



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:27 am GMT

PDB ID : 3UK9  
Title : Galactose-specific lectin from Dolichos lablab  
Authors : Shetty, K.N.; Latha, V.L.; Rao, R.N.; Nadimpalli, S.K.; Suguna, K.  
Deposited on : 2011-11-09  
Resolution : 3.11 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

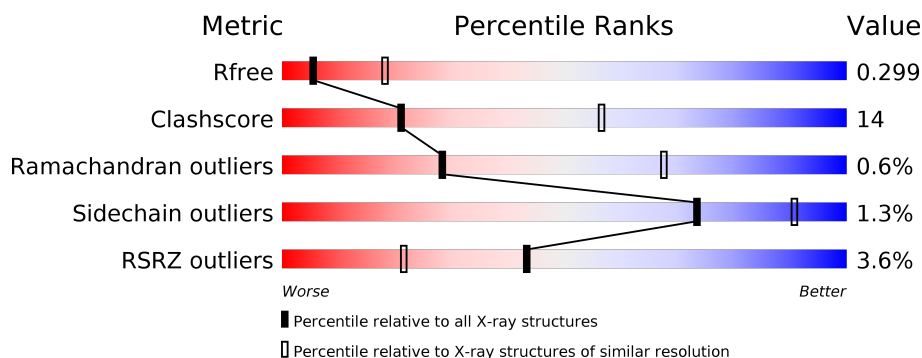
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.11 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))
$R_{free}$	100719	1000 (3.14-3.10)
Clashscore	112137	1099 (3.14-3.10)
Ramachandran outliers	110173	1060 (3.14-3.10)
Sidechain outliers	110143	1060 (3.14-3.10)
RSRZ outliers	101464	1005 (3.14-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	281	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>11%</div> </div> </div>
1	B	281	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>12%</div> <div>11%</div> </div> </div>
1	C	281	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>15%</div> <div>12%</div> </div> </div>
1	D	281	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>17%</div> <div>12%</div> </div> </div>
1	E	281	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>21%</div> <div>12%</div> </div> </div>
1	F	281	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>11%</div> <div>12%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	281	
1	H	281	

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	EDO	C	301	-	-	-	X
2	EDO	D	301	-	-	-	X
2	EDO	F	301	-	-	-	X
2	EDO	G	301	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15116 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 Legume lectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	0	0	0
			1879	1198	309	372			
1	B	249	Total	C	N	O	0	0	0
			1883	1201	308	374			
1	C	247	Total	C	N	O	0	0	0
			1864	1188	307	369			
1	D	248	Total	C	N	O	0	0	0
			1877	1198	309	370			
1	E	247	Total	C	N	O	0	0	0
			1869	1192	307	370			
1	F	247	Total	C	N	O	0	0	0
			1853	1181	304	368			
1	G	247	Total	C	N	O	0	0	0
			1865	1190	304	371			
1	H	250	Total	C	N	O	0	0	0
			1885	1200	312	373			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



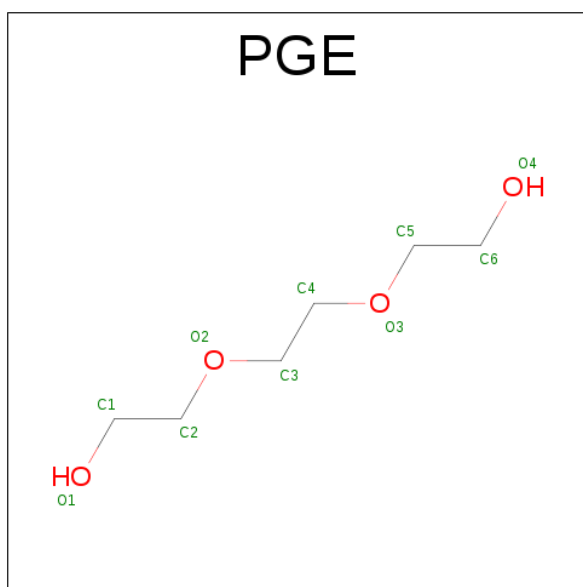
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	F	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	2	2		
2	G	1	Total	C	O	0	0
			4	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	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	C	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	E	1	Total	C	O	0	0
			7	4	3		
3	G	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	E	1	Total	Ca	0	0
			1	1		
5	H	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	A	1	Total	Ca	0	0
			1	1		
5	F	1	Total	Ca	0	0
			1	1		

