



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:14 AM UTC

PDB ID : 7ZGI / pdb_00007zgi
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

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

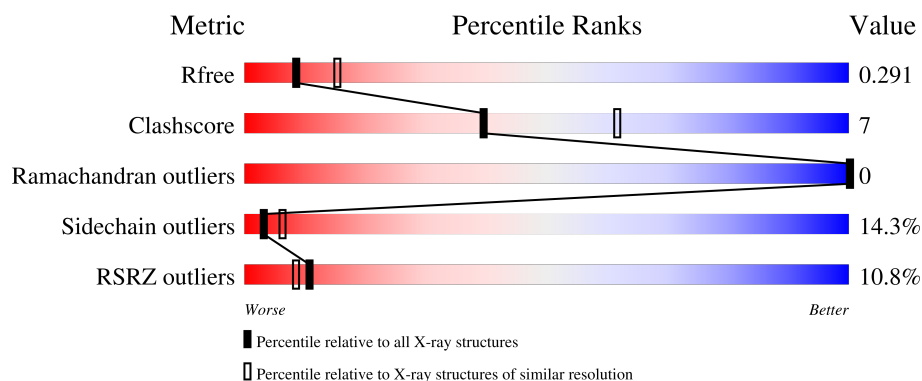
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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	481	9% 51% 15% • 32%
1	B	481	5% 53% 13% • 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
1	A	327	Total	C	N	O	Se	0	0	0
			2597	1630	447	507	13			
1	B	329	Total	C	N	O	Se	0	0	0
			2609	1639	448	509	13			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



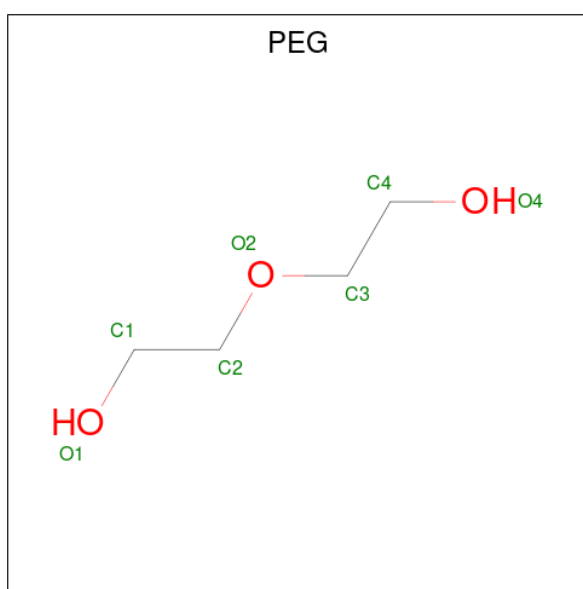
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: PEG) (formula: C₄H₁₀O₃).



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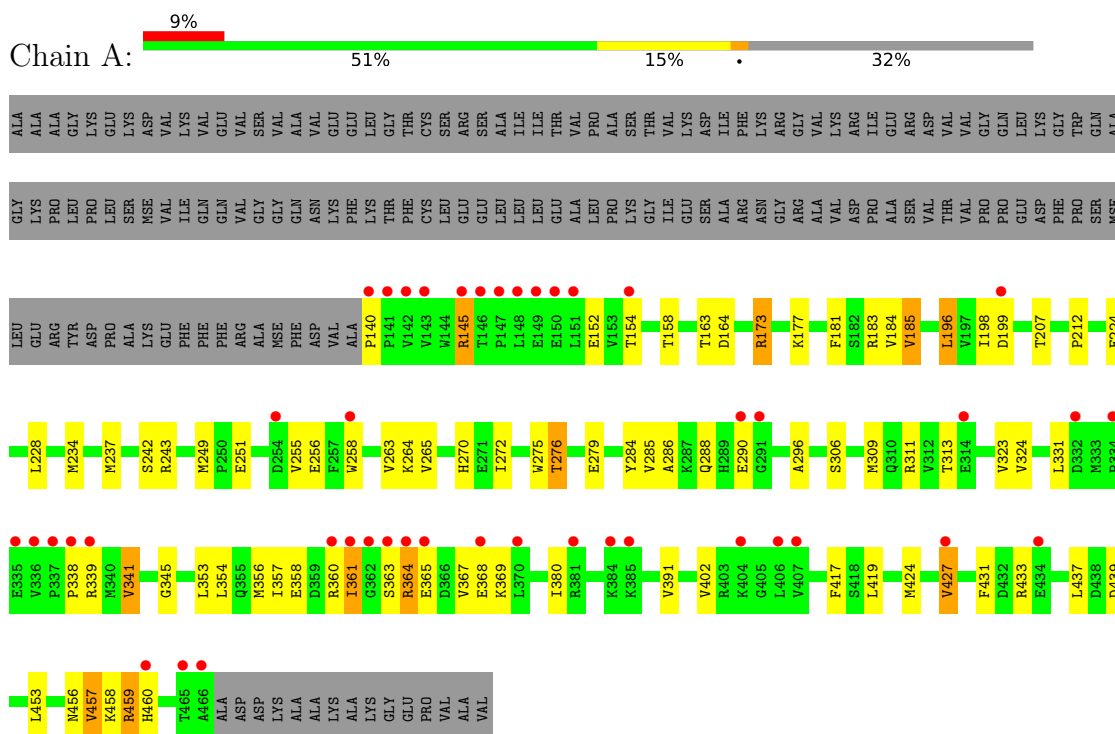
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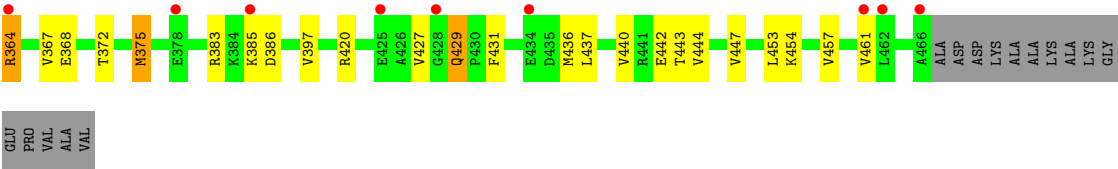
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	13	Total	O	0	0
			13	13		

