



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:11 PM UTC

PDB ID : 1YYU / pdb_00001yyu
Title : D100E Trichodiene Synthase: Complex With Mg, Pyrophosphate, and (4S)-7-azabisabolene
Authors : Vedula, L.S.; Rynkiewicz, M.J.; Pyun, H.J.; Coates, R.M.; Cane, D.E.; Christianson, D.W.
Deposited on : 2005-02-25
Resolution : 2.95 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

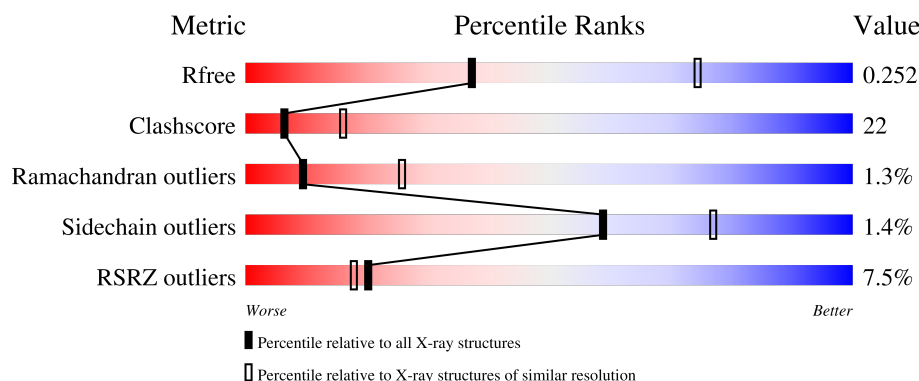
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	3% 57% 36% • 5%
1	B	374	10% 55% 38% • 5%

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	RAZ	A	710	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6008 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	47	0	0
			2941	1883	493	547	18			
1	B	354	Total	C	N	O	S	170	0	0
			2941	1883	493	547	18			

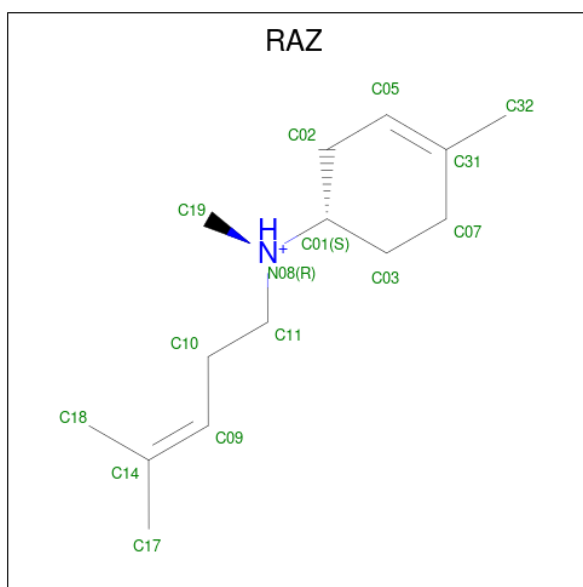
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	GLU	ASP	engineered mutation	UNP P13513
B	100	GLU	ASP	engineered mutation	UNP P13513

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

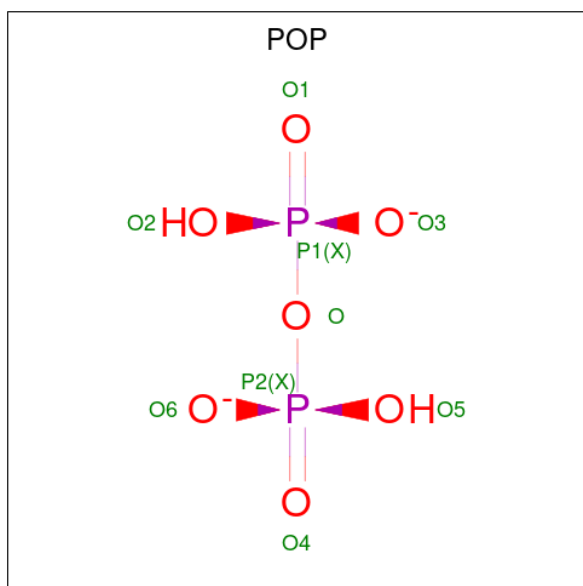
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is (1R)-N,4-DIMETHYL-N-(4-METHYLPENT-3-ENYL)CYCLOHEX-3-ENAMINIUM (CCD ID: RAZ) (formula: C₁₄H₂₆N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			15	14	1		