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total Mn 1 1	0	0
6	D	1	Total Mn 1 1	0	0
6	E	1	Total Mn 1 1	0	0
6	H	1	Total Mn 1 1	0	0
6	B	1	Total Mn 1 1	0	0
6	C	1	Total Mn 1 1	0	0
6	A	1	Total Mn 1 1	0	0
6	F	1	Total Mn 1 1	0	0

- Molecule 7 is water.

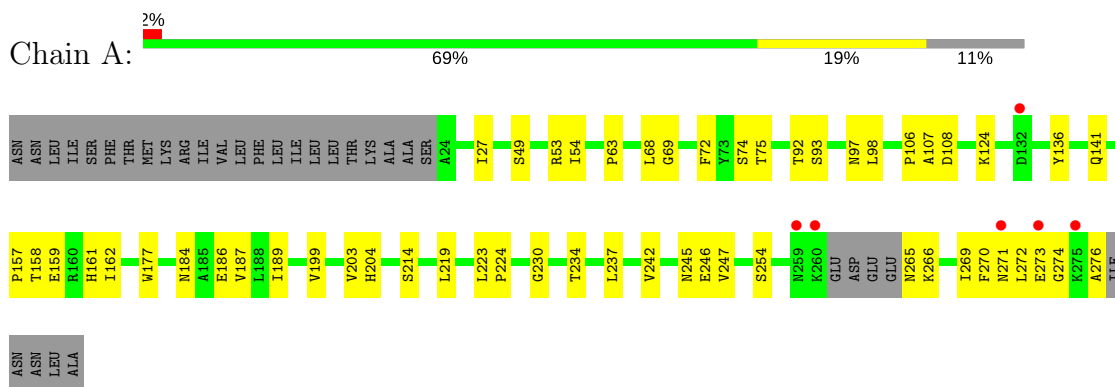
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	B	2	Total O 2 2	0	0
7	C	4	Total O 4 4	0	0
7	D	3	Total O 3 3	0	0
7	E	1	Total O 1 1	0	0
7	F	4	Total O 4 4	0	0
7	G	3	Total O 3 3	0	0
7	H	2	Total O 2 2	0	0



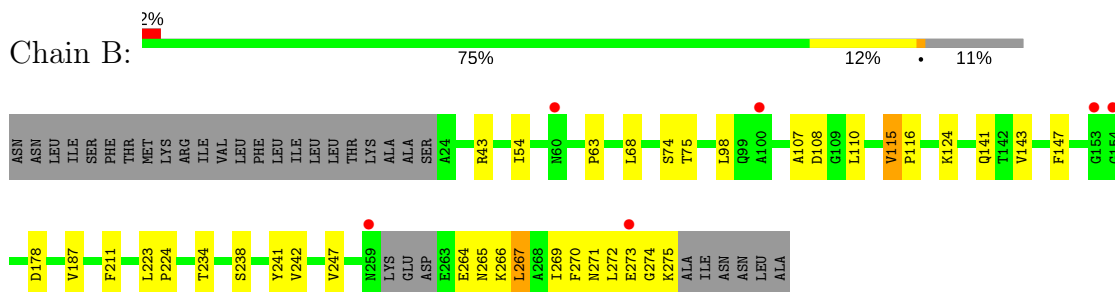
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

