



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 PM UTC

PDB ID : 6IWT / pdb_00006iwt
Title : Crystal structure of methyltransferase COMT-S in *P. praeruptorum*
Authors : Wang, N.N.; Zeng, Z.X.
Deposited on : 2018-12-06
Resolution : 2.53 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

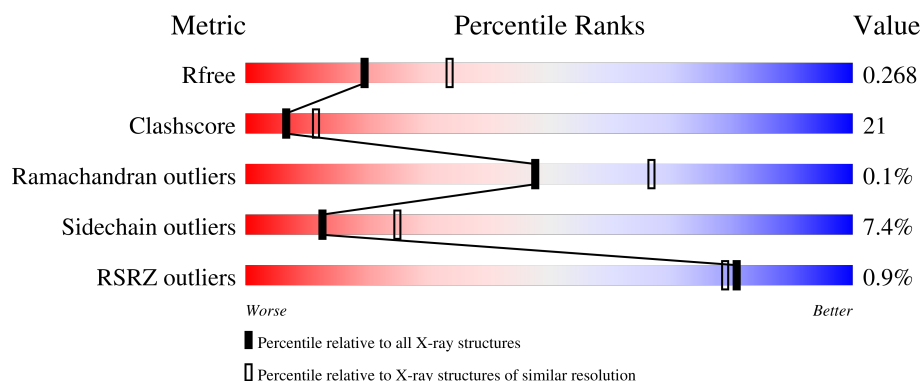
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

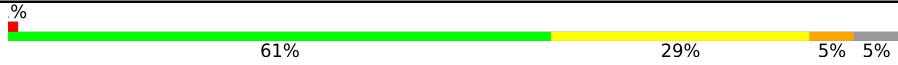
The reported resolution of this entry is 2.53 Å.

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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	364	
1	B	364	

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
2	PEG	A	402	-	-	X	-

2 Entry composition [i](#)

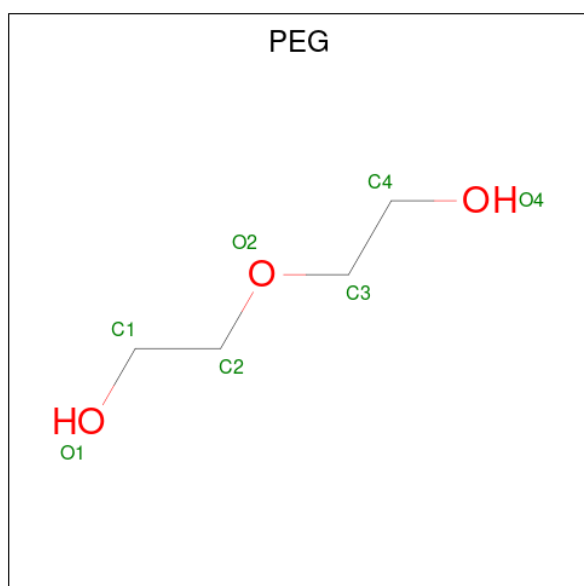
There are 3 unique types of molecules in this entry. The entry contains 5322 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pmethyltransferase pCOMT-S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2652	1704	435	488	25			
1	B	346	Total	C	N	O	S	0	0	0
			2652	1704	435	488	25			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		