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



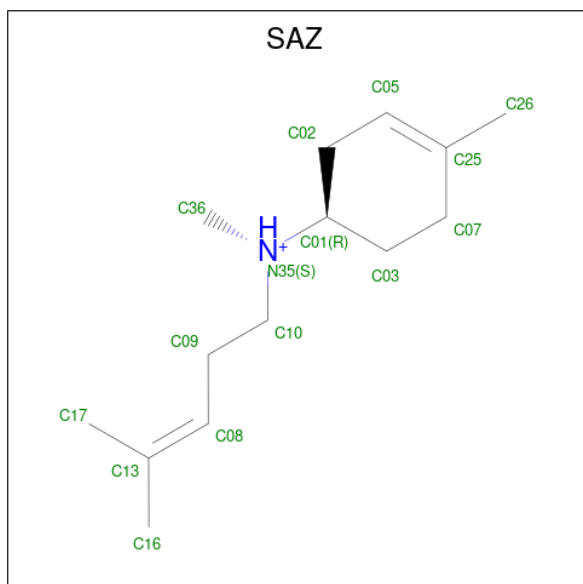
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			9	7	2		
4	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 6 is (1S)-N,4-DIMETHYL-N-(4-METHYLPENT-3-ENYL)CYCLOHEX-3-ENAMINIUM (CCD ID: SAZ) (formula: $C_{14}H_{26}N$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	N	0	0
			15	14	1		

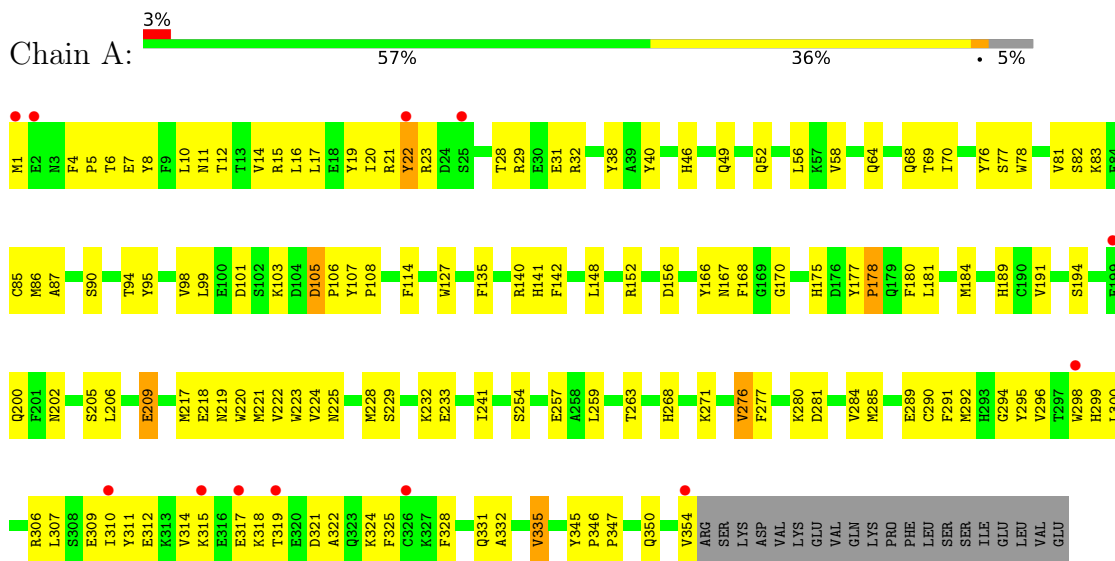
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	39	Total 39	O 39	0	0
7	B	27	Total 27	O 27	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



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.49Å 122.49Å 150.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.95 50.00 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.6 (50.00-2.95) 97.6 (50.00-2.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.255 0.221 , 0.252	Depositor DCC
R_{free} test set	1342 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6008	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: SAZ, MG, EDO, RAZ, POP

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	0.51	1/3026 (0.0%)	0.90	5/4107 (0.1%)
1	B	0.50	0/3026	0.91	9/4107 (0.2%)
All	All	0.50	1/6052 (0.0%)	0.91	14/8214 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	LYS	C-N	-6.58	1.23	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	323	GLN	OE1-CD-NE2	-9.79	112.81	122.60
1	B	276	VAL	N-CA-C	7.11	117.21	110.53
1	A	276	VAL	N-CA-C	6.94	117.05	110.53
1	A	103	LYS	N-CA-C	-6.72	105.12	113.38
1	B	323	GLN	CG-CD-NE2	6.69	126.43	116.40
1	B	2	GLU	N-CA-C	-6.64	104.49	112.59
1	A	105	ASP	CA-C-N	6.05	125.60	119.19
1	A	105	ASP	C-N-CA	6.05	125.60	119.19
1	A	277	PHE	N-CA-C	5.91	120.49	113.28
1	B	277	PHE	N-CA-C	5.90	120.47	113.28
1	B	4	PHE	CA-C-N	5.77	127.05	119.84
1	B	4	PHE	C-N-CA	5.77	127.05	119.84
1	B	105	ASP	CA-C-N	5.32	124.83	119.19
1	B	105	ASP	C-N-CA	5.32	124.83	119.19

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	2941	0	2795	117	0
1	B	2941	0	2795	133	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	15	0	25	3	0
4	A	9	0	0	0	0
4	B	9	0	0	1	0
5	A	4	0	6	0	0
5	B	4	0	6	0	0
6	B	15	0	25	2	0
7	A	39	0	0	1	0
7	B	27	0	0	1	0
All	All	6008	0	5652	245	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 22.

