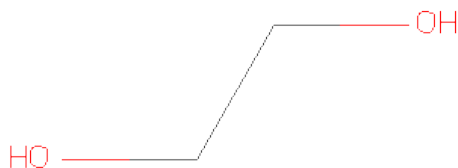
- Molecule 1 is a protein called Trichodiene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2924	1873	490	544	17			
1	B	350	Total	C	N	O	S	0	0	0
			2905	1860	487	541	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	225	ASP	ASN	ENGINEERED	UNP P13513
A	229	THR	SER	ENGINEERED	UNP P13513
B	225	ASP	ASN	ENGINEERED	UNP P13513
B	229	THR	SER	ENGINEERED	UNP P13513

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is water.

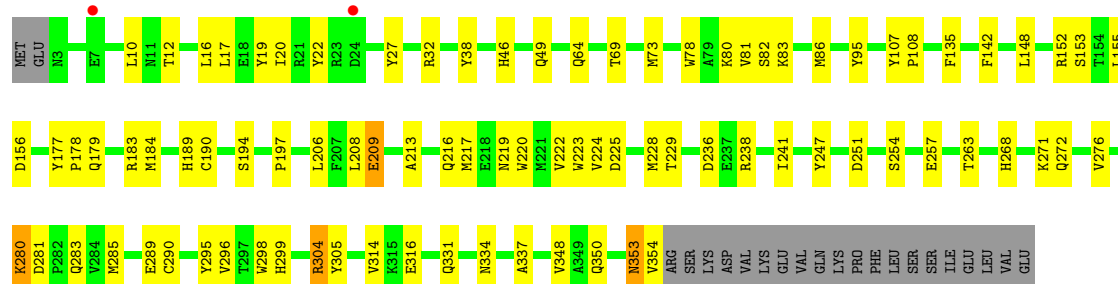
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total 51	O 51	0	0
3	B	21	Total 21	O 21	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

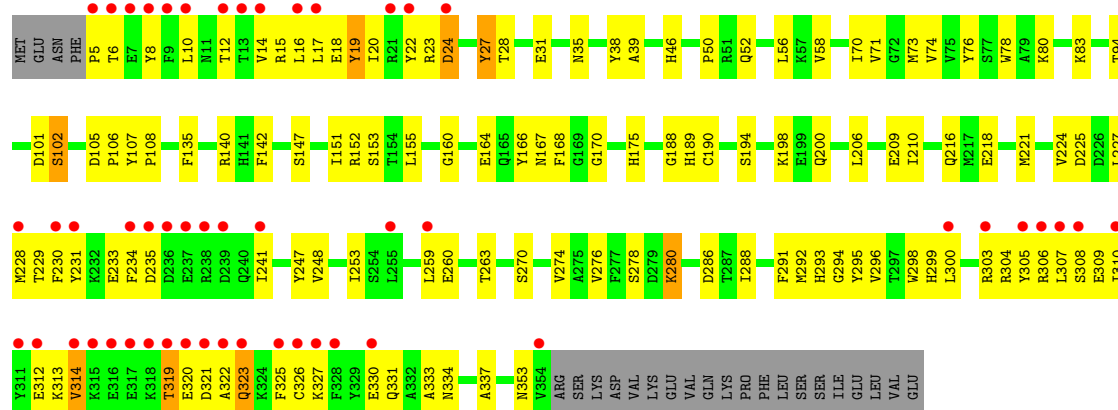
• Molecule 1: Trichodiene synthase

Chain A: 



• Molecule 1: Trichodiene synthase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.23Å 122.23Å 150.17Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.60 61.24 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.60) 95.9 (61.24-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.255 0.238 , 0.264	Depositor DCC
R_{free} test set	1941 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 28.5	EDS
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 38761 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5909	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.39	0/3009	0.55	0/4086
1	B	0.36	0/2989	0.55	0/4058
All	All	0.38	0/5998	0.55	0/8144