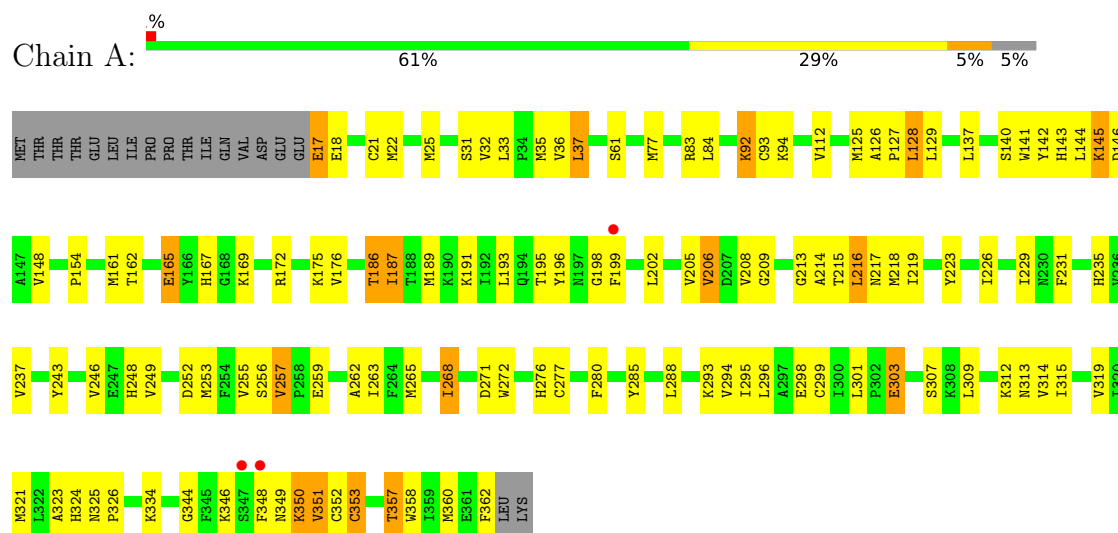
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		

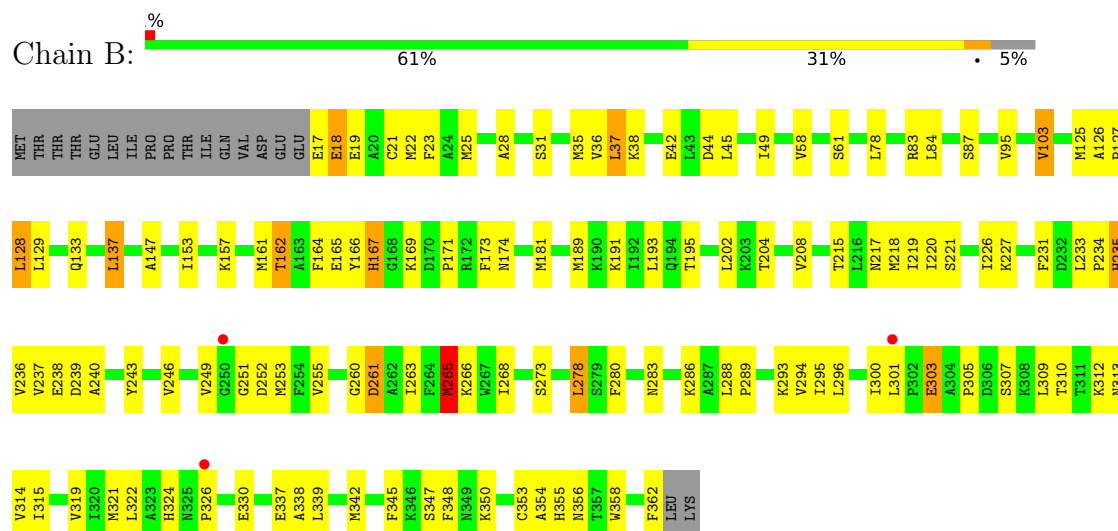
3 Residue-property plots [i](#)

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: Pmethyltransferase pCOMT-S



• Molecule 1: Pmethyltransferase pCOMT-S



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.37Å 70.39Å 59.65Å 90.00° 97.87° 90.00°	Depositor
Resolution (Å)	66.59 – 2.53 66.59 – 2.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (66.59-2.53) 96.0 (66.59-2.53)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.11_2567	Depositor
R, R_{free}	0.189 , 0.261 0.199 , 0.268	Depositor DCC
R_{free} test set	1392 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	74.2	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5322	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% 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: PEG

