



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 07:44 AM GMT

PDB ID : 3BTP
Title : Crystal structure of Agrobacterium tumefaciens VirE2 in complex with its chaperone VirE1: a novel fold and implications for DNA binding
Authors : Dym, O.; Albeck, S.; Unger, T.; Elbaum, M.; Israel Structural Proteomics Center (ISPC)
Deposited on : 2007-12-30
Resolution : 2.30 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>

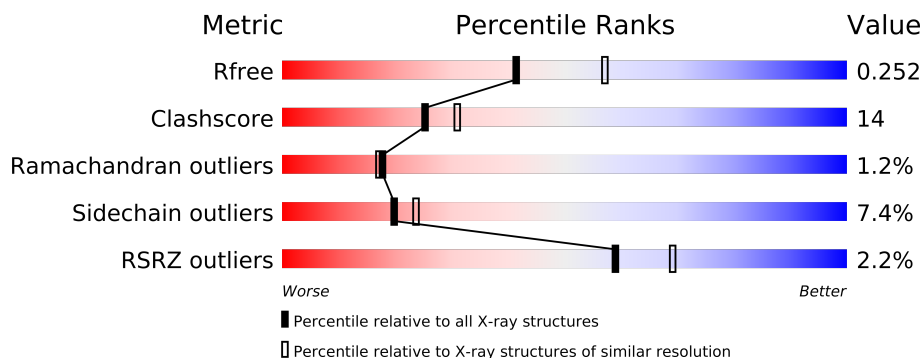
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	556	
2	B	63	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NH4	A	601	-	X
3	NH4	B	602	-	X
4	PEG	A	701	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3466 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 Single-strand DNA-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	1	0
			3158	1980	570	595	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	LEU	ILE	CONFLICT	UNP P08062

- Molecule 2 is a protein called Protein virE1.

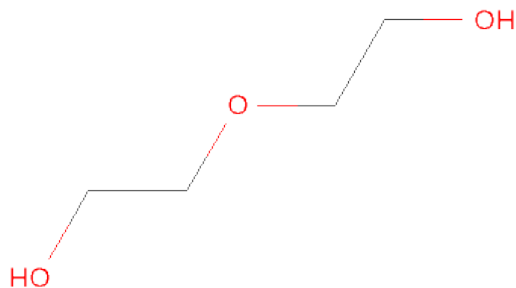
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	28	Total	C	N	O	S	0	0	0
			227	144	37	44	2			

- Molecule 3 is AMMONIUM ION (three-letter code: NH4) (formula: H₄N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N 1 1	0	0
3	B	1	Total N 1 1	0	0
3	B	1	Total N 1 1	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	61	Total O 61 61	0	0
5	B	10	Total O 10 10	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.02Å 96.27Å 112.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.14 – 2.30 48.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.14-2.30) 99.6 (48.14-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.209 , 0.256 0.209 , 0.252	Depositor DCC
R_{free} test set	1288 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 25163 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3466	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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: NH4, 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	1.17	9/3225 (0.3%)	1.14	19/4343 (0.4%)
2	B	1.28	0/233	1.07	1/316 (0.3%)
All	All	1.18	9/3458 (0.3%)	1.13	20/4659 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	GLU	CG-CD	7.83	1.63	1.51
1	A	324	GLU	CB-CG	6.75	1.65	1.52
1	A	165	ALA	CA-CB	6.73	1.66	1.52
1	A	116	GLU	CG-CD	6.12	1.61	1.51
1	A	258	SER	CB-OG	5.43	1.49	1.42
1	A	324	GLU	CD-OE2	5.31	1.31	1.25
1	A	463	GLU	CD-OE2	5.14	1.31	1.25
1	A	318	LYS	CD-CE	5.09	1.64	1.51
1	A	389	GLU	CG-CD	5.01	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	491	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	A	356	GLN	C-N-CD	-10.78	96.87	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	402	ASP	CB-CG-OD1	9.58	126.92	118.30
1	A	356	GLN	N-CA-C	8.81	134.80	111.00
1	A	402	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	A	356	GLN	C-N-CA	8.50	157.71	122.00
1	A	491	ARG	NE-CZ-NH1	8.45	124.53	120.30
1	A	277	ARG	NE-CZ-NH1	-8.01	116.29	120.30
1	A	183	GLU	N-CA-C	7.75	131.92	111.00
1	A	113	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	179	LEU	CA-CB-CG	6.77	130.87	115.30
1	A	243	ARG	NE-CZ-NH1	-6.11	117.25	120.30
2	B	40	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	201	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	A	485	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	277	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	A	357	PRO	CA-N-CD	-5.37	103.99	111.50
1	A	345	GLN	N-CA-C	5.20	125.04	111.00
1	A	353	MET	CB-CG-SD	5.07	127.61	112.40
1	A	340	ARG	NE-CZ-NH2	-5.05	117.77	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	183	GLU	Peptide
1	A	356	GLN	Peptide