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2924	0	2775	76	0
1	B	2905	0	2761	103	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
3	A	51	0	0	0	0
3	B	21	0	0	1	0
All	All	5909	0	5548	175	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (175) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:17:LEU:HD21	1:A:296:VAL:HG11	1.50	0.94
1:B:229:THR:HG22	1:B:233:GLU:HG2	1.51	0.92
1:B:319:THR:H	1:B:323:GLN:HB2	1.36	0.90
1:A:64:GLN:HE22	1:A:348:VAL:H	1.19	0.90
1:A:304:ARG:HH11	1:A:304:ARG:HB2	1.37	0.88
1:A:19:TYR:CE2	1:A:271:LYS:HE3	2.14	0.82
1:B:10:LEU:HD11	1:B:314:VAL:HG11	1.63	0.80
1:B:231:TYR:CE1	1:B:310:ILE:HD11	2.19	0.78
1:A:304:ARG:HB2	1:A:304:ARG:NH1	2.00	0.75
1:A:217:MET:CE	1:A:220:TRP:HB3	2.18	0.73
1:B:10:LEU:O	1:B:14:VAL:HG23	1.90	0.71
1:A:12:THR:HG21	1:A:263:THR:HG21	1.72	0.71
1:A:82:SER:O	1:A:86:MET:HG3	1.91	0.70
1:B:323:GLN:HA	1:B:323:GLN:OE1	1.92	0.69
1:B:24:ASP:HA	1:B:293:HIS:HB3	1.74	0.69
1:B:224:VAL:O	1:B:228:MET:HG2	1.93	0.68
1:A:276:VAL:O	1:A:280:LYS:HD3	1.93	0.68
1:B:276:VAL:O	1:B:280:LYS:HD3	1.93	0.68
1:B:323:GLN:CA	1:B:323:GLN:OE1	2.42	0.67
1:B:153:SER:HB3	1:B:190:CYS:HB2	1.78	0.66
1:B:147:SER:O	1:B:151:ILE:HG13	1.96	0.66
1:A:217:MET:HE1	1:A:220:TRP:HB3	1.76	0.65
1:A:80:LYS:HE2	1:A:290:CYS:SG	2.36	0.64
1:B:17:LEU:HD21	1:B:296:VAL:HG11	1.80	0.64
1:B:319:THR:H	1:B:323:GLN:CB	2.11	0.62
1:A:350:GLN:O	1:A:354:VAL:HG23	2.00	0.62
1:B:319:THR:N	1:B:323:GLN:HB2	2.13	0.62
1:A:78:TRP:O	1:A:81:VAL:HG22	2.00	0.61
1:A:46:HIS:HA	1:A:49:GLN:HE21	1.64	0.61
1:B:46:HIS:O	1:B:52:GLN:HG3	1.98	0.61
1:B:323:GLN:OE1	1:B:323:GLN:O	2.18	0.61
1:B:274:VAL:O	1:B:278:SER:HB2	1.99	0.61
1:A:38:TYR:CD2	1:A:83:LYS:HB3	2.36	0.61
1:B:10:LEU:HD22	1:B:325:PHE:CD2	2.36	0.60
1:B:160:GLY:O	1:B:164:GLU:HG3	2.01	0.60
1:A:304:ARG:HH11	1:A:304:ARG:CB	2.12	0.59
1:B:308:SER:C	1:B:310:ILE:H	2.05	0.59
1:B:10:LEU:CD1	1:B:314:VAL:HG11	2.33	0.59
1:B:5:PRO:N	1:B:234:PHE:HE2	2.00	0.58
1:B:12:THR:HA	1:B:15:ARG:HE	1.69	0.58