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	0.75	7/2714 (0.3%)	0.68	5/3675 (0.1%)
1	B	0.60	2/2714 (0.1%)	0.64	0/3675
All	All	0.68	9/5428 (0.2%)	0.66	5/7350 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	146	ASP	C-O	-7.57	1.15	1.24
1	A	145	LYS	C-O	-6.28	1.16	1.24
1	A	357	THR	C-O	-6.11	1.16	1.24
1	A	143	HIS	C-O	-5.82	1.16	1.24
1	A	142	TYR	C-O	-5.61	1.16	1.24
1	A	353	CYS	C-O	-5.39	1.17	1.23
1	B	266	LYS	CA-C	-5.38	1.46	1.52
1	A	141	TRP	C-O	-5.03	1.17	1.24
1	B	265	MET	C-O	-5.02	1.18	1.24

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	PRO	CA-C-N	-6.57	112.49	122.28
1	A	326	PRO	C-N-CA	-6.57	112.49	122.28
1	A	93	CYS	N-CA-C	5.82	118.60	108.76
1	A	186	THR	CA-C-N	-5.52	112.04	121.97
1	A	186	THR	C-N-CA	-5.52	112.04	121.97

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	2652	0	2664	115	1
1	B	2652	0	2664	140	1
2	A	14	0	20	8	0
3	A	4	0	0	0	0
All	All	5322	0	5348	229	1

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 21.

