



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 06:42 AM EDT

PDB ID : 7AAS  
Title : Crystal structure of nitrosogluthione reductase (GSNOR) from *Chlamydomonas reinhardtii*  
Authors : Fermani, S.; Zaffagnini, M.; Falini, G.; Lemaire, S.D.  
Deposited on : 2020-09-04  
Resolution : 1.80 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 : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 1.20.1  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

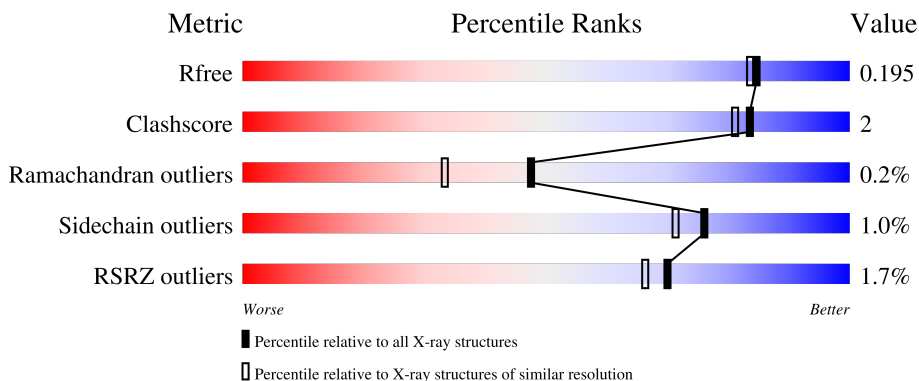
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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.



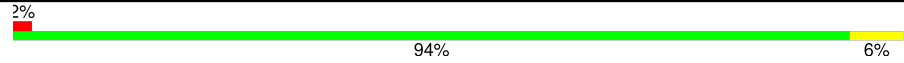
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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  $\leq 5\%$ . 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	378	 96%
1	B	378	 96%
1	C	378	 94% 5%
1	D	378	 95%
1	E	378	 95% 5%

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Mol	Chain	Length	Quality of chain
1	F	378	 <p>A horizontal bar chart representing the quality of the chain. The bar is divided into three segments: a small red segment on the left labeled '2%', a large green segment in the middle labeled '94%', and a small yellow segment on the right labeled '6%'.</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19327 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 S-(hydroxymethyl)glutathione dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	377	2831	1795	482	530	24	0	2	0
1	B	376	2829	1793	481	530	25	0	3	0
1	C	377	2832	1794	482	531	25	0	3	0
1	D	377	2835	1796	482	534	23	0	2	0
1	E	376	2817	1785	481	528	23	0	0	0
1	F	377	2829	1792	482	532	23	0	1	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- 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 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	D	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	E	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0
3	F	1	Total C O 7 4 3	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0

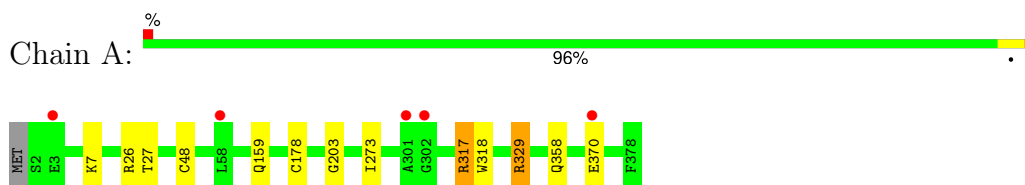
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	419	Total O 419 419	0	0
5	B	413	Total O 413 413	0	0
5	C	373	Total O 373 373	0	0
5	D	416	Total O 416 416	0	0
5	E	308	Total O 308 308	0	0
5	F	320	Total O 320 320	0	0

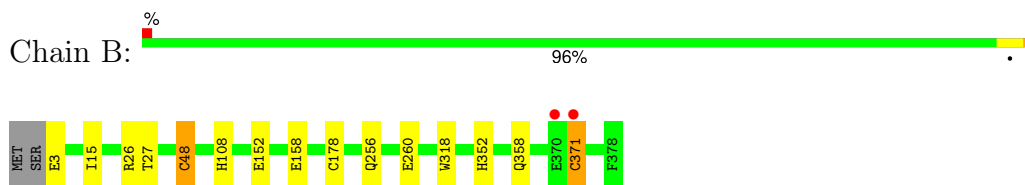
### 3 Residue-property plots [i](#)

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.