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	3158	0	3089	84	0
2	B	227	0	209	7	0
3	A	1	0	0	1	0
3	B	2	0	0	1	0
4	A	7	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	61	0	0	2	0
5	B	10	0	0	1	0
All	All	3466	0	3308	92	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 14.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:356:GLN:H	1:A:364:THR:HG22	1.09	1.15
1:A:277:ARG:HH11	1:A:277:ARG:CG	1.61	1.12
1:A:325:ARG:CG	1:A:325:ARG:HH11	1.65	1.07
1:A:277:ARG:NH1	1:A:277:ARG:HG2	1.63	1.03
2:B:37:THR:HG22	2:B:40:ASP:H	1.19	1.01
1:A:325:ARG:HG3	1:A:325:ARG:NH1	1.68	1.00
1:A:325:ARG:HG3	1:A:325:ARG:HH11	0.85	1.00
1:A:356:GLN:N	1:A:364:THR:HG22	1.77	0.99
1:A:315:HIS:HD2	1:A:331:ARG:HH12	1.15	0.93
1:A:447:PHE:N	1:A:447:PHE:HD2	1.66	0.91
1:A:277:ARG:HH11	1:A:277:ARG:HG2	0.78	0.91
1:A:447:PHE:N	1:A:447:PHE:CD2	2.28	0.89
1:A:315:HIS:CD2	1:A:331:ARG:HH12	1.92	0.88
1:A:507:LYS:HE3	1:A:508:LEU:O	1.76	0.85
1:A:476:SER:HB2	1:A:502:GLU:OE1	1.77	0.84
1:A:137:ASP:OD1	1:A:138:HIS:HD2	1.63	0.81
1:A:184:PRO:O	1:A:186:GLU:N	2.15	0.80
2:B:37:THR:HG21	5:B:607:HOH:O	1.81	0.78
1:A:350:THR:HG23	1:A:368:HIS:HB3	1.66	0.77
1:A:121:ARG:HH12	1:A:131:THR:HG22	1.49	0.77
3:A:601:NH4:N	3:B:603:NH4:N	2.33	0.76
1:A:413:GLU:HG3	1:A:420:PHE:CD2	2.20	0.75
1:A:413:GLU:HG3	1:A:420:PHE:CE2	2.23	0.73
1:A:178:GLN:O	1:A:178:GLN:HG2	1.89	0.73
1:A:152:TYR:OH	1:A:203:HIS:HE1	1.73	0.71
1:A:179:LEU:C	1:A:182:LEU:HA	2.14	0.67
1:A:178:GLN:O	1:A:179:LEU:HB2	1.93	0.66
1:A:350:THR:CG2	1:A:368:HIS:HB3	2.25	0.66
2:B:31:HIS:CE1	2:B:32:GLN:NE2	2.65	0.65
1:A:325:ARG:CG	1:A:325:ARG:NH1	2.39	0.65
1:A:368:HIS:HD2	5:A:708:HOH:O	1.80	0.64
1:A:171:LEU:CD1	1:A:191:CYS:SG	2.86	0.64
1:A:199:TRP:O	1:A:203:HIS:HD2	1.82	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:LEU:HD13	1:A:191:CYS:SG	2.40	0.62
1:A:450:GLN:O	1:A:491:ARG:NH2	2.34	0.60
1:A:239:GLU:HG2	1:A:240:LYS:HG3	1.83	0.59
1:A:173:GLU:HG3	1:A:174:GLN:NE2	2.16	0.59
1:A:201:ARG:O	1:A:205:GLU:HG3	2.03	0.59
1:A:277:ARG:CD	1:A:332:PHE:O	2.51	0.59
1:A:356:GLN:HB3	1:A:357:PRO:HD2	1.84	0.59
1:A:315:HIS:HD2	1:A:331:ARG:NH1	1.95	0.59
1:A:397:GLN:HE22	1:A:495:TYR:HD2	1.53	0.57