All (229) 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:278:LEU:HD21	1:B:342:MET:HG2	1.11	1.06
1:B:301:LEU:HG	1:B:314:VAL:CG1	1.88	1.02
1:A:22:MET:HE2	1:B:310:THR:HG22	1.39	1.01
1:B:301:LEU:HD12	1:B:330:GLU:HB2	1.53	0.91
1:B:231:PHE:HD1	1:B:249:VAL:HG23	1.33	0.90
1:B:191:LYS:HD3	1:B:355:HIS:HB2	1.55	0.89
1:B:301:LEU:HG	1:B:314:VAL:HG12	1.53	0.87
1:B:233:LEU:HD13	1:B:235:HIS:CD2	2.10	0.86
1:A:237:VAL:HG11	1:A:248:HIS:HB3	1.58	0.84
1:B:265:MET:HG3	1:B:296:LEU:HD23	1.57	0.84
1:B:301:LEU:HG	1:B:314:VAL:HG11	1.56	0.84
1:A:172:ARG:O	1:A:175:LYS:HG2	1.78	0.83
1:A:208:VAL:HG22	1:A:265:MET:HG2	1.58	0.83
1:B:37:LEU:HD13	1:B:129:LEU:HD11	1.61	0.82
1:A:161:MET:HB2	1:A:165:GLU:HG3	1.62	0.81
1:A:253:MET:HE2	1:A:280:PHE:CG	2.15	0.81
1:B:37:LEU:HD13	1:B:129:LEU:CD1	2.11	0.81
1:B:233:LEU:HD11	1:B:236:VAL:HG23	1.62	0.80
1:A:285:TYR:CE1	1:A:344:GLY:O	2.36	0.79
1:A:17:GLU:N	1:A:17:GLU:OE1	2.15	0.79
1:A:186:THR:O	1:A:187:ILE:C	2.22	0.79
1:A:237:VAL:CG1	1:A:248:HIS:HB3	2.13	0.78
1:A:272:TRP:CE3	2:A:402:PEG:H21	2.19	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:LEU:HD21	1:B:342:MET:CG	2.05	0.77
1:B:164:PHE:HD1	1:B:165:GLU:HG3	1.49	0.76
1:A:202:LEU:HD21	1:A:262:ALA:HB3	1.69	0.75
1:A:265:MET:HB3	1:A:268:ILE:CG2	2.17	0.74
1:A:265:MET:HB3	1:A:268:ILE:HG21	1.70	0.74
1:A:21:CYS:SG	1:B:191:LYS:NZ	2.60	0.73
1:B:162:THR:OG1	1:B:164:PHE:HB3	1.87	0.73
1:A:252:ASP:O	1:A:255:VAL:HG22	1.90	0.72
1:B:233:LEU:HD12	1:B:236:VAL:H	1.54	0.72
1:B:137:LEU:HD12	1:B:324:HIS:CE1	2.25	0.72
1:A:208:VAL:CG2	1:A:265:MET:HG2	2.20	0.72
1:B:162:THR:HG23	1:B:165:GLU:OE1	1.91	0.71
1:A:37:LEU:HD13	1:A:129:LEU:CD1	2.20	0.71
1:A:162:THR:HG23	1:A:165:GLU:OE2	1.90	0.70
1:A:191:LYS:NZ	1:B:21:CYS:SG	2.64	0.70
1:A:216:LEU:HD23	1:A:217:ASN:N	2.07	0.70
1:B:217:ASN:CG	1:B:243:TYR:HD2	1.99	0.70
1:B:22:MET:HA	1:B:22:MET:HE2	1.74	0.70
1:B:217:ASN:CG	1:B:243:TYR:CD2	2.70	0.70
1:A:350:LYS:HD3	1:A:358:TRP:CZ3	2.27	0.68
1:B:233:LEU:HD13	1:B:235:HIS:CG	2.27	0.68
1:B:301:LEU:HD12	1:B:330:GLU:CB	2.22	0.67
1:B:253:MET:HE2	1:B:280:PHE:CG	2.29	0.67
1:A:216:LEU:HD21	1:A:246:VAL:HB	1.76	0.67
1:A:125:MET:HE2	1:B:25:MET:HG3	1.77	0.67
1:B:231:PHE:CD1	1:B:249:VAL:HG23	2.24	0.67
1:B:253:MET:HE2	1:B:280:PHE:CD2	2.29	0.67
1:B:293:LYS:HE3	1:B:295:ILE:HD11	1.75	0.67
1:B:153:ILE:HG23	1:B:326:PRO:HD3	1.76	0.66
1:B:337:GLU:HG3	1:B:338:ALA:N	2.10	0.66
1:B:353:CYS:HB2	1:B:358:TRP:CD2	2.30	0.66
1:B:161:MET:HE2	1:B:165:GLU:C	2.20	0.66
1:A:202:LEU:HD21	1:A:262:ALA:CB	2.25	0.66
1:A:125:MET:HE2	1:B:25:MET:CG	2.26	0.65