All (245) 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	1.32	1.08
1:A:1:MET:HE2	1:A:5:PRO:HG3	1.45	0.95
1:A:10:LEU:HD11	1:A:314:VAL:HG11	1.51	0.92
1:B:314:VAL:HB	1:B:322:ALA:HB1	1.55	0.89
1:A:64:GLN:HE21	1:A:68:GLN:HE21	1.26	0.83
1:B:14:VAL:O	1:B:18:GLU:HG3	1.79	0.82
1:B:17:LEU:HD23	1:B:22:TYR:CD2	2.15	0.81
1:B:64:GLN:HE21	1:B:68:GLN:HE21	1.31	0.76
1:A:19:TYR:CD2	1:A:271:LYS:HG3	2.19	0.76
1:A:290:CYS:SG	7:A:764:HOH:O	2.44	0.75
1:A:19:TYR:HD2	1:A:271:LYS:HG3	1.52	0.72
1:B:228:MET:HE1	1:B:296:VAL:HA	1.71	0.72
1:A:217:MET:HE1	1:A:220:TRP:CE3	2.25	0.71
1:B:49:GLN:HB2	1:B:52:GLN:HG2	1.72	0.71
1:B:12:THR:HG21	1:B:263:THR:HG21	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:CYS:HA	1:A:141:HIS:CE1	2.25	0.71
1:A:228:MET:HE1	1:A:296:VAL:HA	1.72	0.71
1:B:85:CYS:HA	1:B:141:HIS:CE1	2.26	0.70
1:A:49:GLN:HB2	1:A:52:GLN:HG2	1.72	0.70
1:A:152:ARG:CZ	1:B:184:MET:HE1	2.21	0.70
1:A:184:MET:HE1	1:B:152:ARG:CZ	2.22	0.69
1:A:328:PHE:O	1:A:331:GLN:HB2	1.93	0.69
1:B:228:MET:HE1	1:B:296:VAL:HG13	1.75	0.69
1:A:15:ARG:O	1:A:19:TYR:HD1	1.75	0.68
1:B:12:THR:HA	1:B:15:ARG:HD3	1.75	0.68
1:B:310:ILE:O	1:B:314:VAL:HG22	1.94	0.68
1:A:19:TYR:CE2	1:A:271:LYS:HE3	2.29	0.68
1:B:14:VAL:HG12	1:B:18:GLU:OE1	1.94	0.67
1:A:217:MET:HE3	1:A:220:TRP:HB3	1.75	0.66
1:B:46:HIS:O	1:B:49:GLN:HG3	1.96	0.66
1:A:191:VAL:HG21	1:A:221:MET:HE2	1.78	0.65
1:A:228:MET:HE1	1:A:296:VAL:HG13	1.79	0.64
1:B:300:LEU:HA	1:B:307:LEU:HD12	1.78	0.64
1:A:46:HIS:O	1:A:49:GLN:HG3	1.98	0.64
1:B:331:GLN:HA	1:B:334:ASN:HD22	1.62	0.64
1:B:217:MET:HE3	1:B:220:TRP:HB3	1.79	0.63
1:B:15:ARG:O	1:B:19:TYR:HD1	1.81	0.62
1:A:219:ASN:HB3	1:A:223:TRP:CZ3	2.35	0.62
1:B:217:MET:HE1	1:B:220:TRP:CE3	2.33	0.62
1:A:152:ARG:NH1	1:B:184:MET:HE1	2.14	0.62
1:B:77:SER:HB3	1:B:291:PHE:CD1	2.35	0.62
1:A:225:ASN:ND2	3:A:710:RAZ:H102	2.14	0.61
1:B:4:PHE:HE2	1:B:9:PHE:HD1	1.46	0.61
1:A:148:LEU:O	1:A:152:ARG:HG3	1.99	0.61
1:B:254:SER:OG	1:B:257:GLU:HG3	2.00	0.60
1:B:4:PHE:CE2	1:B:9:PHE:HD1	2.19	0.60
1:A:77:SER:HB3	1:A:291:PHE:CD1	2.37	0.59
1:B:82:SER:O	1:B:86:MET:HG3	2.02	0.59
1:A:300:LEU:HA	1:A:307:LEU:HD12	1.85	0.59
1:B:217:MET:HE3	1:B:217:MET:HA	1.84	0.59
1:A:254:SER:OG	1:A:257:GLU:HG3	2.03	0.58
1:A:17:LEU:HD22	1:A:22:TYR:CG	2.38	0.58
1:B:191:VAL:HG21	1:B:221:MET:HE2	1.85	0.58
1:B:32:ARG:HD2	1:B:335:VAL:O	2.04	0.58
1:A:11:ASN:O	1:A:15:ARG:HG3	2.03	0.58
1:A:206:LEU:HD22	1:A:209:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HD23	1:B:307:LEU:HD13	1.86	0.57
1:A:217:MET:HE3	1:A:217:MET:HA	1.86	0.57
1:A:38:TYR:CD2	1:A:83:LYS:HB3	2.40	0.57
1:A:82:SER:O	1:A:86:MET:HG3	2.04	0.57
1:B:148:LEU:O	1:B:152:ARG:HG3	2.05	0.57
1:B:11:ASN:ND2	1:B:15:ARG:HD2	2.20	0.57
