



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2022 – 05:00 pm BST

PDB ID : 7ZGI  
Title : chloroplast trigger factor (TIG1)  
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Deposited on : 2022-04-03  
Resolution : 2.60 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

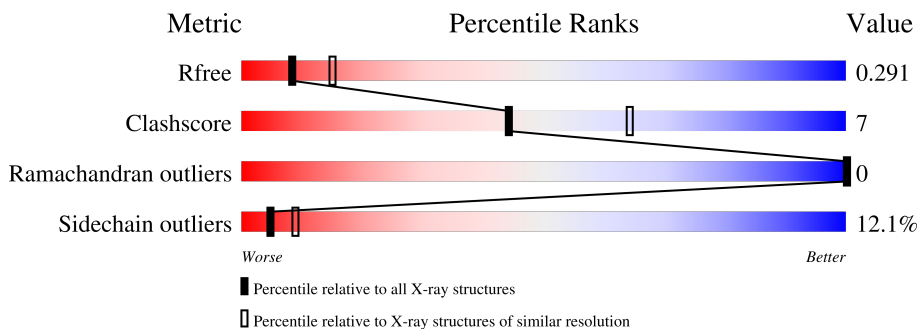
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	481	 53% 14% • 32%
1	B	481	 54% 12% • 32%

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5300 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 Peptidylprolyl isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	327	Total 2597	C 1630	N 447	O 507	Se 13	0	0	0
1	B	329	Total 2609	C 1639	N 448	O 509	Se 13	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



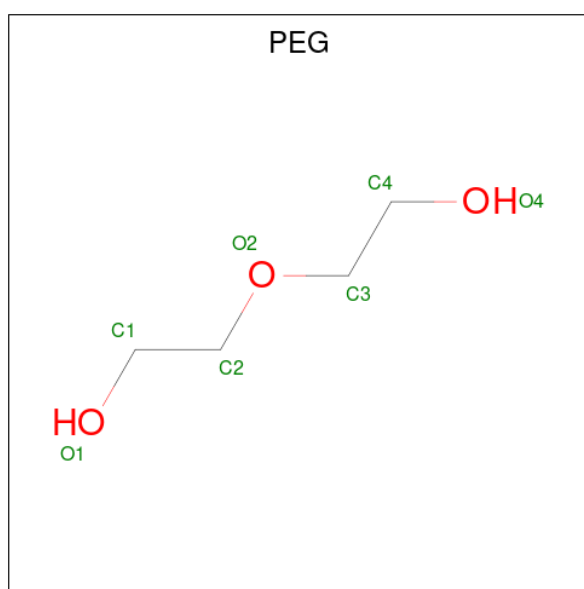
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total	O	0	0
			13	13		

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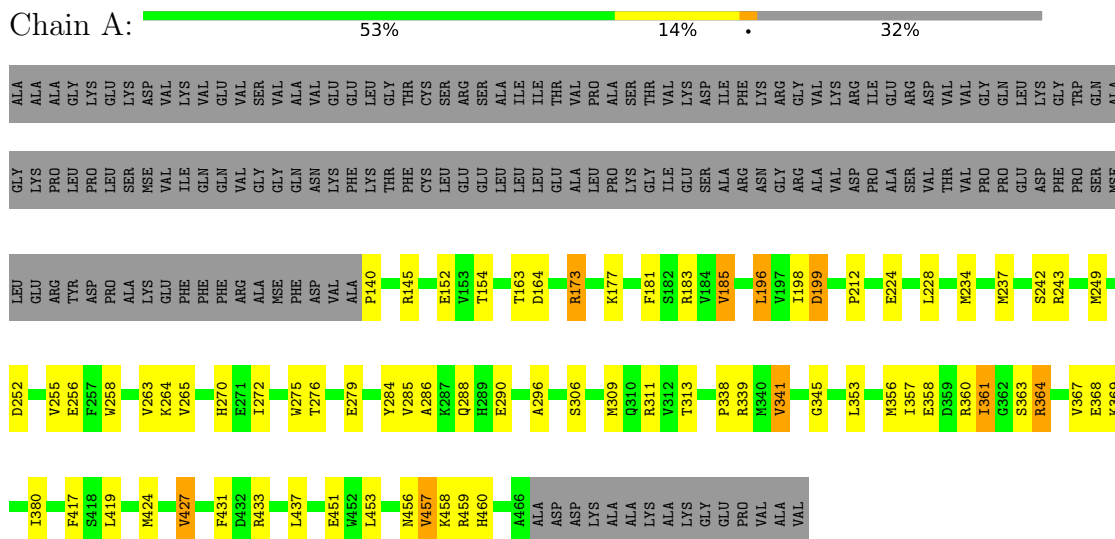
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	13	Total	O	0	0
			13	13		