1:B:278:LEU:CD2	1:B:342:MET:HG2	2.06	0.64
1:B:353:CYS:HB2	1:B:358:TRP:CE3	2.32	0.64
1:A:353:CYS:HB2	1:A:358:TRP:CD2	2.32	0.64
1:A:272:TRP:HA	2:A:402:PEG:H22	1.78	0.64
1:B:233:LEU:HD12	1:B:233:LEU:O	1.97	0.64
1:A:324:HIS:NE2	2:A:401:PEG:H21	2.13	0.64
1:A:22:MET:HE3	1:B:313:ASN:HD22	1.62	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:LEU:CD1	1:B:330:GLU:HB2	2.27	0.63
1:A:206:VAL:HG13	1:A:263:ILE:HG12	1.80	0.63
1:B:208:VAL:HB	1:B:265:MET:HE3	1.80	0.63
1:A:265:MET:HE2	1:A:296:LEU:CD2	2.29	0.62
1:A:216:LEU:HA	1:A:219:ILE:HD12	1.80	0.62
1:A:293:LYS:HG3	1:A:295:ILE:HD11	1.80	0.62
1:B:265:MET:HB3	1:B:268:ILE:HG21	1.81	0.62
1:B:161:MET:HE2	1:B:166:TYR:HA	1.81	0.61
1:B:300:ILE:HG13	1:B:358:TRP:CD1	2.36	0.61
1:B:191:LYS:NZ	1:B:355:HIS:HD2	2.00	0.60
1:A:37:LEU:HD13	1:A:129:LEU:HD11	1.82	0.59
1:B:265:MET:HE2	1:B:268:ILE:HG21	1.85	0.58
1:A:206:VAL:CG1	1:A:263:ILE:HG12	2.33	0.58
1:A:202:LEU:HD23	1:A:205:VAL:CG2	2.33	0.58
1:A:265:MET:HE3	1:A:268:ILE:HG23	1.84	0.58
1:B:191:LYS:O	1:B:195:THR:HG23	2.03	0.58
1:B:161:MET:HE2	1:B:166:TYR:N	2.18	0.58
1:B:161:MET:HE3	1:B:165:GLU:HB3	1.84	0.57
1:A:126:ALA:HB3	1:A:127:PRO:HD3	1.87	0.57
1:B:164:PHE:CD1	1:B:165:GLU:HG3	2.37	0.56
1:A:112:VAL:HG21	1:B:23:PHE:CE2	2.41	0.56
1:A:257:VAL:HG21	1:A:263:ILE:CD1	2.36	0.56
1:A:22:MET:CE	1:B:313:ASN:HD22	2.18	0.56
1:B:243:TYR:HB2	1:B:246:VAL:HG22	1.88	0.56
1:A:293:LYS:HE3	1:A:295:ILE:HD11	1.87	0.56
1:B:217:ASN:HB2	1:B:243:TYR:CD2	2.41	0.56
1:A:313:ASN:ND2	1:B:25:MET:HE2	2.21	0.55
1:A:22:MET:HE3	1:B:313:ASN:ND2	2.22	0.55
1:B:126:ALA:HB3	1:B:127:PRO:HD3	1.89	0.55
1:B:303:GLU:OE1	1:B:303:GLU:N	2.35	0.54
1:A:25:MET:HG2	1:B:125:MET:HE2	1.90	0.54
1:B:191:LYS:CD	1:B:355:HIS:HB2	2.31	0.54
1:B:147:ALA:HA	1:B:157:LYS:HE3	1.90	0.54
1:B:261:ASP:OD1	1:B:261:ASP:N	2.41	0.54
1:A:216:LEU:HD23	1:A:216:LEU:C	2.33	0.54
1:B:243:TYR:HB2	1:B:246:VAL:CG2	2.38	0.54
1:A:319:VAL:HG11	1:B:36:VAL:HG21	1.90	0.53
1:B:49:ILE:HG12	1:B:58:VAL:HG21	1.88	0.53
1:A:25:MET:CG	1:B:125:MET:HE2	2.39	0.53
1:B:161:MET:HE2	1:B:166:TYR:CA	2.38	0.53
1:B:265:MET:CB	1:B:268:ILE:HG21	2.38	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:LYS:HD3	1:B:358:TRP:CE3	2.44	0.53
1:A:216:LEU:HD21	1:A:246:VAL:CB	2.38	0.52
1:A:276:HIS:ND1	2:A:402:PEG:H12	2.24	0.52
1:A:350:LYS:HD3	1:A:358:TRP:CE3	2.44	0.52
1:B:303:GLU:H	1:B:303:GLU:CD	2.17	0.52
1:A:301:LEU:HD13	1:B:83:ARG:NH1	2.25	0.52
1:A:83:ARG:HG3	1:B:305:PRO:HG3	1.90	0.51
1:B:137:LEU:HD22	1:B:173:PHE:CE1	2.44	0.51
1:A:196:TYR:CZ	1:A:198:GLY:HA3	2.45	0.51