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 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: Peptidylprolyl isomerase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	175.29Å 69.88Å 106.04Å 90.00° 110.99° 90.00°	Depositor
Resolution (Å)	54.31 – 2.60 54.31 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (54.31-2.60) 99.6 (54.31-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.61Å)	Xtriage
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 (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5300	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage'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.*

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 [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	1.05	1/2629 (0.0%)	1.52	4/3530 (0.1%)
1	B	1.04	0/2641	1.45	5/3550 (0.1%)
All	All	1.05	1/5270 (0.0%)	1.48	9/7080 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	391	VAL	C-O	5.16	1.29	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	THR	CB-CA-C	6.44	121.66	109.37
1	A	439	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	221	PHE	CA-CB-CG	6.16	119.96	113.80
1	A	158	THR	CA-CB-OG1	-5.52	101.31	109.60
1	A	184	VAL	CA-C-O	-5.34	114.94	121.13
1	B	162	SER	CA-C-N	5.16	127.46	120.44
1	B	162	SER	C-N-CA	5.16	127.46	120.44
1	B	194	ASP	CA-C-N	5.12	130.74	122.29
1	B	194	ASP	C-N-CA	5.12	130.74	122.29

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	38	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	70	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 (70) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ARG:HA	1:B:360:ARG:HD2	1.68	0.42
1:A:417:PHE:CD1	1:A:417:PHE:C	2.98	0.41
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%)	234 (85%)	42 (15%)	3	5
1	B	278/387 (72%)	241 (87%)	37 (13%)	4	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	554/774 (72%)	475 (86%)	79 (14%)	3 6

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140	PRO
1	A	145	ARG
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	207	THR
1	A	242	SER
1	A	243	ARG
1	A	251	GLU
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
1	A	313	THR
1	A	323	VAL
1	A	324	VAL
1	A	331	LEU
1	A	339	ARG
1	A	341	VAL
1	A	353	LEU
1	A	354	LEU
1	A	358	GLU
1	A	360	ARG
1	A	361	ILE
1	A	363	SER
1	A	364	ARG
1	A	365	GLU
1	A	368	GLU
1	A	369	LYS
1	A	402	VAL
1	A	419	LEU

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Mol	Chain	Res	Type
1	A	427	VAL
1	A	456	ASN
1	A	457	VAL
1	A	458	LYS
1	A	459	ARG
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	163	THR
1	B	171	LEU
1	B	173	ARG
1	B	195	THR
1	B	203	THR
1	B	205	LYS
1	B	221	PHE
1	B	223	THR
1	B	232	SER
1	B	242	SER
1	B	263	VAL
1	B	297	LYS
1	B	310	GLN
1	B	313	THR
1	B	335	GLU
1	B	342	GLU
1	B	343	GLN
1	B	350	GLN
1	B	355	GLN
1	B	360	ARG
1	B	361	ILE
1	B	364	ARG
1	B	372	THR
1	B	375	MSE
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. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	GLN
1	A	352	GLN
1	A	394	ASN
1	A	456	ASN
1	B	178	GLN
1	B	179	HIS
1	B	246	ASN
1	B	343	GLN
1	B	352	GLN
1	B	456	ASN

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](#)