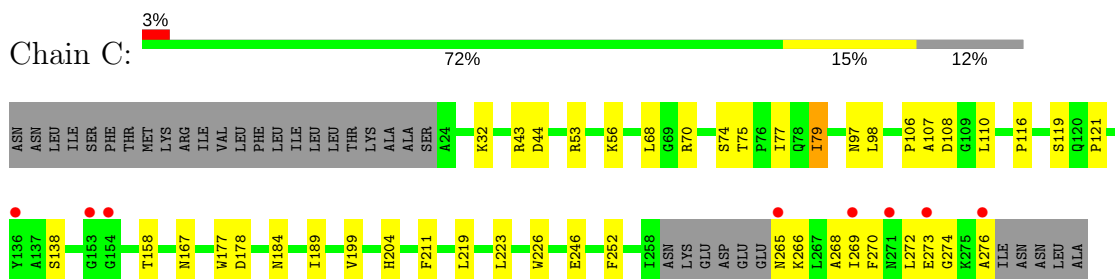
- Molecule 1: Legume lectin



- Molecule 1: Legume lectin

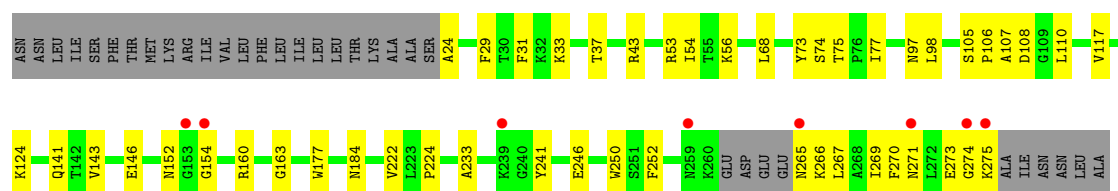


- Molecule 1: Legume lectin

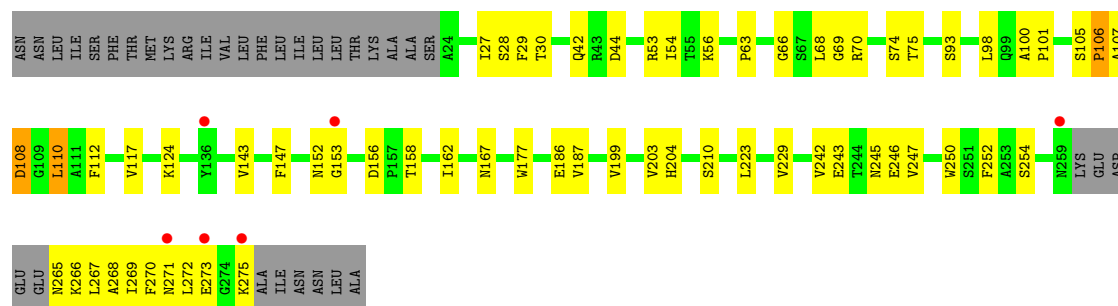


- Molecule 1: Legume lectin

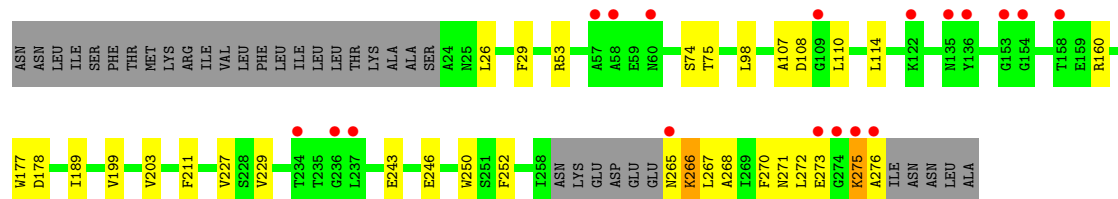
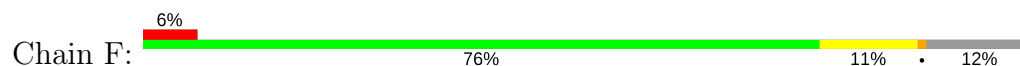