1:A:125:MET:HE3	1:A:128:LEU:HD12	1.92	0.51
1:B:217:ASN:CB	1:B:243:TYR:CD2	2.93	0.51
1:B:233:LEU:HD11	1:B:236:VAL:CG2	2.39	0.51
1:B:283:ASN:HA	1:B:286:LYS:HD3	1.93	0.51
1:A:265:MET:HE3	1:A:268:ILE:CG2	2.41	0.51
1:A:299:CYS:HB3	1:A:314:VAL:HG22	1.93	0.50
1:B:303:GLU:N	1:B:303:GLU:CD	2.68	0.50
1:B:265:MET:HG3	1:B:296:LEU:CD2	2.36	0.50
1:A:277:CYS:HA	1:A:280:PHE:CE2	2.47	0.50
1:A:293:LYS:HG3	1:A:295:ILE:CD1	2.40	0.50
1:A:154:PRO:HG2	1:A:323:ALA:HA	1.94	0.49
1:B:204:THR:HA	1:B:227:LYS:O	2.11	0.49
1:A:262:ALA:HB1	1:A:295:ILE:CD1	2.42	0.49
1:B:233:LEU:CD1	1:B:236:VAL:H	2.24	0.49
1:A:189:MET:HG3	1:A:215:THR:HG23	1.94	0.49
1:B:202:LEU:O	1:B:226:ILE:HG12	2.12	0.49
1:A:315:ILE:HG21	1:B:84:LEU:HA	1.95	0.49
1:A:32:VAL:HG23	1:A:33:LEU:N	2.28	0.49
1:A:288:LEU:HD11	1:A:294:VAL:HG23	1.95	0.48
1:B:129:LEU:HD23	1:B:129:LEU:C	2.38	0.48
1:B:167:HIS:O	1:B:174:ASN:HB2	2.12	0.48
1:B:265:MET:HB2	1:B:268:ILE:CG2	2.43	0.48
1:A:243:TYR:HB2	1:A:246:VAL:CG2	2.43	0.48
1:A:262:ALA:HB1	1:A:295:ILE:HD13	1.95	0.48
1:A:144:LEU:O	1:A:148:VAL:HG23	2.13	0.48
1:B:220:ILE:HD12	1:B:221:SER:N	2.29	0.48
1:B:294:VAL:HB	1:B:362:PHE:HB2	1.96	0.48
1:B:301:LEU:CG	1:B:314:VAL:HG12	2.33	0.48
1:A:276:HIS:HD1	2:A:402:PEG:H12	1.78	0.48
1:A:271:ASP:O	2:A:402:PEG:H32	2.13	0.47
1:A:353:CYS:HB2	1:A:358:TRP:CE3	2.49	0.47
1:B:191:LYS:HZ3	1:B:355:HIS:HD2	1.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:HD12	1:A:218:MET:HE2	1.96	0.47
1:B:252:ASP:O	1:B:255:VAL:HG22	2.14	0.47
1:A:186:THR:OG1	1:A:187:ILE:N	2.47	0.47
1:A:145:LYS:HD2	1:B:42:GLU:HB3	1.97	0.47
1:A:161:MET:HB2	1:A:165:GLU:CG	2.40	0.47
1:A:112:VAL:HG21	1:B:23:PHE:CD2	2.50	0.46
1:A:348:PHE:N	1:A:348:PHE:CD1	2.82	0.46
1:B:129:LEU:HD23	1:B:129:LEU:O	2.15	0.46
1:B:17:GLU:HG3	1:B:18:GLU:H	1.81	0.46
1:A:243:TYR:HB2	1:A:246:VAL:HG22	1.97	0.46
1:B:153:ILE:HD13	1:B:326:PRO:CD	2.46	0.46
1:A:265:MET:HE2	1:A:296:LEU:HD22	1.97	0.45
1:A:321:MET:HG3	1:A:325:ASN:O	2.17	0.45
1:A:125:MET:HE2	1:B:25:MET:HG2	1.97	0.45
1:B:309:LEU:HD12	1:B:309:LEU:HA	1.76	0.45
1:A:32:VAL:O	1:A:36:VAL:HG23	2.16	0.45
1:A:193:LEU:CD1	1:A:218:MET:HE2	2.46	0.45
1:A:128:LEU:HD13	1:B:28:ALA:HB1	1.98	0.45
1:B:95:VAL:HG13	1:B:103:VAL:HG13	1.99	0.45
1:B:348:PHE:HD1	1:B:362:PHE:HE1	1.63	0.45
1:A:351:VAL:HG22	1:A:352:CYS:N	2.32	0.45
1:A:129:LEU:C	1:A:129:LEU:HD23	2.42	0.45
1:B:193:LEU:HD21	1:B:219:ILE:HG12	1.98	0.45
1:A:199:PHE:HB2	1:A:223:TYR:CE2	2.52	0.45
1:B:260:GLY:O	1:B:289:PRO:HD3	2.16	0.44
1:A:293:LYS:HA	1:A:362:PHE:O	2.18	0.44
1:A:175:LYS:HG3	1:A:176:VAL:N	2.32	0.44
1:A:206:VAL:HA	1:A:229:ILE:O	2.18	0.44