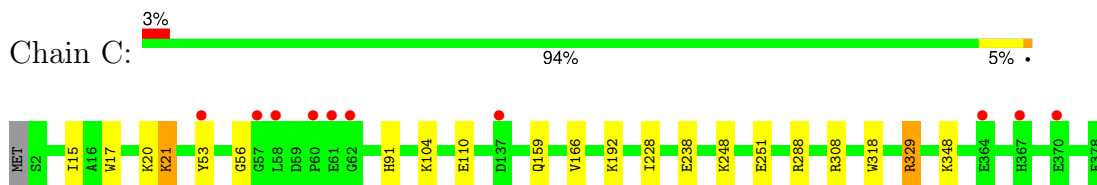
- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase



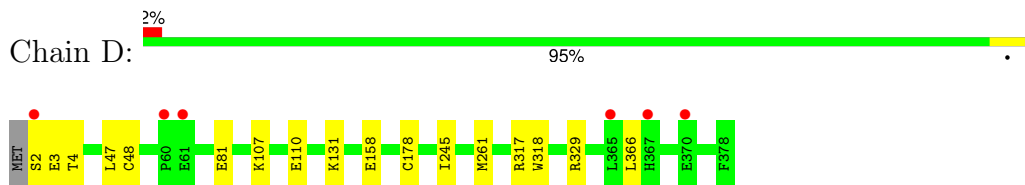
- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase



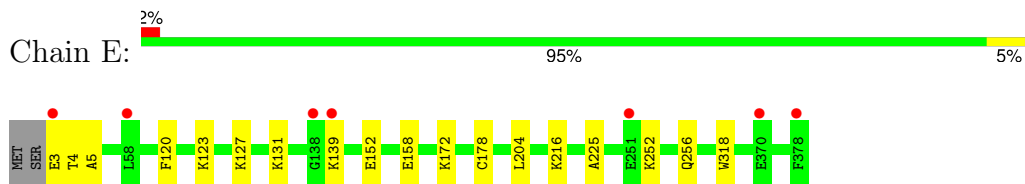
- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase



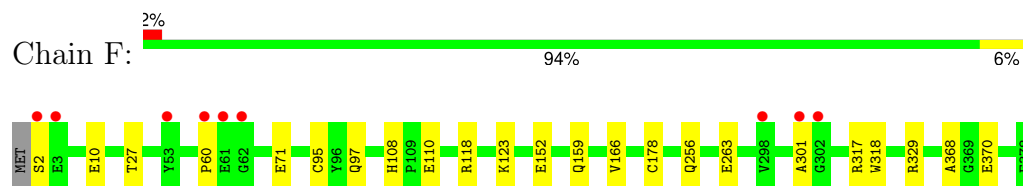
- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase



- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase



- Molecule 1: S-(hydroxymethyl)glutathione dehydrogenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.83Å 143.00Å 206.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.97 – 1.80 56.97 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (56.97-1.80) 97.9 (56.97-1.80)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.14 (at 1.80Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.173 , 0.204 0.164 , 0.195	Depositor DCC
$R_{free}$ test set	10398 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtrriage
Anisotropy	0.117	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19327	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: CL, ZN, 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	0.49	1/2899 (0.0%)	0.62	2/3935 (0.1%)
1	B	0.48	1/2900 (0.0%)	0.61	0/3936
1	C	0.46	0/2903	0.61	2/3940 (0.1%)
1	D	0.49	0/2903	0.61	0/3940
1	E	0.44	0/2879	0.57	0/3908
1	F	0.45	0/2894	0.57	0/3928
All	All	0.47	2/17378 (0.0%)	0.60	4/23587 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	CYS	CB-SG	-5.99	1.72	1.82
1	B	48	CYS	CB-SG	-5.04	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	329	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	C	329	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	329	ARG	NE-CZ-NH1	5.49	123.04	120.30

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	2831	0	2816	6	0
1	B	2829	0	2811	11	0
1	C	2832	0	2815	20	0
1	D	2835	0	2812	10	0
1	E	2817	0	2795	13	0
1	F	2829	0	2806	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	21	0	30	0	0
3	B	7	0	10	0	0
3	C	14	0	20	2	0
3	D	21	0	30	2	0
3	E	14	0	20	0	0
3	F	14	0	20	3	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	419	0	0	3	0
5	B	413	0	0	7	2
5	C	373	0	0	11	2
5	D	416	0	0	6	0
5	E	308	0	0	4	2
5	F	320	0	0	9	2
All	All	19327	0	16985	80	4

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 2.