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	B	507	-	6,6,6	0.37	0	5,5,5	0.19	0
2	SO4	A	502	-	4,4,4	0.27	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	505	-	4,4,4	1.92	1 (25%)	6,6,6	0.30	0
2	SO4	A	501	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	503	-	4,4,4	1.78	2 (50%)	6,6,6	0.41	0
2	SO4	B	504	-	4,4,4	0.33	0	6,6,6	0.15	0
2	SO4	B	501	-	4,4,4	0.29	0	6,6,6	0.13	0
2	SO4	B	503	-	4,4,4	0.33	0	6,6,6	0.24	0
2	SO4	B	502	-	4,4,4	0.29	0	6,6,6	0.14	0
3	PEG	A	505	-	6,6,6	0.21	0	5,5,5	0.14	0
3	PEG	A	504	-	6,6,6	0.39	0	5,5,5	0.23	0
3	PEG	B	506	-	6,6,6	0.18	0	5,5,5	0.18	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	B	507	-	-	4/4/4/4	-
3	PEG	A	505	-	-	2/4/4/4	-
3	PEG	A	504	-	-	3/4/4/4	-
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	2.63	1.60	1.44
2	A	503	SO4	O2-S	2.24	1.58	1.44
2	A	503	SO4	O1-S	2.20	1.57	1.44

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

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Mol	Chain	Res	Type	Atoms
3	B	506	PEG	O1-C1-C2-O2
3	B	507	PEG	C1-C2-O2-C3
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	B	505	SO4	1	0
2	A	503	SO4	1	0
2	B	504	SO4	1	0
2	B	503	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

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	314/481 (65%)	0.77	44 (14%) 6 5	24, 56, 93, 139	0
1	B	316/481 (65%)	0.59	24 (7%) 20 16	23, 53, 86, 118	0
All	All	630/962 (65%)	0.68	68 (10%) 11 8	23, 55, 93, 139	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	291	GLY	7.3
1	A	466	ALA	6.6
1	A	140	PRO	6.4
1	B	466	ALA	4.9
1	B	138	VAL	4.8
1	A	361	ILE	4.7
1	A	339	ARG	4.4
1	B	361	ILE	4.2
1	A	141	PRO	4.0
1	A	254	ASP	3.8
1	A	384	LYS	3.7
1	A	381	ARG	3.6
1	A	146	THR	3.6
1	A	147	PRO	3.6
1	A	291	GLY	3.3
1	A	385	LYS	3.3
1	A	363	SER	3.2
1	A	290	GLU	3.2
1	A	151	LEU	3.1
1	B	315	LEU	3.1
1	A	314	GLU	3.0
1	A	145	ARG	3.0
1	B	360	ARG	2.9
1	A	460	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	378	GLU	2.8
1	A	332	ASP	2.8
1	A	338	PRO	2.8
1	B	364	ARG	2.8
1	A	337	PRO	2.8
1	B	199	ASP	2.7
1	A	465	THR	2.7
1	A	258	TRP	2.6
1	B	292	LYS	2.6
1	A	336	VAL	2.6
1	B	425	GLU	2.5
1	B	428	GLY	2.5
1	B	139	ALA	2.5
1	A	150	GLU	2.5
1	A	360	ARG	2.5
1	B	316	ASP	2.5
1	B	140	PRO	2.5
1	B	434	GLU	2.4
1	B	314	GLU	2.4
1	A	407	VAL	2.4
1	A	335	GLU	2.4
1	A	434	GLU	2.4
1	B	212	PRO	2.3
1	A	148	LEU	2.3
1	B	385	LYS	2.3
1	B	461	VAL	2.3
1	B	347	ARG	2.3
1	B	294	GLY	2.3
1	B	462	LEU	2.2
1	A	142	VAL	2.2
1	A	154	THR	2.2
1	A	368	GLU	2.1
1	A	365	GLU	2.1
1	A	149	GLU	2.1
1	A	334	PRO	2.1
1	A	370	LEU	2.1
1	B	251	GLU	2.1
1	A	404	LYS	2.1
1	A	362	GLY	2.0
1	A	143	VAL	2.0
1	A	427	VAL	2.0
1	A	199	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	406	LEU	2.0
1	A	364	ARG	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	SO4	A	503	5/5	0.77	0.28	41,42,47,50	0
2	SO4	B	505	5/5	0.81	0.25	43,44,47,50	0
2	SO4	B	504	5/5	0.82	0.13	82,86,102,118	0
3	PEG	B	507	7/7	0.85	0.19	56,63,71,72	0
3	PEG	B	506	7/7	0.88	0.23	59,64,71,74	0
2	SO4	B	501	5/5	0.90	0.13	63,70,74,80	0
3	PEG	A	504	7/7	0.90	0.18	53,61,66,68	0
2	SO4	B	502	5/5	0.91	0.17	73,79,85,86	0
2	SO4	B	503	5/5	0.92	0.15	61,68,70,72	0
2	SO4	A	501	5/5	0.93	0.13	73,76,80,84	0
3	PEG	A	505	7/7	0.93	0.11	46,50,54,57	0
2	SO4	A	502	5/5	0.95	0.15	60,60,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.