1:B:321:MET:HE2	1:B:321:MET:HB2	1.86	0.44
1:A:36:VAL:HG21	1:B:319:VAL:HG11	1.98	0.44
1:B:38:LYS:HD2	1:B:133:GLN:HB3	1.99	0.44
1:A:223:TYR:HB2	1:A:226:ILE:HD12	2.00	0.44
1:A:307:SER:O	1:A:312:LYS:HE3	2.18	0.44
1:B:234:PRO:HD3	1:B:251:GLY:H	1.82	0.44
1:B:278:LEU:HD13	1:B:339:LEU:CD2	2.47	0.44
1:B:95:VAL:HG13	1:B:103:VAL:CG1	2.48	0.43
1:B:265:MET:CB	1:B:268:ILE:CG2	2.95	0.43
1:A:334:LYS:HB2	1:A:334:LYS:HE3	1.83	0.43
1:B:153:ILE:HG12	1:B:326:PRO:HG3	1.99	0.43
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.81	0.43
1:B:345:PHE:C	1:B:347:SER:H	2.25	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LEU:HA	1:B:315:ILE:HG21	2.00	0.43
1:A:294:VAL:HB	1:A:362:PHE:HB2	2.00	0.43
1:B:307:SER:O	1:B:312:LYS:HE3	2.18	0.43
1:B:191:LYS:HB3	1:B:354:ALA:HB1	2.00	0.43
1:B:265:MET:HB3	1:B:265:MET:HE2	1.56	0.42
1:B:278:LEU:HD13	1:B:339:LEU:HD22	2.01	0.42
1:A:298:GLU:HB2	1:A:360:MET:HE1	2.01	0.42
1:B:45:LEU:HD11	1:B:78:LEU:HD22	2.01	0.42
1:A:309:LEU:HD22	1:B:19:GLU:OE2	2.19	0.42
1:B:153:ILE:HD13	1:B:326:PRO:HD2	2.02	0.42
1:B:234:PRO:HD3	1:B:251:GLY:N	2.35	0.42
1:B:233:LEU:HD12	1:B:233:LEU:C	2.44	0.42
1:A:253:MET:HE2	1:A:280:PHE:CD1	2.51	0.42
1:B:350:LYS:HD3	1:B:358:TRP:CZ3	2.55	0.42
1:A:77:MET:HG2	1:B:322:LEU:HD11	2.02	0.41
1:A:216:LEU:HD21	1:A:246:VAL:CG1	2.50	0.41
1:B:235:HIS:ND1	1:B:235:HIS:N	2.68	0.41
1:A:303:GLU:H	1:A:303:GLU:HG2	1.43	0.41
1:B:128:LEU:HD22	1:B:128:LEU:HA	1.81	0.41
1:B:153:ILE:CG2	1:B:326:PRO:HD3	2.45	0.41
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.92	0.41
1:B:239:ASP:O	1:B:240:ALA:C	2.61	0.41
1:B:246:VAL:O	1:B:246:VAL:HG23	2.20	0.41
1:A:137:LEU:HD13	2:A:401:PEG:H12	2.01	0.41
1:A:237:VAL:O	1:A:237:VAL:HG12	2.19	0.41
1:B:189:MET:HG3	1:B:215:THR:HG23	2.02	0.41
1:A:213:GLY:O	1:A:214:ALA:C	2.63	0.41
1:A:22:MET:HE1	1:B:356:ASN:ND2	2.36	0.41
1:A:312:LYS:HE2	1:B:87:SER:O	2.21	0.41
1:A:324:HIS:CD2	2:A:401:PEG:H21	2.55	0.41
1:A:209:GLY:N	1:A:231:PHE:O	2.54	0.41
1:B:137:LEU:CD2	1:B:173:PHE:CZ	3.04	0.41
1:A:31:SER:O	1:A:35:MET:HG2	2.20	0.40
1:B:217:ASN:OD1	1:B:220:ILE:HD11	2.20	0.40
1:B:263:ILE:HD13	1:B:288:LEU:HG	2.03	0.40
1:A:253:MET:HE2	1:A:280:PHE:CD2	2.55	0.40
1:B:161:MET:HE3	1:B:165:GLU:CB	2.48	0.40
1:B:181:MET:HE3	1:B:181:MET:HA	2.03	0.40
1:B:193:LEU:HD12	1:B:218:MET:HE2	2.02	0.40
1:B:263:ILE:CD1	1:B:288:LEU:HG	2.51	0.40
1:A:255:VAL:O	1:A:256:SER:HB3	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:SER:O	1:B:35:MET:HG2	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:LYS:NZ	1:B:238:GLU:OE2[1_554]	1.73	0.47