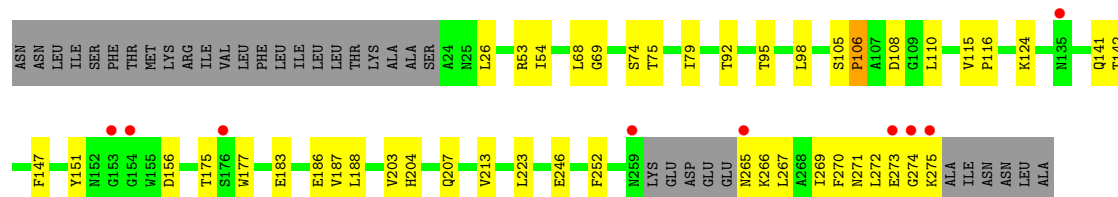
• Molecule 1: Legume lectin



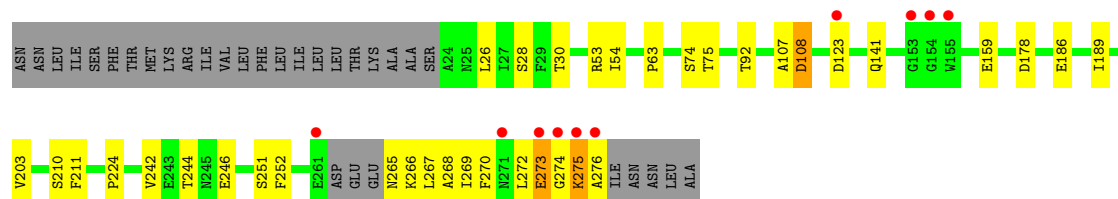
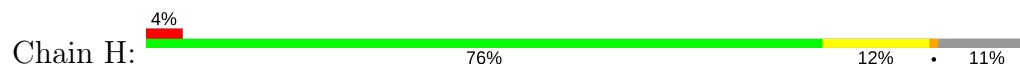
• Molecule 1: Legume lectin



• Molecule 1: Legume lectin



• Molecule 1: Legume lectin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.99Å 84.13Å 93.16Å 89.92° 76.01° 77.00°	Depositor
Resolution (Å)	90.17 – 3.11 23.46 – 3.11	Depositor EDS
% Data completeness (in resolution range)	95.7 (90.17-3.11) 94.3 (23.46-3.11)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 3.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.251 , 0.306 0.249 , 0.299	Depositor DCC
$R_{free}$ test set	1820 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 32.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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: PEG, CA, PGE, EDO, MN

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	0.36	0/1921	0.52	0/2618
1	B	0.35	0/1925	0.50	0/2624
1	C	0.36	0/1906	0.52	0/2599
1	D	0.36	0/1919	0.52	0/2615
1	E	0.36	0/1911	0.52	0/2607
1	F	0.34	0/1895	0.49	0/2587
1	G	0.35	0/1907	0.51	0/2601
1	H	0.35	0/1927	0.50	0/2627
All	All	0.36	0/15311	0.51	0/20878

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	1879	0	1809	95	0
1	B	1883	0	1810	53	0
1	C	1864	0	1792	92	0
1	D	1877	0	1813	67	0
1	E	1869	0	1802	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1853	0	1766	67	0
1	G	1865	0	1787	88	0
1	H	1885	0	1811	71	0
2	A	8	0	12	0	0
2	B	4	0	6	0	0
2	C	8	0	12	1	0
2	D	4	0	6	0	0
2	E	4	0	6	1	0
2	F	8	0	12	0	0
2	G	8	0	12	0	0
3	A	14	0	20	0	0
3	B	7	0	10	0	0
3	C	7	0	10	0	0
3	D	7	0	10	1	0
3	E	7	0	10	0	0
3	G	7	0	10	0	0
4	A	10	0	14	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	3	0	0	0	0
7	B	2	0	0	0	0
7	C	4	0	0	0	0
7	D	3	0	0	0	0
7	E	1	0	0	0	0
7	F	4	0	0	0	0
7	G	3	0	0	0	0
7	H	2	0	0	0	0
All	All	15116	0	14540	405	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 14.