1:B:219:ASN:HB3	1:B:223:TRP:CZ3	2.39	0.57
1:A:98:VAL:O	1:A:101:ASP:HB2	2.05	0.57
1:A:202:ASN:HB3	1:A:205:SER:HB2	1.86	0.56
1:A:107:TYR:HB3	1:A:108:PRO:CD	2.35	0.56
1:A:78:TRP:O	1:A:81:VAL:HG22	2.05	0.56
1:A:12:THR:HG21	1:A:263:THR:HG22	1.87	0.56
1:B:206:LEU:HD22	1:B:209:GLU:HG3	1.86	0.55
1:A:184:MET:HE1	1:B:152:ARG:NH1	2.21	0.55
1:B:328:PHE:HA	1:B:331:GLN:HE21	1.71	0.55
1:B:140:ARG:HG3	1:B:141:HIS:HD2	1.72	0.55
1:B:38:TYR:CD2	1:B:83:LYS:HB3	2.41	0.55
1:B:107:TYR:HB3	1:B:108:PRO:CD	2.37	0.54
1:B:78:TRP:O	1:B:81:VAL:HG22	2.07	0.54
1:B:202:ASN:HB3	1:B:205:SER:HB2	1.89	0.54
1:A:217:MET:CE	1:A:220:TRP:HB3	2.37	0.54
1:B:140:ARG:HG3	1:B:141:HIS:CD2	2.43	0.54
1:B:168:PHE:CE2	1:B:170:GLY:HA2	2.42	0.54
1:A:19:TYR:HE2	1:A:271:LYS:HE3	1.73	0.54
1:A:232:LYS:HG3	1:A:233:GLU:N	2.23	0.54
1:B:167:ASN:HA	1:B:241:ILE:HD13	1.90	0.54
1:B:11:ASN:ND2	1:B:15:ARG:HH11	2.05	0.53
1:B:350:GLN:O	1:B:354:VAL:HG23	2.09	0.53
1:A:22:TYR:OH	1:A:332:ALA:HB2	2.08	0.53
1:A:140:ARG:HG3	1:A:141:HIS:CD2	2.44	0.53
1:A:140:ARG:HG3	1:A:141:HIS:HD2	1.73	0.53
1:B:105:ASP:OD2	1:B:107:TYR:HB3	2.09	0.53
1:A:177:TYR:HB3	1:A:178:PRO:HD3	1.91	0.52
1:A:300:LEU:HD23	1:A:307:LEU:HD13	1.91	0.52
1:A:177:TYR:O	1:A:180:PHE:HB3	2.09	0.52
1:A:350:GLN:O	1:A:354:VAL:HG23	2.10	0.52
1:B:98:VAL:O	1:B:101:ASP:HB2	2.09	0.52
1:B:231:TYR:HE2	1:B:306:ARG:HH21	1.56	0.52
1:A:10:LEU:O	1:A:14:VAL:HG23	2.10	0.52
1:A:8:TYR:HD2	1:A:8:TYR:O	1.93	0.52
1:B:28:THR:OG1	1:B:31:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HG23	1:A:298:TRP:HZ2	1.74	0.51
1:B:333:ALA:O	1:B:337:ALA:HB3	2.10	0.51
1:B:13:THR:O	1:B:16:LEU:HB3	2.10	0.51
1:A:28:THR:OG1	1:A:31:GLU:HG3	2.11	0.51
1:A:20:ILE:O	1:A:21:ARG:HB2	2.10	0.51
1:B:308:SER:HA	1:B:329:TYR:OH	2.11	0.51
1:B:13:THR:O	1:B:17:LEU:HD13	2.11	0.50
3:A:710:RAZ:H173	3:A:710:RAZ:H021	1.92	0.50
1:A:168:PHE:CE2	1:A:170:GLY:HA2	2.46	0.50
1:B:76:TYR:O	1:B:294:GLY:HA3	2.12	0.50
1:A:17:LEU:CD2	1:A:296:VAL:HG11	2.23	0.50
1:A:268:HIS:NE2	1:B:175:HIS:HD2	2.10	0.50
1:B:217:MET:CE	1:B:220:TRP:HB3	2.41	0.50
1:B:69:THR:HG23	1:B:298:TRP:HZ2	1.76	0.50
1:B:29:ARG:HG3	1:B:335:VAL:HA	1.94	0.49
1:A:285:MET:HE3	1:A:289:GLU:HB2	1.94	0.49
1:B:234:PHE:C	1:B:236:ASP:H	2.20	0.49
1:B:234:PHE:O	1:B:236:ASP:N	2.41	0.49
1:A:217:MET:CE	1:A:220:TRP:HE3	2.25	0.49
1:B:46:HIS:HE1	1:B:95:TYR:OH	1.95	0.49
1:B:311:TYR:HD2	1:B:312:GLU:OE1	1.95	0.48
1:A:46:HIS:HE1	1:A:95:TYR:OH	1.94	0.48
1:B:56:LEU:HG	1:B:58:VAL:HG23	1.95	0.48
1:A:184:MET:HE1	1:B:152:ARG:NH2	2.29	0.48
1:A:175:HIS:HD2	1:B:268:HIS:NE2	2.12	0.48
1:A:85:CYS:CA	1:A:141:HIS:CE1	2.97	0.48
1:A:7:GLU:HG3	1:A:8:TYR:N	2.28	0.47
1:A:99:LEU:HD13	1:A:127:TRP:CG	2.50	0.47