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	344/364 (94%)	334 (97%)	10 (3%)	0	100	100
1	B	344/364 (94%)	331 (96%)	12 (4%)	1 (0%)	36	53
All	All	688/728 (94%)	665 (97%)	22 (3%)	1 (0%)	48	67

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	PRO

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	290/309 (94%)	264 (91%)	26 (9%)	9	18
1	B	290/309 (94%)	273 (94%)	17 (6%)	18	35
All	All	580/618 (94%)	537 (93%)	43 (7%)	13	25

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	18	GLU
1	A	37	LEU
1	A	61	SER
1	A	92	LYS
1	A	94	LYS
1	A	128	LEU
1	A	140	SER
1	A	165	GLU
1	A	167	HIS
1	A	169	LYS
1	A	187	ILE
1	A	195	THR
1	A	206	VAL
1	A	216	LEU
1	A	235	HIS
1	A	249	VAL
1	A	257	VAL
1	A	259	GLU
1	A	268	ILE
1	A	303	GLU
1	A	346	LYS
1	A	349	ASN
1	A	350	LYS
1	A	351	VAL
1	A	357	THR
1	B	18	GLU
1	B	37	LEU
1	B	44	ASP
1	B	61	SER
1	B	103	VAL
1	B	128	LEU
1	B	137	LEU
1	B	162	THR
1	B	167	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	LYS
1	B	235	HIS
1	B	237	VAL
1	B	261	ASP
1	B	265	MET
1	B	273	SER
1	B	278	LEU
1	B	303	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	178	ASN
1	A	197	ASN
1	B	174	ASN
1	B	184	HIS
1	B	194	GLN
1	B	313	ASN
1	B	324	HIS
1	B	355	HIS

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](#)

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	PEG	A	402	-	6,6,6	0.48	0	5,5,5	1.09	1 (20%)
2	PEG	A	401	-	6,6,6	0.48	0	5,5,5	0.39	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	PEG	A	402	-	-	1/4/4/4	-
2	PEG	A	401	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	402	PEG	O1-C1-C2	-2.28	98.43	111.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	PEG	O1-C1-C2-O2
2	A	401	PEG	C4-C3-O2-C2
2	A	402	PEG	C4-C3-O2-C2
2	A	401	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	PEG	5	0
2	A	401	PEG	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	346/364 (95%)	0.02	3 (0%) 81 79	50, 80, 123, 151	0
1	B	346/364 (95%)	0.09	3 (0%) 81 79	47, 79, 116, 137	0
All	All	692/728 (95%)	0.05	6 (0%) 81 79	47, 80, 121, 151	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	348	PHE	2.5
1	B	301	LEU	2.5
1	B	326	PRO	2.3
1	B	250	GLY	2.3
1	A	199	PHE	2.0
1	A	347	SER	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($\text{\AA}^2$)	Q<0.9
2	PEG	A	401	7/7	0.83	0.18	62,83,90,93	0
2	PEG	A	402	7/7	0.89	0.19	51,64,78,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.