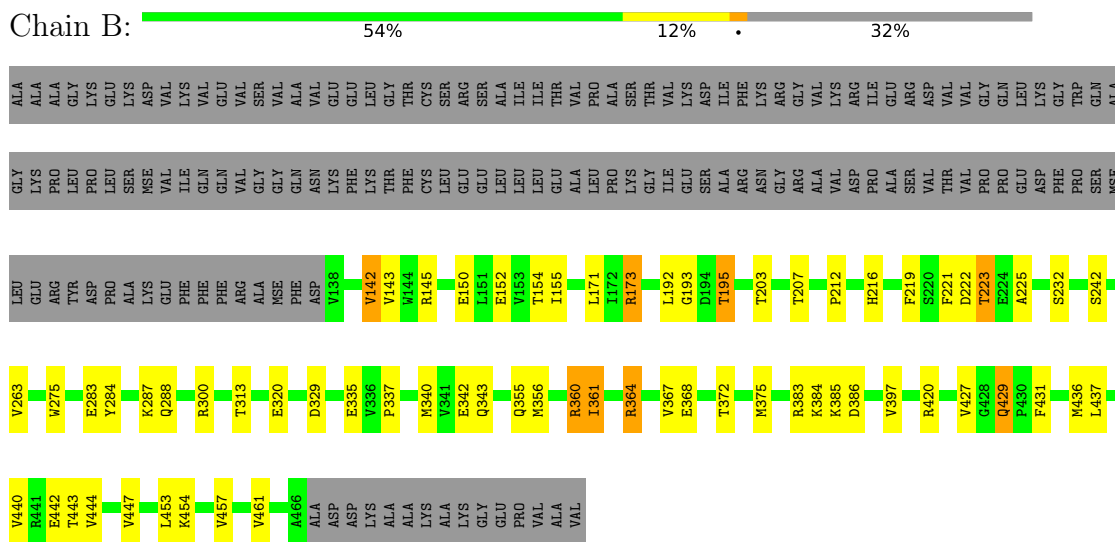
### 3 Residue-property plots

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. 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. 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: Peptidylprolyl isomerase



- Molecule 1: Peptidylprolyl isomerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.29Å 69.88Å 106.04Å 90.00° 110.99° 90.00°	Depositor
Resolution (Å)	54.31 – 2.60 54.25 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (54.31-2.60) 99.6 (54.25-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.235 , 0.283 0.243 , 0.291	Depositor DCC
$R_{free}$ test set	1738 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.3	Xtrriage
Anisotropy	0.036	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5300	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.0060e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.71	0/2629	0.89	0/3530
1	B	0.70	0/2641	0.85	0/3550
All	All	0.70	0/5270	0.87	0/7080

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2597	0	2552	37	0
1	B	2609	0	2568	32	0
2	A	15	0	0	1	0
2	B	25	0	0	3	0
3	A	14	0	20	0	0
3	B	14	0	20	0	0
4	A	13	0	0	0	0
4	B	13	0	0	1	0
All	All	5300	0	5160	69	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 7.