1:A:153:SER:HB3	1:A:190:CYS:HB2	1.85	0.58
1:B:333:ALA:O	1:B:337:ALA:HB3	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:321:ASP:C	1:B:323:GLN:H	2.06	0.57
1:B:288:ILE:O	1:B:292:MET:HG3	2.05	0.57
1:B:230:PHE:CE2	1:B:259:LEU:HD22	2.39	0.57
1:A:217:MET:HE3	1:A:217:MET:HA	1.84	0.57
1:B:229:THR:HG22	1:B:229:THR:O	2.06	0.56
1:A:73:MET:HB2	1:A:298:TRP:CE2	2.40	0.56
1:A:206:LEU:HD22	1:A:209:GLU:HG3	1.89	0.55
1:B:80:LYS:HE3	1:B:286:ASP:OD2	2.07	0.55
1:B:17:LEU:CD2	1:B:296:VAL:HG11	2.36	0.55
1:B:167:ASN:HA	1:B:241:ILE:HD13	1.89	0.55
1:A:64:GLN:NE2	1:A:348:VAL:H	1.98	0.54
1:B:260:GLU:HA	1:B:263:THR:HG22	1.90	0.54
1:A:295:TYR:O	1:A:299:HIS:HD2	1.91	0.53
1:B:229:THR:O	1:B:233:GLU:HG2	2.08	0.53
1:B:300:LEU:HA	1:B:307:LEU:HD12	1.89	0.53
1:B:310:ILE:HG22	1:B:325:PHE:CE2	2.44	0.53
1:B:74:VAL:HA	1:B:78:TRP:CE3	2.44	0.53
1:B:38:TYR:CD2	1:B:83:LYS:HB3	2.43	0.52
1:B:23:ARG:O	1:B:24:ASP:HB3	2.08	0.52
1:A:206:LEU:CD2	1:A:209:GLU:HG3	2.39	0.52
1:B:20:ILE:HG12	1:B:20:ILE:O	2.09	0.52
1:B:314:VAL:HG23	1:B:326:CYS:SG	2.49	0.52
1:B:310:ILE:HG22	1:B:325:PHE:HE2	1.75	0.52
1:B:14:VAL:O	1:B:18:GLU:HG3	2.11	0.51
1:A:219:ASN:HB3	1:A:223:TRP:CZ3	2.45	0.51
1:B:300:LEU:HD23	1:B:307:LEU:CD1	2.41	0.51
1:B:152:ARG:NH2	1:B:189:HIS:ND1	2.58	0.51
1:A:280:LYS:HD2	1:A:280:LYS:N	2.24	0.51
1:A:217:MET:HE3	1:A:220:TRP:HB3	1.93	0.51
1:A:12:THR:HG21	1:A:263:THR:CG2	2.41	0.50
1:A:353:ASN:HD22	1:A:353:ASN:C	2.12	0.50
1:B:216:GLN:HE22	1:B:276:VAL:HG11	1.77	0.50
1:B:248:VAL:HG13	1:B:253:ILE:O	2.11	0.50
1:B:188:GLY:HA3	1:B:218:GLU:HG3	1.94	0.49
1:B:142:PHE:CE2	1:B:194:SER:HA	2.48	0.49
1:A:142:PHE:CE2	1:A:194:SER:HA	2.47	0.49
1:A:152:ARG:HG2	1:B:155:LEU:CD2	2.43	0.48
1:B:308:SER:O	1:B:310:ILE:N	2.47	0.48
1:A:208:LEU:HD22	1:B:168:PHE:CG	2.48	0.48
1:A:10:LEU:HD11	1:A:314:VAL:HG11	1.94	0.48
1:A:155:LEU:HD23	1:B:152:ARG:HG2	1.96	0.48
1:B:28:THR:HG23	1:B:31:GLU:OE1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:177:TYR:HB3	1:A:178:PRO:HD3	1.96	0.48
1:A:213:ALA:O	1:A:217:MET:HB2	2.14	0.47