1:B:166:TYR:O	1:B:167:ASN:C	2.56	0.47
1:B:228:MET:CE	1:B:296:VAL:HG13	2.43	0.47
1:A:40:TYR:C	1:A:40:TYR:CD2	2.92	0.47
1:B:11:ASN:O	1:B:15:ARG:HG3	2.14	0.47
1:A:276:VAL:O	1:A:280:LYS:HD3	2.14	0.47
1:B:177:TYR:O	1:B:180:PHE:HB3	2.14	0.47
1:A:76:TYR:O	1:A:294:GLY:HA3	2.14	0.47
1:A:225:ASN:ND2	1:A:299:HIS:HE1	2.13	0.47
1:A:217:MET:HE1	1:A:220:TRP:HE3	1.72	0.47
1:B:22:TYR:HD2	1:B:328:PHE:CD1	2.32	0.47
1:B:29:ARG:O	1:B:33:ILE:HG13	2.14	0.47
1:B:99:LEU:HD13	1:B:127:TRP:CG	2.50	0.47
1:A:69:THR:CG2	1:A:298:TRP:HZ2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TYR:OH	1:A:181:LEU:HD22	2.15	0.47
1:B:295:TYR:O	1:B:299:HIS:HD2	1.97	0.47
1:B:329:TYR:CD1	1:B:329:TYR:C	2.93	0.47
1:A:292:MET:O	1:A:296:VAL:HG23	2.15	0.47
1:A:206:LEU:HB3	1:A:209:GLU:HG2	1.97	0.47
1:B:142:PHE:CE2	1:B:194:SER:HA	2.50	0.47
1:B:231:TYR:C	1:B:231:TYR:CD2	2.94	0.46
1:A:22:TYR:HD2	1:A:328:PHE:CD1	2.33	0.46
1:B:23:ARG:HH22	1:B:289:GLU:CD	2.24	0.46
1:B:292:MET:O	1:B:296:VAL:HG23	2.16	0.46
1:B:276:VAL:O	1:B:280:LYS:HD3	2.15	0.46
1:A:259:LEU:O	1:A:263:THR:HG23	2.15	0.46
1:A:295:TYR:O	1:A:299:HIS:HD2	1.99	0.46
1:B:218:GLU:O	1:B:222:VAL:HG22	2.15	0.46
1:B:311:TYR:HE1	1:B:326:CYS:HB3	1.81	0.46
1:B:347:PRO:HG2	1:B:350:GLN:HB2	1.98	0.46
1:A:347:PRO:HG2	1:A:350:GLN:HB2	1.98	0.46
1:A:218:GLU:O	1:A:222:VAL:HG22	2.16	0.46
1:A:7:GLU:HG3	1:A:8:TYR:H	1.81	0.46
1:B:40:TYR:C	1:B:40:TYR:CD2	2.94	0.46
1:B:17:LEU:HB3	1:B:22:TYR:CB	2.45	0.45
1:A:16:LEU:O	1:A:20:ILE:HG12	2.16	0.45
1:B:280:LYS:O	1:B:281:ASP:C	2.58	0.45
1:B:328:PHE:O	1:B:329:TYR:C	2.59	0.45
1:A:114:PHE:HB2	1:B:151:ILE:HD11	1.98	0.45
1:A:225:ASN:O	1:A:229:SER:HB3	2.17	0.45
1:B:231:TYR:C	1:B:231:TYR:HD2	2.24	0.45
3:A:710:RAZ:H032	3:A:710:RAZ:H111	1.62	0.45
1:B:69:THR:CG2	1:B:298:TRP:HZ2	2.30	0.45
1:A:105:ASP:OD2	1:A:107:TYR:HB3	2.16	0.45
1:B:326:CYS:HA	1:B:329:TYR:HB3	1.99	0.45
1:A:317:GLU:HG2	1:A:319:THR:HG23	1.98	0.45
1:A:56:LEU:HG	1:A:58:VAL:HG23	1.99	0.45
1:A:142:PHE:CE2	1:A:194:SER:HA	2.51	0.45
1:B:177:TYR:HB3	1:B:178:PRO:HD3	1.99	0.45
1:A:23:ARG:HH22	1:A:289:GLU:CD	2.24	0.45
1:A:14:VAL:HG11	1:A:324:LYS:HD3	1.99	0.44
1:A:241:ILE:HG13	1:A:241:ILE:O	2.15	0.44
1:B:16:LEU:HD22	1:B:227:LEU:HD23	2.00	0.44
1:A:8:TYR:C	1:A:8:TYR:CD2	2.95	0.44
1:B:225:ASN:ND2	1:B:299:HIS:HE1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:HIS:O	1:A:52:GLN:HG3	2.18	0.44
1:A:189:HIS:CE1	1:B:180:PHE:HE1	2.36	0.44
1:B:177:TYR:OH	1:B:181:LEU:HD22	2.17	0.43
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.17	0.43
1:A:105:ASP:HA	1:A:106:PRO:HD3	1.80	0.43
1:A:311:TYR:O	1:A:315:LYS:HB2	2.18	0.43
1:A:166:TYR:O	1:A:167:ASN:C	2.60	0.43
1:A:12:THR:HG21	1:A:263:THR:CG2	2.48	0.43