All (69) 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:212:PRO:HG3	1:B:356:MSE:HE3	1.20	1.12
1:B:212:PRO:HG3	1:B:356:MSE:CE	1.93	0.97
1:B:212:PRO:CG	1:B:356:MSE:HE3	1.98	0.92
1:A:145:ARG:HG2	1:A:145:ARG:HH11	1.40	0.86
1:B:356:MSE:HE2	1:B:367:VAL:HG22	1.63	0.80
1:B:356:MSE:HA	1:B:361:ILE:HD11	1.70	0.73
1:A:356:MSE:HE2	1:A:367:VAL:HG22	1.69	0.72
1:A:459:ARG:HH11	1:A:459:ARG:CG	2.04	0.71
1:B:192:LEU:HD12	1:B:223:THR:HG23	1.77	0.66
1:B:207:THR:HG21	1:B:375:MSE:HG2	1.77	0.65
1:A:255:VAL:HG22	1:A:361:ILE:HD12	1.79	0.64
1:A:459:ARG:HH11	1:A:459:ARG:HG3	1.63	0.64
1:A:145:ARG:HH11	1:A:145:ARG:CG	2.11	0.63
1:B:300:ARG:NH1	2:B:504:SO4:O4	2.25	0.62
1:A:173:ARG:NH1	2:A:503:SO4:O1	2.35	0.59
1:A:234:MSE:O	1:A:237:MSE:HG3	2.02	0.59
1:B:284:TYR:CE1	1:B:288:GLN:HG3	2.37	0.59
1:B:283:GLU:N	1:B:283:GLU:OE1	2.34	0.58
1:B:443:THR:O	1:B:447:VAL:HG23	2.03	0.57
1:A:338:PRO:HA	1:A:341:VAL:HG13	1.86	0.57
1:B:195:THR:HB	1:B:275:TRP:HE1	1.69	0.57
1:A:199:ASP:OD1	1:A:270:HIS:NE2	2.36	0.56
1:A:212:PRO:HD2	1:A:258:TRP:CZ2	2.40	0.56
1:A:212:PRO:HD2	1:A:258:TRP:HZ2	1.71	0.55
1:B:431:PHE:CD2	1:B:436:MSE:HG3	2.42	0.55
1:B:337:PRO:HG2	1:B:340:MSE:HG3	1.90	0.54
1:A:198:ILE:HG21	1:A:234:MSE:HE1	1.91	0.53
1:A:145:ARG:HG2	1:A:145:ARG:NH1	2.19	0.53
1:B:436:MSE:O	1:B:440:VAL:HG23	2.09	0.53
1:B:356:MSE:HG2	1:B:361:ILE:HG13	1.92	0.51
1:A:459:ARG:HG3	1:A:459:ARG:NH1	2.24	0.51
1:A:154:THR:HA	1:A:460:HIS:O	2.11	0.50
1:A:286:ALA:O	1:A:290:GLU:HB3	2.11	0.49
1:A:284:TYR:CE1	1:A:288:GLN:HG3	2.47	0.49
1:B:216:HIS:HB2	1:B:219:PHE:HB2	1.94	0.48
1:B:383:ARG:HD3	4:B:602:HOH:O	2.12	0.48
1:A:357:ILE:HG21	1:A:427:VAL:HG23	1.96	0.47
1:A:196:LEU:N	1:A:196:LEU:HD23	2.30	0.47
1:A:364:ARG:HE	1:A:364:ARG:HB3	1.29	0.47
1:B:420:ARG:HB2	1:B:436:MSE:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:ARG:CG	1:A:145:ARG:NH1	2.72	0.46
1:B:427:VAL:HG23	1:B:429:GLN:HB2	1.97	0.46
1:B:453:LEU:O	1:B:457:VAL:HG12	2.17	0.45
1:B:320:GLU:HG2	1:B:454:LYS:HE3	1.99	0.45
1:A:285:VAL:HG21	1:A:296:ALA:HA	1.98	0.45
1:B:440:VAL:O	1:B:444:VAL:HG23	2.17	0.45
1:A:177:LYS:NZ	1:A:224:GLU:OE1	2.50	0.45
1:B:145:ARG:NH2	1:B:329:ASP:O	2.50	0.44
1:B:364:ARG:O	1:B:368:GLU:CG	2.66	0.44
1:B:173:ARG:NH2	2:B:505:SO4:O2	2.51	0.44
1:A:433:ARG:HG3	1:A:433:ARG:HH11	1.82	0.44
1:A:181:PHE:O	1:A:275:TRP:HA	2.17	0.44
1:A:417:PHE:CD2	1:A:437:LEU:CD1	3.00	0.44
1:A:309:MSE:HA	1:A:309:MSE:HE2	2.00	0.43
1:B:287:LYS:NZ	2:B:503:SO4:O4	2.29	0.43
1:A:228:LEU:HD22	1:A:249:MSE:HE1	1.99	0.43
1:B:193:GLY:H	1:B:223:THR:CG2	2.32	0.43
1:A:212:PRO:HG2	1:A:356:MSE:HE1	2.00	0.43
1:A:357:ILE:HG13	1:A:367:VAL:HG11	2.01	0.43
1:A:424:MSE:HG2	1:A:431:PHE:CD1	2.54	0.43
1:A:185:VAL:HG13	1:A:272:ILE:HG22	2.02	0.42
1:A:345:GLY:HA3	1:A:380:ILE:HG12	2.02	0.42
1:A:361:ILE:H	1:A:361:ILE:HG12	1.66	0.42
1:A:453:LEU:O	1:A:457:VAL:HB	2.20	0.42
1:B:360:ARG:HA	1:B:360:ARG:HD2	1.68	0.42
1:B:142:VAL:O	1:B:142:VAL:CG2	2.69	0.41
1:B:356:MSE:HG2	1:B:361:ILE:CG1	2.51	0.40
1:A:164:ASP:OD2	1:A:311:ARG:NH1	2.53	0.40
1:B:222:ASP:HB3	1:B:225:ALA:HB3	2.04	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	325/481 (68%)	310 (95%)	15 (5%)	0	100	100
1	B	327/481 (68%)	317 (97%)	10 (3%)	0	100	100
All	All	652/962 (68%)	627 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	276/387 (71%)	241 (87%)	35 (13%)	4	8
1	B	278/387 (72%)	246 (88%)	32 (12%)	5	10
All	All	554/774 (72%)	487 (88%)	67 (12%)	5	9