1:A:325:ARG:N	1:A:325:ARG:HD2	2.19	0.57
1:A:413:GLU:OE1	1:A:434:GLY:O	2.23	0.56
1:A:486:ASN:OD1	1:A:490:GLN:HG2	2.05	0.56
1:A:137:ASP:OD1	1:A:138:HIS:CD2	2.53	0.56
1:A:138:HIS:HE1	1:A:144:GLU:OE1	1.89	0.55
1:A:469:PRO:HA	1:A:472:LEU:CD1	2.38	0.54
1:A:482:ILE:HD11	1:A:498:VAL:HG13	1.91	0.53
1:A:296:LYS:HB2	1:A:301:SER:HA	1.90	0.53
1:A:325:ARG:H	1:A:325:ARG:HD2	1.73	0.53
1:A:469:PRO:HA	1:A:472:LEU:HD11	1.89	0.53
1:A:350:THR:HG22	5:A:708:HOH:O	2.09	0.53
1:A:175:LEU:HD23	1:A:179:LEU:HD22	1.91	0.53
1:A:367:ARG:HE	1:A:460:ASN:ND2	2.07	0.52
1:A:277:ARG:HD3	1:A:332:PHE:O	2.10	0.51
2:B:37:THR:CG2	2:B:40:ASP:H	2.07	0.51
2:B:37:THR:HG22	2:B:40:ASP:N	2.05	0.51
1:A:114:THR:HB	1:A:134:CYS:HB3	1.92	0.51
1:A:171:LEU:HD11	1:A:191:CYS:SG	2.51	0.50
1:A:326:GLY:O	1:A:330:ILE:HG13	2.12	0.50
1:A:155:GLY:CA	4:A:701:PEG:H21	2.42	0.50
1:A:329:ASP:OD2	1:A:340:ARG:HD2	2.12	0.50
1:A:486:ASN:CG	1:A:490:GLN:HG2	2.32	0.49
1:A:173:GLU:HG3	1:A:174:GLN:HE21	1.77	0.49
1:A:292:GLU:O	1:A:296:LYS:HG2	2.12	0.49
1:A:121:ARG:NH1	1:A:131:THR:HG22	2.24	0.49
1:A:152:TYR:OH	1:A:203:HIS:CE1	2.61	0.49
1:A:486:ASN:ND2	1:A:490:GLN:HG2	2.27	0.49
1:A:182:LEU:C	1:A:183:GLU:HG3	2.34	0.48
1:A:397:GLN:NE2	1:A:495:TYR:HD2	2.12	0.48
1:A:178:GLN:O	1:A:178:GLN:CG	2.56	0.48
1:A:155:GLY:HA3	4:A:701:PEG:H21	1.97	0.47
4:A:701:PEG:H41	2:B:51:LEU:HD21	1.95	0.46
1:A:146:ASN:HD21	1:A:212:ASP:H	1.62	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:477:GLN:HG3	1:A:479:ASP:H	1.80	0.46
1:A:324:GLU:HB3	1:A:327:SER:OG	2.15	0.46
1:A:469:PRO:O	1:A:472:LEU:HD12	2.15	0.46
1:A:296:LYS:HB3	1:A:296:LYS:HE2	1.74	0.46
2:B:46:LEU:O	2:B:50:VAL:HB	2.15	0.45
1:A:277:ARG:NH1	1:A:277:ARG:CG	2.38	0.45
1:A:476:SER:O	1:A:476:SER:OG	2.34	0.44
1:A:179:LEU:O	1:A:182:LEU:HD12	2.18	0.44
1:A:486:ASN:HD21	1:A:490:GLN:CG	2.30	0.44
1:A:511:ASP:OD1	1:A:512:ALA:N	2.51	0.43
1:A:186:GLU:O	1:A:190:GLN:HG3	2.18	0.43
1:A:338:GLU:OE1	1:A:340:ARG:NH2	2.50	0.43
1:A:486:ASN:ND2	1:A:490:GLN:CG	2.82	0.42
1:A:504:LEU:HB2	1:A:506[B]:MET:HG3	2.01	0.42
1:A:277:ARG:HD3	1:A:335:PHE:HB2	1.99	0.42
1:A:225:ARG:HG3	1:A:225:ARG:H	1.60	0.41
1:A:277:ARG:NH1	1:A:281:ASP:OD2	2.54	0.41