1:A:69:THR:HG22	1:A:298:TRP:HZ2	1.79	0.47
1:B:300:LEU:HD23	1:B:307:LEU:HD13	1.96	0.47
1:B:56:LEU:O	1:B:58:VAL:HG12	2.14	0.47
1:A:217:MET:HE2	1:A:220:TRP:HE3	1.80	0.47
1:A:220:TRP:CE2	1:A:224:VAL:HG21	2.50	0.47
1:B:327:LYS:O	1:B:331:GLN:HG3	2.13	0.47
1:B:206:LEU:HD22	1:B:209:GLU:HG3	1.97	0.47
1:A:229:THR:HG22	1:A:305:TYR:CE1	2.50	0.47
1:A:16:LEU:O	1:A:20:ILE:HG12	2.14	0.46
1:B:260:GLU:HA	1:B:263:THR:CG2	2.45	0.46
1:A:152:ARG:HG2	1:B:155:LEU:HD23	1.98	0.46
1:B:323:GLN:OE1	1:B:323:GLN:C	2.54	0.46
1:A:272:GLN:O	1:A:276:VAL:HG23	2.15	0.46
1:A:152:ARG:NH2	1:A:189:HIS:ND1	2.63	0.46
1:B:101:ASP:O	1:B:102:SER:C	2.53	0.46
1:B:319:THR:HG23	1:B:320:GLU:H	1.80	0.46
1:B:16:LEU:O	1:B:20:ILE:HG22	2.15	0.46
1:A:19:TYR:CD2	1:A:271:LYS:HG3	2.51	0.45
1:B:291:PHE:O	1:B:295:TYR:HB2	2.16	0.45
1:A:17:LEU:HD23	1:A:20:ILE:HD11	1.99	0.45
1:B:230:PHE:HE2	1:B:259:LEU:HD22	1.81	0.45
1:B:308:SER:C	1:B:310:ILE:N	2.69	0.45
1:B:6:THR:OG1	1:B:8:TYR:HB3	2.17	0.45
1:B:166:TYR:O	1:B:167:ASN:C	2.54	0.45
1:B:50:PRO:HG2	3:B:709:HOH:O	2.15	0.45
1:A:285:MET:HE2	1:A:289:GLU:HB2	1.99	0.45
1:A:225:ASP:OD2	1:A:299:HIS:HE1	2.00	0.45
1:B:225:ASP:OD2	1:B:299:HIS:HE1	1.99	0.45
1:A:353:ASN:ND2	1:A:353:ASN:C	2.70	0.45
1:B:73:MET:HB2	1:B:298:TRP:CE2	2.52	0.45
1:B:107:TYR:HB3	1:B:108:PRO:CD	2.47	0.45
1:B:321:ASP:O	1:B:322:ALA:HB3	2.17	0.44
1:A:148:LEU:O	1:A:152:ARG:HG3	2.17	0.44
1:A:353:ASN:O	1:A:353:ASN:ND2	2.47	0.44
1:B:39:ALA:HB3	1:B:71:VAL:HG13	1.99	0.44
1:A:220:TRP:CZ2	1:A:224:VAL:HG21	2.53	0.44
1:A:17:LEU:HD22	1:A:22:TYR:CG	2.53	0.44
1:B:330:GLU:O	1:B:334:ASN:ND2	2.51	0.44
1:B:27:TYR:CE1	1:B:35:ASN:ND2	2.86	0.44
1:B:206:LEU:O	1:B:210:ILE:HG13	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:236:ASP:OD1	1:A:238:ARG:HB2	2.18	0.44
1:A:46:HIS:HE1	1:A:95:TYR:OH	1.99	0.43
1:A:80:LYS:CE	1:A:290:CYS:SG	3.06	0.43
1:B:319:THR:OG1	1:B:320:GLU:N	2.50	0.43
1:B:188:GLY:HA2	1:B:221:MET:CE	2.49	0.43
1:A:254:SER:OG	1:A:257:GLU:HG3	2.18	0.43
1:A:156:ASP:HB3	1:A:184:MET:HE3	2.00	0.43