1:A:19:TYR:CE2	1:A:271:LYS:HG3	2.54	0.43
1:A:284:VAL:O	1:A:285:MET:C	2.62	0.43
1:B:46:HIS:O	1:B:52:GLN:HG3	2.19	0.43
1:A:321:ASP:O	1:A:322:ALA:C	2.59	0.43
1:B:85:CYS:CA	1:B:141:HIS:CE1	2.98	0.43
1:B:285:MET:HE3	1:B:289:GLU:HB2	2.01	0.43
1:B:105:ASP:HA	1:B:106:PRO:HD3	1.82	0.43
1:B:3:ASN:O	1:B:4:PHE:HB2	2.19	0.43
1:B:160:GLY:O	1:B:164:GLU:HG2	2.19	0.43
1:A:232:LYS:HG3	1:A:233:GLU:HG3	2.01	0.42
1:B:300:LEU:HD23	1:B:307:LEU:CD1	2.48	0.42
1:A:4:PHE:C	1:A:6:THR:H	2.27	0.42
1:A:306:ARG:NH1	1:A:309:GLU:OE2	2.52	0.42
1:B:345:TYR:HA	1:B:346:PRO:C	2.44	0.42
1:A:220:TRP:CZ2	1:A:224:VAL:HG21	2.54	0.42
1:A:307:LEU:O	1:A:310:ILE:HG12	2.19	0.42
6:B:709:SAZ:H162	4:B:706:POP:O6	2.19	0.42
1:A:280:LYS:O	1:A:281:ASP:C	2.61	0.42
1:B:9:PHE:C	1:B:9:PHE:CD2	2.98	0.42
1:B:59:ASP:OD1	1:B:60:PRO:HD2	2.20	0.42
1:B:314:VAL:HG21	1:B:325:PHE:CD2	2.55	0.42
1:B:168:PHE:CZ	1:B:170:GLY:HA2	2.54	0.42
1:B:229:SER:C	1:B:231:TYR:H	2.27	0.42
1:B:217:MET:CE	1:B:220:TRP:HE3	2.33	0.41
1:B:284:VAL:O	1:B:285:MET:C	2.64	0.41
1:B:206:LEU:HB3	1:B:209:GLU:HG2	2.02	0.41
1:B:231:TYR:CE2	1:B:306:ARG:NH2	2.88	0.41
1:B:311:TYR:CE1	1:B:326:CYS:HB3	2.54	0.41
1:B:217:MET:CE	1:B:220:TRP:CE3	3.03	0.41
1:B:307:LEU:O	1:B:310:ILE:HG12	2.20	0.41
1:B:92:HIS:HB2	1:B:138:VAL:HG21	2.03	0.41
1:B:111:VAL:HA	7:B:758:HOH:O	2.19	0.41
1:A:345:TYR:HA	1:A:346:PRO:C	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HD2	1:A:335:VAL:O	2.20	0.41
1:B:220:TRP:CZ2	1:B:224:VAL:HG21	2.55	0.41
1:A:58:VAL:HG21	1:A:98:VAL:HG11	2.03	0.41
1:A:232:LYS:NZ	1:A:233:GLU:HG2	2.36	0.41
1:B:70:ILE:HG13	1:B:94:THR:HA	2.03	0.41
1:B:107:TYR:HB3	1:B:108:PRO:HD3	2.03	0.41
1:B:209:GLU:CD	1:B:209:GLU:H	2.29	0.41
1:B:231:TYR:HE2	1:B:306:ARG:NH2	2.19	0.41
1:A:70:ILE:HG13	1:A:94:THR:HA	2.03	0.41
1:A:311:TYR:HD2	1:A:312:GLU:OE1	2.03	0.41
1:B:46:HIS:HA	1:B:49:GLN:HE21	1.85	0.41
1:B:306:ARG:NH1	1:B:309:GLU:OE2	2.54	0.41
1:B:156:ASP:HA	1:B:184:MET:HE2	2.02	0.40
1:B:234:PHE:C	1:B:236:ASP:N	2.80	0.40
1:A:156:ASP:HA	1:A:184:MET:HE2	2.03	0.40
1:A:228:MET:CE	1:A:296:VAL:HG13	2.47	0.40
1:B:179:GLN:O	1:B:183:ARG:HG3	2.21	0.40
1:B:187:LEU:O	1:B:191:VAL:HG23	2.21	0.40
1:B:328:PHE:HA	1:B:331:GLN:NE2	2.36	0.40
1:A:87:ALA:O	1:A:90:SER:HB2	2.21	0.40
1:A:209:GLU:CD	1:A:209:GLU:H	2.30	0.40
6:B:709:SAZ:H102	6:B:709:SAZ:H032	1.85	0.40
1:A:310:ILE:HD11	1:A:325:PHE:CZ	2.56	0.40
1:B:27:TYR:HA	1:B:31:GLU:OE1	2.22	0.40
1:B:225:ASN:O	1:B:229:SER:HB3	2.21	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%)	319 (91%)	31 (9%)	2 (1%)	21	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	352/374 (94%)	306 (87%)	39 (11%)	7 (2%)	6	16
All	All	704/748 (94%)	625 (89%)	70 (10%)	9 (1%)	9	26