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	375/556 (67%)	361 (96%)	9 (2%)	5 (1%)	18	17
2	B	26/63 (41%)	26 (100%)	0	0	100	100
All	All	401/619 (65%)	387 (96%)	9 (2%)	5 (1%)	18	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	356	GLN
1	A	183	GLU

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Mol	Chain	Res	Type
1	A	184	PRO
1	A	173	GLU

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	337/483 (70%)	312 (93%)	25 (7%)	20	24
2	B	27/58 (47%)	25 (93%)	2 (7%)	20	24
All	All	364/541 (67%)	337 (93%)	27 (7%)	20	24

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	THR
1	A	142	LYS
1	A	178	GLN
1	A	182	LEU
1	A	190	GLN
1	A	197	GLU
1	A	222	LYS
1	A	232	GLU
1	A	240	LYS
1	A	275	SER
1	A	277	ARG
1	A	307	LEU
1	A	314	MET
1	A	325	ARG
1	A	350	THR
1	A	356	GLN
1	A	376	GLN
1	A	427	VAL
1	A	447	PHE
1	A	448	ASP
1	A	461	LEU
1	A	470	GLU
1	A	472	LEU

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Mol	Chain	Res	Type
1	A	498	VAL
1	A	508	LEU
2	B	37	THR
2	B	50	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	146	ASN
1	A	174	GLN
1	A	190	GLN
1	A	200	ASN
1	A	203	HIS
1	A	270	ASN
1	A	315	HIS
1	A	368	HIS
1	A	377	ASN
1	A	404	ASN
1	A	460	ASN
2	B	31	HIS

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 ⓘ

Of 4 ligands modelled in this entry, 3 are modelled with single atom - leaving 1 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	$\# Z > 2$
4	PEG	A	701	-	6,6,6	0.68	0	5,5,5	0.77	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
4	PEG	A	701	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

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	386/556 (69%)	0.07	9 (2%) 57 67	15, 30, 55, 68	0
2	B	28/63 (44%)	-0.07	0 100 100	17, 24, 46, 51	0
All	All	414/619 (66%)	0.06	9 (2%) 59 69	15, 30, 55, 68	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	476	SER	4.6
1	A	449	ARG	3.1
1	A	226	ASN	2.6
1	A	356	GLN	2.5
1	A	341	ALA	2.3
1	A	447	PHE	2.3
1	A	173	GLU	2.2
1	A	517	ALA	2.1
1	A	357	PRO	2.1

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
3	NH4	B	602	1/1	0.35	4.75	33,33,33,33	0
3	NH4	A	601	1/1	0.23	3.49	27,27,27,27	0
4	PEG	A	701	7/7	0.15	3.22	30,34,36,37	0
3	NH4	B	603	1/1	0.14	0.16	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.