1:A:316:GLU:O	1:A:316:GLU:HG3	2.19	0.43
1:B:105:ASP:OD2	1:B:107:TYR:HB3	2.19	0.43
1:B:303:ARG:O	1:B:305:TYR:N	2.52	0.43
1:B:76:TYR:O	1:B:294:GLY:HA3	2.18	0.43
1:B:260:GLU:CA	1:B:263:THR:HG22	2.49	0.43
1:A:285:MET:CE	1:A:289:GLU:HB2	2.49	0.42
1:A:280:LYS:O	1:A:281:ASP:C	2.56	0.42
1:B:5:PRO:N	1:B:234:PHE:CE2	2.86	0.42
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.84	0.42
1:B:17:LEU:HD21	1:B:296:VAL:CG1	2.46	0.42
1:B:260:GLU:C	1:B:263:THR:HG22	2.39	0.42
1:B:330:GLU:HG2	1:B:334:ASN:HD21	1.83	0.42
1:B:70:ILE:HG13	1:B:94:THR:HA	2.02	0.42
1:B:168:PHE:CZ	1:B:170:GLY:HA2	2.54	0.42
1:A:81:VAL:HG12	1:A:197:PRO:HG2	2.01	0.42
1:A:216:GLN:HE22	1:A:276:VAL:HG11	1.85	0.42
1:B:140:ARG:O	1:B:198:LYS:HE2	2.20	0.42
1:B:17:LEU:HD22	1:B:22:TYR:CD2	2.54	0.41
1:B:16:LEU:HD22	1:B:227:LEU:HD23	2.01	0.41
1:A:107:TYR:CD1	1:A:107:TYR:C	2.94	0.41
1:A:217:MET:CE	1:A:217:MET:HA	2.49	0.41
1:B:229:THR:HG22	1:B:233:GLU:CG	2.36	0.41
1:A:217:MET:CE	1:A:220:TRP:HE3	2.34	0.41
1:A:241:ILE:HG13	1:A:241:ILE:O	2.21	0.41
1:A:281:ASP:OD1	1:A:283:GLN:N	2.54	0.41
1:B:312:GLU:O	1:B:313:LYS:HG3	2.20	0.41
1:A:228:MET:HE1	1:A:296:VAL:HG13	2.03	0.41
1:B:8:TYR:CE2	1:B:259:LEU:HD23	2.56	0.41
1:B:321:ASP:C	1:B:323:GLN:N	2.73	0.41
1:B:105:ASP:HA	1:B:106:PRO:HD3	1.79	0.41
1:B:270:SER:O	1:B:274:VAL:HG23	2.21	0.41
1:B:107:TYR:CD1	1:B:107:TYR:C	2.93	0.41
1:A:247:TYR:O	1:A:251:ASP:HB2	2.21	0.41
1:A:19:TYR:CD1	1:A:19:TYR:N	2.90	0.40
1:A:222:VAL:HG23	1:A:223:TRP:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.51	0.40
1:A:268:HIS:O	1:A:272:GLN:HG2	2.22	0.40
1:A:179:GLN:HB3	1:A:183:ARG:NH1	2.37	0.40
1:A:27:TYR:HB3	1:A:32:ARG:HH12	1.85	0.40
1:B:292:MET:O	1:B:296:VAL:HG23	2.22	0.40
1:A:331:GLN:HA	1:A:334:ASN:HD22	1.87	0.40
1:B:19:TYR:HD2	1:B:19:TYR:O	2.03	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	350/374 (94%)	338 (97%)	11 (3%)	1 (0%)	50	77
1	B	348/374 (93%)	310 (89%)	29 (8%)	9 (3%)	8	13
All	All	698/748 (93%)	648 (93%)	40 (6%)	10 (1%)	16	32