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	TYR
1	B	22	TYR
1	B	235	ASP
1	B	239	ASP
1	B	319	THR
1	B	333	ALA
1	B	5	PRO
1	B	178	PRO
1	A	178	PRO

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%)	315 (98%)	5 (2%)	55	75
1	B	320/340 (94%)	316 (99%)	4 (1%)	61	78
All	All	640/680 (94%)	631 (99%)	9 (1%)	59	77

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	135	PHE
1	A	200	GLN
1	A	209	GLU
1	A	335	VAL
1	B	29	ARG
1	B	135	PHE

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Mol	Chain	Res	Type
1	B	200	GLN
1	B	209	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	165	GLN
1	A	167	ASN
1	A	175	HIS
1	A	216	GLN
1	A	256	HIS
1	A	272	GLN
1	A	299	HIS
1	A	334	ASN
1	B	11	ASN
1	B	46	HIS
1	B	49	GLN
1	B	68	GLN
1	B	137	ASN
1	B	165	GLN
1	B	175	HIS
1	B	179	GLN
1	B	240	GLN
1	B	272	GLN
1	B	299	HIS
1	B	331	GLN
1	B	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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$
6	SAZ	B	709	-	14,15,15	2.15	5 (35%)	18,19,19	1.97	6 (33%)
3	RAZ	A	710	-	14,15,15	2.17	6 (42%)	18,19,19	2.10	7 (38%)
4	POP	B	706	2	6,8,8	1.51	1 (16%)	12,13,13	1.52	1 (8%)
5	EDO	B	751	-	3,3,3	0.60	0	2,2,2	0.59	0
4	POP	A	701	2	6,8,8	1.42	1 (16%)	12,13,13	1.54	2 (16%)
5	EDO	A	750	-	3,3,3	0.49	0	2,2,2	0.47	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
6	SAZ	B	709	-	-	0/10/20/20	0/1/1/1
3	RAZ	A	710	-	1/1/4/6	6/10/20/20	0/1/1/1
4	POP	B	706	2	-	0/6/6/6	-
5	EDO	B	751	-	-	0/1/1/1	-
4	POP	A	701	2	-	0/6/6/6	-
5	EDO	A	750	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	709	SAZ	C05-C25	5.16	1.52	1.33
3	A	710	RAZ	C05-C31	5.03	1.52	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	710	RAZ	C07-C31	-3.74	1.35	1.49
6	B	709	SAZ	C07-C25	-3.48	1.36	1.49
6	B	709	SAZ	C02-C01	3.08	1.57	1.52
3	A	710	RAZ	C02-C01	2.71	1.57	1.52
3	A	710	RAZ	C01-N08	-2.64	1.44	1.47
4	A	701	POP	P2-O6	-2.63	1.45	1.54
6	B	709	SAZ	C02-C05	2.56	1.55	1.50
3	A	710	RAZ	C03-C01	2.54	1.58	1.52
4	B	706	POP	P2-O6	-2.42	1.45	1.54
6	B	709	SAZ	C03-C01	2.36	1.58	1.52
3	A	710	RAZ	C02-C05	2.16	1.54	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	706	POP	O2-P1-O	4.63	120.17	104.64
4	A	701	POP	O2-P1-O	4.28	118.99	104.64
6	B	709	SAZ	C36-N35-C10	-3.85	104.86	110.51
3	A	710	RAZ	C01-C02-C05	3.68	116.68	111.32
6	B	709	SAZ	C01-C02-C05	3.54	116.48	111.32
3	A	710	RAZ	C11-N08-C01	3.35	119.91	112.62
6	B	709	SAZ	C03-C07-C25	3.29	124.56	113.51
3	A	710	RAZ	C03-C07-C31	3.22	124.32	113.51
3	A	710	RAZ	C19-N08-C11	-3.15	105.89	110.51
3	A	710	RAZ	C02-C05-C31	-2.87	112.42	123.96
3	A	710	RAZ	C03-C01-C02	2.78	113.08	109.52
3	A	710	RAZ	C07-C03-C01	2.72	117.16	111.66
6	B	709	SAZ	C02-C05-C25	-2.65	113.31	123.96
6	B	709	SAZ	C10-N35-C01	2.34	117.71	112.62
6	B	709	SAZ	C07-C03-C01	2.27	116.27	111.66
4	A	701	POP	O6-P2-O5	2.12	115.75	107.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	710	RAZ	C01