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	PRO
1	A	152	GLU
1	A	163	THR
1	A	173	ARG
1	A	183	ARG
1	A	185	VAL
1	A	196	LEU
1	A	199	ASP
1	A	242	SER
1	A	243	ARG
1	A	252	ASP
1	A	256	GLU
1	A	263	VAL
1	A	264	LYS
1	A	265	VAL
1	A	276	THR
1	A	279	GLU
1	A	306	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	313	THR
1	A	339	ARG
1	A	341	VAL
1	A	353	LEU
1	A	358	GLU
1	A	360	ARG
1	A	361	ILE
1	A	363	SER
1	A	364	ARG
1	A	368	GLU
1	A	369	LYS
1	A	419	LEU
1	A	427	VAL
1	A	451	GLU
1	A	456	ASN
1	A	457	VAL
1	A	458	LYS
1	B	142	VAL
1	B	143	VAL
1	B	150	GLU
1	B	152	GLU
1	B	154	THR
1	B	155	ILE
1	B	171	LEU
1	B	173	ARG
1	B	195	THR
1	B	203	THR
1	B	221	PHE
1	B	223	THR
1	B	232	SER
1	B	242	SER
1	B	263	VAL
1	B	313	THR
1	B	335	GLU
1	B	342	GLU
1	B	343	GLN
1	B	355	GLN
1	B	360	ARG
1	B	361	ILE
1	B	364	ARG
1	B	372	THR
1	B	384	LYS

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Mol	Chain	Res	Type
1	B	385	LYS
1	B	386	ASP
1	B	397	VAL
1	B	429	GLN
1	B	437	LEU
1	B	442	GLU
1	B	461	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 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	$\# Z  > 2$
3	PEG	A	505	-	6,6,6	0.21	0	5,5,5	0.14	0
2	SO4	A	502	-	4,4,4	0.34	0	6,6,6	0.31	0
3	PEG	A	504	-	6,6,6	0.39	0	5,5,5	0.24	0
2	SO4	A	501	-	4,4,4	0.38	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	503	-	4,4,4	1.78	2 (50%)	6,6,6	0.40	0
3	PEG	B	507	-	6,6,6	0.36	0	5,5,5	0.19	0
2	SO4	B	502	-	4,4,4	0.31	0	6,6,6	0.14	0
3	PEG	B	506	-	6,6,6	0.18	0	5,5,5	0.18	0
2	SO4	B	503	-	4,4,4	0.30	0	6,6,6	0.21	0
2	SO4	B	504	-	4,4,4	0.36	0	6,6,6	0.17	0
2	SO4	B	505	-	4,4,4	1.94	1 (25%)	6,6,6	0.31	0
2	SO4	B	501	-	4,4,4	0.30	0	6,6,6	0.14	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
3	PEG	A	504	-	-	3/4/4/4	-
3	PEG	A	505	-	-	2/4/4/4	-
3	PEG	B	507	-	-	4/4/4/4	-
3	PEG	B	506	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	505	SO4	O1-S	2.67	1.60	1.46
2	A	503	SO4	O2-S	2.24	1.58	1.46
2	A	503	SO4	O1-S	2.20	1.57	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	504	PEG	O2-C3-C4-O4
3	B	507	PEG	O1-C1-C2-O2
3	A	505	PEG	C1-C2-O2-C3
3	A	504	PEG	O1-C1-C2-O2
3	A	505	PEG	O2-C3-C4-O4
3	B	507	PEG	O2-C3-C4-O4
3	B	506	PEG	O1-C1-C2-O2
3	B	507	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
3	A	504	PEG	C4-C3-O2-C2
3	B	507	PEG	C4-C3-O2-C2
3	B	506	PEG	C1-C2-O2-C3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	SO4	1	0
2	B	503	SO4	1	0
2	B	504	SO4	1	0
2	B	505	SO4	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.