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	ASP
1	B	27	TYR
1	B	304	ARG
1	B	309	GLU
1	B	24	ASP
1	B	306	ARG
1	B	353	ASN
1	A	337	ALA
1	B	314	VAL
1	B	102	SER

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	318/340 (94%)	313 (98%)	5 (2%)	75	93
1	B	316/340 (93%)	308 (98%)	8 (2%)	60	86
All	All	634/680 (93%)	621 (98%)	13 (2%)	66	90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	PHE
1	A	209	GLU
1	A	280	LYS
1	A	304	ARG
1	A	353	ASN
1	B	19	TYR
1	B	135	PHE
1	B	175	HIS
1	B	200	GLN
1	B	247	TYR
1	B	280	LYS
1	B	319	THR
1	B	323	GLN

Some 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	64	GLN
1	A	68	GLN
1	A	137	ASN
1	A	165	GLN
1	A	167	ASN
1	A	216	GLN
1	A	299	HIS
1	A	334	ASN
1	A	350	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	353	ASN
1	B	46	HIS
1	B	49	GLN
1	B	137	ASN
1	B	200	GLN
1	B	216	GLN
1	B	219	ASN
1	B	240	GLN
1	B	264	GLN
1	B	272	GLN
1	B	331	GLN
1	B	334	ASN
1	B	350	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	700	-	3,3,3	2.24	2 (66%)	2,2,2	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	701	-	3,3,3	2.10	2 (66%)	2,2,2	0.59	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	700	-	-	0/1/1/1	0/0/0/0
2	EDO	B	701	-	-	0/1/1/1	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700	EDO	O2-C2	2.89	1.57	1.42
2	B	701	EDO	O2-C2	2.59	1.55	1.42
2	B	701	EDO	O1-C1	2.41	1.54	1.42
2	A	700	EDO	O1-C1	2.41	1.54	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	352/374 (94%)	0.13	2 (0%) 86 89	27, 45, 72, 94	0
1	B	350/374 (93%)	0.71	51 (14%) 3 2	28, 51, 104, 137	0
All	All	702/748 (93%)	0.42	53 (7%) 14 11	27, 47, 94, 137	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	10	LEU	9.2
1	B	316	GLU	8.0
1	B	9	PHE	6.8
1	B	321	ASP	6.3
1	B	236	ASP	6.2
1	B	239	ASP	6.1
1	B	238	ARG	5.8
1	B	235	ASP	5.5
1	B	8	TYR	5.4
1	B	312	GLU	4.9
1	B	322	ALA	4.9
1	B	315	LYS	4.7
1	B	323	GLN	4.6
1	B	234	PHE	4.6
1	B	237	GLU	4.6
1	B	325	PHE	4.5
1	B	320	GLU	4.5
1	B	317	GLU	4.4
1	B	230	PHE	4.2
1	B	314	VAL	4.2
1	B	307	LEU	4.0
1	B	7	GLU	3.9
1	B	303	ARG	3.8
1	B	5	PRO	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	24	ASP	3.6
1	B	22	TYR	3.5
1	B	17	LEU	3.4
1	B	231	TYR	3.3
1	B	319	THR	3.3
1	B	328	PHE	3.2
1	B	311	TYR	3.2
1	B	318	LYS	3.1
1	B	255	LEU	3.1
1	B	21	ARG	3.0
1	B	330	GLU	2.9
1	B	354	VAL	2.8
1	B	327	LYS	2.7
1	B	24	ASP	2.7
1	B	259	LEU	2.5
1	B	14	VAL	2.5
1	B	241	ILE	2.5
1	B	326	CYS	2.4
1	A	7	GLU	2.4
1	B	305	TYR	2.3
1	B	12	THR	2.3
1	B	16	LEU	2.3
1	B	6	THR	2.2
1	B	300	LEU	2.2
1	B	306	ARG	2.1
1	B	310	ILE	2.1
1	B	228	MET	2.0
1	B	13	THR	2.0
1	B	308	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	EDO	B	701	4/4	0.27	5.90	32,34,38,39	0
2	EDO	A	700	4/4	0.25	4.95	42,43,43,46	0

6.5 Other polymers

There are no such residues in this entry.