All (80) 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:F:118:ARG:NH1	5:F:501:HOH:O	1.92	1.01
1:B:358:GLN:NE2	5:B:501:HOH:O	2.08	0.85
1:C:21:LYS:HE3	5:C:627:HOH:O	1.80	0.81
1:F:263:GLU:OE2	5:F:502:HOH:O	1.96	0.81
1:A:26:ARG:NH1	1:A:27:THR:O	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:GLU:OE1	5:D:501:HOH:O	1.99	0.80
1:F:108:HIS:HE2	3:F:404:PEG:H21	1.47	0.79
1:C:251:GLU:OE2	5:C:501:HOH:O	2.01	0.78
1:C:110:GLU:OE1	5:C:503:HOH:O	2.03	0.76
1:C:15:ILE:O	5:C:502:HOH:O	2.03	0.76
1:C:20:LYS:HD3	1:C:56:GLY:HA2	1.67	0.75
1:A:159:GLN:O	1:A:329:ARG:HD2	1.88	0.73
1:A:358:GLN:NE2	5:A:502:HOH:O	2.20	0.72
1:D:81[B]:GLU:OE1	5:D:502:HOH:O	2.08	0.71
1:F:166:VAL:HG12	5:F:558:HOH:O	1.90	0.71
1:B:26:ARG:NH2	1:B:27:THR:O	2.24	0.70
1:B:108:HIS:HE2	3:C:403:PEG:H12	1.55	0.70
1:C:159:GLN:O	1:C:329:ARG:HD2	1.92	0.69
1:D:329:ARG:NH2	5:D:505:HOH:O	2.25	0.69
1:F:110[A]:GLU:OE1	3:F:404:PEG:O4	2.08	0.68
1:C:53:TYR:OH	5:C:504:HOH:O	2.09	0.67
1:A:317:ARG:NH2	5:A:501:HOH:O	2.19	0.67
1:C:192:LYS:NZ	5:C:503:HOH:O	2.24	0.66
1:C:308:ARG:NH1	5:C:506:HOH:O	2.28	0.64
1:D:47:LEU:HD13	1:D:366:LEU:HD22	1.80	0.63
1:F:256:GLN:NE2	5:F:504:HOH:O	2.21	0.63
1:E:3:GLU:CD	1:E:4:THR:H	2.00	0.63
1:B:108:HIS:HE2	3:C:403:PEG:C1	2.10	0.62
1:E:158:GLU:OE2	5:E:501:HOH:O	2.16	0.62
1:C:104:LYS:NZ	5:C:507:HOH:O	2.31	0.62
1:D:131:LYS:NZ	5:D:506:HOH:O	2.33	0.60
1:D:245:ILE:HD11	1:D:261:MET:SD	2.41	0.59
1:F:95:CYS:HA	5:F:512:HOH:O	2.03	0.58
1:F:159:GLN:O	1:F:329:ARG:HD2	2.03	0.58
1:C:17:TRP:N	5:C:502:HOH:O	2.18	0.58
1:E:3:GLU:O	1:E:4:THR:OG1	2.20	0.57
1:A:203:GLY:HA3	1:A:273:ILE:HG12	1.87	0.57
1:D:110:GLU:OE2	3:D:404:PEG:O1	2.18	0.56
1:B:3:GLU:N	5:B:507:HOH:O	2.39	0.56
1:C:21:LYS:NZ	5:C:502:HOH:O	2.04	0.56
1:B:256:GLN:NE2	5:B:505:HOH:O	2.33	0.55
1:F:317:ARG:NH2	5:F:506:HOH:O	2.29	0.54
1:C:288:ARG:NH2	5:C:511:HOH:O	2.41	0.53
1:A:7:LYS:NZ	5:A:511:HOH:O	2.39	0.53
1:E:3:GLU:C	1:E:5:ALA:H	2.13	0.52
5:B:701:HOH:O	1:C:104:LYS:HD3	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLN:NE2	5:B:503:HOH:O	2.26	0.51
1:F:152:GLU:OE2	5:F:503:HOH:O	2.19	0.50
1:B:371[A]:CYS:SG	5:B:695:HOH:O	2.29	0.50
1:E:152:GLU:OE2	5:E:502:HOH:O	2.20	0.49
1:F:10:GLU:HG2	1:F:27:THR:CG2	2.43	0.48
1:B:15:ILE:HD12	1:B:26:ARG:HD3	1.96	0.48
1:C:20:LYS:HD3	1:C:56:GLY:CA	2.42	0.47
1:D:3:GLU:HG3	1:D:4:THR:HG23	1.96	0.47
1:D:81[A]:GLU:OE1	5:D:503:HOH:O	2.20	0.47
1:E:252:LYS:HE3	1:E:256:GLN:OE1	2.15	0.46
1:E:120:PHE:CE2	1:E:127:LYS:HG3	2.51	0.46
1:E:216:LYS:HD3	5:E:649:HOH:O	2.16	0.46
1:F:71:GLU:HG2	1:F:178:CYS:HB3	1.98	0.45
1:C:238:GLU:OE2	1:C:348:LYS:HE2	2.16	0.45
1:B:260:GLU:OE1	5:B:502:HOH:O	2.21	0.45
1:F:108:HIS:NE2	3:F:404:PEG:H21	2.25	0.45
1:F:97:GLN:NE2	5:F:501:HOH:O	2.50	0.44
1:E:139:LYS:HD2	1:E:139:LYS:HA	1.73	0.44
1:E:3:GLU:OE2	1:E:4:THR:N	2.46	0.44
1:F:368:ALA:HB3	1:F:370:GLU:HG3	2.00	0.44
1:E:204:LEU:HD21	1:E:225:ALA:HB1	2.00	0.44
1:C:159:GLN:C	1:C:329:ARG:HD2	2.38	0.43
1:F:317:ARG:NH1	5:F:513:HOH:O	2.44	0.43
3:D:404:PEG:H11	3:D:404:PEG:H31	1.62	0.42
1:E:123:LYS:HB2	1:E:123:LYS:HE2	1.68	0.42
1:F:108:HIS:CE1	1:F:110[A]:GLU:HB2	2.54	0.42
1:C:228:ILE:H	1:C:228:ILE:HG13	1.67	0.41
1:B:352:HIS:NE2	1:B:371[B]:CYS:SG	2.88	0.41
1:E:172:LYS:NZ	5:E:520:HOH:O	2.53	0.41
1:C:248:LYS:HE3	1:C:248:LYS:HB3	1.92	0.41
1:C:91:HIS:CD2	1:C:166:VAL:HG23	2.56	0.41
1:D:107:LYS:HE2	5:D:846:HOH:O	2.19	0.40
1:F:123:LYS:HA	1:F:123:LYS:HD3	1.85	0.40
1:F:60:PRO:HD3	1:F:301:ALA:HB2	2.03	0.40