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	710	RAZ	C02-C01-N08-C11
3	A	710	RAZ	C03-C01-N08-C11

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Mol	Chain	Res	Type	Atoms
3	A	710	RAZ	C09-C10-C11-N08
3	A	710	RAZ	C02-C01-N08-C19
3	A	710	RAZ	C03-C01-N08-C19
3	A	710	RAZ	C10-C11-N08-C19
5	A	750	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	709	SAZ	2	0
3	A	710	RAZ	3	0
4	B	706	POP	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	349/374 (93%)	0.16	12 (3%) 48 41	40, 57, 86, 114	0
1	B	335/374 (89%)	0.48	39 (11%) 9 8	41, 57, 116, 141	0
All	All	684/748 (91%)	0.32	51 (7%) 20 18	40, 57, 103, 141	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	PRO	7.6
1	B	322	ALA	6.5
1	B	319	THR	6.0
1	B	8	TYR	5.4
1	B	9	PHE	5.1
1	B	328	PHE	4.8
1	B	329	TYR	4.7
1	A	317	GLU	4.7
1	B	230	PHE	4.6
1	B	4	PHE	4.1
1	B	326	CYS	4.1
1	B	239	ASP	3.9
1	B	317	GLU	3.9
1	A	354	VAL	3.7
1	B	314	VAL	3.6
1	B	325	PHE	3.4
1	B	310	ILE	3.1
1	B	22	TYR	3.0
1	B	241	ILE	3.0
1	B	259	LEU	3.0
1	B	19	TYR	3.0
1	B	335	VAL	3.0
1	A	298	TRP	3.0
1	A	319	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	321	ASP	2.9
1	B	13	THR	2.9
1	A	310	ILE	2.8
1	B	331	GLN	2.7
1	B	11	ASN	2.6
1	A	25	SER	2.6
1	B	307	LEU	2.5
1	B	236	ASP	2.4
1	A	1	MET	2.4
1	A	315	LYS	2.3
1	B	14	VAL	2.3
1	A	326	CYS	2.3
1	B	251	ASP	2.3
1	B	312	GLU	2.2
1	B	333	ALA	2.2
1	B	104	ASP	2.2
1	B	175	HIS	2.2
1	B	258	ALA	2.2
1	A	2	GLU	2.2
1	A	199	GLU	2.2
1	B	304	ARG	2.2
1	B	231	TYR	2.1
1	B	102	SER	2.1
1	B	313	LYS	2.1
1	A	22	TYR	2.1
1	B	25	SER	2.0
1	B	2	GLU	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	A	703	1/1	0.86	0.18	54,54,54,54	0
2	MG	B	708	1/1	0.88	0.16	53,53,53,53	0
5	EDO	B	751	4/4	0.92	0.12	50,51,53,53	0
6	SAZ	B	709	15/15	0.92	0.23	84,86,87,87	0
3	RAZ	A	710	15/15	0.93	0.19	69,74,76,76	0
2	MG	A	702	1/1	0.94	0.06	41,41,41,41	0
4	POP	A	701	9/9	0.94	0.07	80,80,83,84	0
5	EDO	A	750	4/4	0.95	0.11	44,45,46,47	0
4	POP	B	706	9/9	0.96	0.07	81,82,84,85	0
2	MG	B	707	1/1	0.96	0.06	58,58,58,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.