All (4) 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)
5:B:641:HOH:O	5:F:558:HOH:O[3_655]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:867:HOH:O	5:F:507:HOH:O[3_655]	2.14	0.06
5:C:810:HOH:O	5:E:770:HOH:O[4_555]	2.17	0.03
5:C:810:HOH:O	5:E:512:HOH:O[4_555]	2.19	0.01

## 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	377/378 (100%)	371 (98%)	5 (1%)	1 (0%)	41	27
1	B	377/378 (100%)	367 (97%)	9 (2%)	1 (0%)	41	27
1	C	378/378 (100%)	369 (98%)	9 (2%)	0	100	100
1	D	377/378 (100%)	369 (98%)	7 (2%)	1 (0%)	41	27
1	E	374/378 (99%)	361 (96%)	12 (3%)	1 (0%)	41	27
1	F	376/378 (100%)	366 (97%)	10 (3%)	0	100	100
All	All	2259/2268 (100%)	2203 (98%)	52 (2%)	4 (0%)	47	33

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	CYS
1	B	178	CYS
1	D	178	CYS
1	E	178	CYS

### 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	301/300 (100%)	298 (99%)	3 (1%)	76	71
1	B	301/300 (100%)	295 (98%)	6 (2%)	55	44
1	C	302/300 (101%)	300 (99%)	2 (1%)	84	81
1	D	301/300 (100%)	297 (99%)	4 (1%)	69	62
1	E	298/300 (99%)	296 (99%)	2 (1%)	84	81
1	F	300/300 (100%)	298 (99%)	2 (1%)	84	81
All	All	1803/1800 (100%)	1784 (99%)	19 (1%)	76	68

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	317	ARG
1	A	318	TRP
1	A	370	GLU
1	B	48	CYS
1	B	152	GLU
1	B	158	GLU
1	B	318	TRP
1	B	371[A]	CYS
1	B	371[B]	CYS
1	C	21	LYS
1	C	318	TRP
1	D	2	SER
1	D	48	CYS
1	D	317	ARG
1	D	318	TRP
1	E	131	LYS
1	E	318	TRP
1	F	2	SER
1	F	318	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	303	GLN
1	E	167	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 14 are monoatomic - leaving 13 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	$\# Z  > 2$
3	PEG	F	403	-	6,6,6	0.51	0	5,5,5	0.50	0
3	PEG	B	403	-	6,6,6	0.50	0	5,5,5	0.16	0
3	PEG	A	404	-	6,6,6	0.47	0	5,5,5	0.29	0
3	PEG	D	405	-	6,6,6	0.46	0	5,5,5	0.23	0
3	PEG	A	405	-	6,6,6	0.51	0	5,5,5	0.34	0
3	PEG	F	404	-	6,6,6	0.45	0	5,5,5	0.59	0
3	PEG	C	403	-	6,6,6	0.39	0	5,5,5	0.49	0
3	PEG	E	403	-	6,6,6	0.53	0	5,5,5	0.37	0
3	PEG	C	404	-	6,6,6	0.47	0	5,5,5	0.33	0
3	PEG	D	403	-	6,6,6	0.39	0	5,5,5	0.50	0
3	PEG	D	404	-	6,6,6	0.48	0	5,5,5	0.35	0
3	PEG	E	404	-	6,6,6	0.54	0	5,5,5	0.69	0
3	PEG	A	403	-	6,6,6	0.54	0	5,5,5	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
3	PEG	F	403	-	-	1/4/4/4	-
3	PEG	B	403	-	-	0/4/4/4	-
3	PEG	A	404	-	-	1/4/4/4	-
3	PEG	D	405	-	-	1/4/4/4	-
3	PEG	A	405	-	-	1/4/4/4	-
3	PEG	F	404	-	-	1/4/4/4	-
3	PEG	C	403	-	-	2/4/4/4	-
3	PEG	E	403	-	-	1/4/4/4	-
3	PEG	C	404	-	-	1/4/4/4	-
3	PEG	D	403	-	-	4/4/4/4	-
3	PEG	D	404	-	-	3/4/4/4	-
3	PEG	E	404	-	-	2/4/4/4	-
3	PEG	A	403	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	404	PEG	C1-C2-O2-C3
3	D	403	PEG	C1-C2-O2-C3
3	D	403	PEG	O1-C1-C2-O2
3	E	404	PEG	O1-C1-C2-O2
3	C	403	PEG	O2-C3-C4-O4
3	C	404	PEG	O1-C1-C2-O2
3	E	404	PEG	O2-C3-C4-O4
3	C	403	PEG	O1-C1-C2-O2
3	A	405	PEG	O2-C3-C4-O4
3	D	405	PEG	O1-C1-C2-O2
3	D	404	PEG	O1-C1-C2-O2
3	A	403	PEG	C4-C3-O2-C2
3	F	404	PEG	C4-C3-O2-C2
3	D	403	PEG	C4-C3-O2-C2
3	A	404	PEG	O2-C3-C4-O4
3	F	403	PEG	O2-C3-C4-O4
3	E	403	PEG	C1-C2-O2-C3
3	D	403	PEG	O2-C3-C4-O4
3	D	404	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	404	PEG	3	0
3	C	403	PEG	2	0
3	D	404	PEG	2	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	377/378 (99%)	-0.24	5 (1%) 77 74	12, 18, 39, 57	0
1	B	376/378 (99%)	-0.33	2 (0%) 91 89	11, 19, 35, 60	0
1	C	377/378 (99%)	-0.20	10 (2%) 54 49	11, 19, 44, 68	0
1	D	377/378 (99%)	-0.27	6 (1%) 72 68	12, 18, 34, 63	0
1	E	376/378 (99%)	-0.03	7 (1%) 66 63	14, 24, 46, 66	0
1	F	377/378 (99%)	-0.00	9 (2%) 59 54	13, 24, 42, 65	0
All	All	2260/2268 (99%)	-0.18	39 (1%) 70 66	11, 20, 41, 68	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	ALA	7.4
1	E	370	GLU	6.2
1	B	370	GLU	5.2
1	F	60	PRO	5.0
1	A	302	GLY	5.0
1	C	60	PRO	4.6
1	D	370	GLU	4.4
1	A	370	GLU	3.8
1	D	367	HIS	3.7
1	A	58	LEU	3.4
1	D	61	GLU	3.4
1	F	61	GLU	3.3
1	E	251	GLU	3.1
1	E	3	GLU	3.0
1	F	2	SER	2.9
1	F	302	GLY	2.9
1	D	365	LEU	2.8
1	C	137	ASP	2.8
1	C	53	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	301	ALA	2.7
1	A	3	GLU	2.7
1	C	367	HIS	2.7
1	F	298	VAL	2.7
1	C	370	GLU	2.7
1	C	61	GLU	2.6
1	E	139	LYS	2.6
1	D	2	SER	2.6
1	E	138	GLY	2.5
1	C	58	LEU	2.5
1	F	53	TYR	2.5
1	D	60	PRO	2.3
1	C	62	GLY	2.2
1	F	3	GLU	2.2
1	E	378	PHE	2.2
1	C	57	GLY	2.1
1	B	371[A]	CYS	2.1
1	E	58	LEU	2.1
1	C	364	GLU	2.1
1	F	62	GLY	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	PEG	D	404	7/7	0.79	0.19	37,45,48,50	0
3	PEG	D	405	7/7	0.84	0.17	32,35,42,45	0
3	PEG	A	403	7/7	0.85	0.14	28,30,40,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	D	403	7/7	0.88	0.12	21,27,31,38	0
3	PEG	A	405	7/7	0.89	0.13	28,36,44,46	0
3	PEG	E	403	7/7	0.89	0.11	25,26,31,33	0
3	PEG	B	403	7/7	0.90	0.10	24,31,35,37	0
3	PEG	C	403	7/7	0.90	0.14	20,28,38,39	0
3	PEG	E	404	7/7	0.90	0.10	26,30,34,35	0
3	PEG	F	403	7/7	0.90	0.13	20,23,25,26	0
3	PEG	C	404	7/7	0.91	0.11	31,34,38,42	0
3	PEG	F	404	7/7	0.93	0.10	25,30,38,38	0
3	PEG	A	404	7/7	0.95	0.10	24,28,30,37	0
2	ZN	C	401	1/1	0.99	0.06	25,25,25,25	1
2	ZN	E	401	1/1	0.99	0.08	19,19,19,19	1
2	ZN	F	401	1/1	0.99	0.07	21,21,21,21	0
2	ZN	A	401	1/1	0.99	0.07	19,19,19,19	1
4	CL	A	406	1/1	0.99	0.04	27,27,27,27	0
4	CL	C	405	1/1	0.99	0.05	24,24,24,24	0
2	ZN	F	402	1/1	1.00	0.08	20,20,20,20	0
2	ZN	A	402	1/1	1.00	0.08	15,15,15,15	0
2	ZN	C	402	1/1	1.00	0.09	15,15,15,15	0
2	ZN	D	401	1/1	1.00	0.06	18,18,18,18	1
2	ZN	D	402	1/1	1.00	0.08	16,16,16,16	0
2	ZN	B	401	1/1	1.00	0.04	25,25,25,25	0
2	ZN	E	402	1/1	1.00	0.06	17,17,17,17	0
2	ZN	B	402	1/1	1.00	0.10	13,13,13,13	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.