All (405) 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:E:270:PHE:H	1:G:270:PHE:CB	1.08	1.67
1:A:270:PHE:CB	1:C:270:PHE:H	0.99	1.64
1:F:265:ASN:CA	1:H:276:ALA:HB3	1.19	1.60
1:A:266:LYS:CG	1:C:273:GLU:HB2	1.27	1.55
1:A:266:LYS:HG3	1:C:273:GLU:CB	1.32	1.53
1:F:275:LYS:HA	1:F:275:LYS:NZ	1.21	1.52
1:E:270:PHE:N	1:G:270:PHE:HB2	1.27	1.47
1:A:266:LYS:HG3	1:C:273:GLU:CA	0.99	1.44
1:H:275:LYS:HA	1:H:275:LYS:NZ	1.10	1.42
1:A:276:ALA:C	1:C:265:ASN:N	1.72	1.42
1:A:270:PHE:CB	1:C:270:PHE:N	1.82	1.42
1:A:266:LYS:CG	1:C:273:GLU:CB	1.82	1.37
1:B:274:GLY:O	1:D:266:LYS:CE	1.74	1.36
1:A:266:LYS:CD	1:C:273:GLU:HB2	1.13	1.35
1:A:266:LYS:CG	1:C:273:GLU:C	1.94	1.35
1:A:266:LYS:HG2	1:C:274:GLY:N	1.43	1.32
1:A:266:LYS:HG3	1:C:273:GLU:C	1.48	1.30
1:H:275:LYS:CA	1:H:275:LYS:HZ3	1.44	1.29
1:A:266:LYS:CG	1:C:273:GLU:CA	1.96	1.26
1:F:268:ALA:CB	1:H:270:PHE:CE1	1.93	1.26
1:F:268:ALA:HB3	1:H:270:PHE:CE1	1.42	1.25
1:E:270:PHE:N	1:G:270:PHE:CB	1.84	1.25
1:F:275:LYS:HZ3	1:F:275:LYS:CA	1.49	1.23
1:D:274:GLY:O	1:D:275:LYS:O	1.54	1.21
1:F:265:ASN:N	1:H:276:ALA:CA	2.05	1.20
1:A:270:PHE:CA	1:C:270:PHE:H	1.42	1.19
1:A:266:LYS:CG	1:C:274:GLY:N	2.02	1.19
1:A:270:PHE:HB2	1:C:270:PHE:N	1.45	1.19
1:A:266:LYS:CD	1:C:273:GLU:CB	1.85	1.19
1:B:274:GLY:O	1:D:266:LYS:HE3	1.00	1.18
1:E:265:ASN:OD1	1:G:272:LEU:N	1.62	1.16
1:C:75:THR:HG22	1:D:74:SER:HB2	1.26	1.16
1:A:266:LYS:CA	1:C:274:GLY:H	1.59	1.15
1:H:275:LYS:CA	1:H:275:LYS:NZ	2.06	1.15
1:A:270:PHE:CA	1:C:270:PHE:N	1.91	1.14
1:A:272:LEU:N	1:C:266:LYS:O	1.72	1.14
1:E:275:LYS:H	1:G:266:LYS:HA	1.09	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:THR:HG22	1:H:74:SER:HB3	1.13	1.12
1:F:275:LYS:NZ	1:F:275:LYS:CA	2.08	1.11
1:E:270:PHE:N	1:G:270:PHE:CA	2.06	1.10
1:A:265:ASN:HB3	1:C:276:ALA:HB3	1.14	1.09
1:E:275:LYS:N	1:G:266:LYS:HA	1.65	1.09
1:A:270:PHE:O	1:C:266:LYS:HB3	1.49	1.08
1:A:274:GLY:H	1:C:266:LYS:HA	0.92	1.08
1:A:266:LYS:HA	1:C:274:GLY:H	1.16	1.06
1:E:272:LEU:N	1:G:265:ASN:OD1	1.65	1.06
1:B:267:LEU:HD13	1:D:271:ASN:O	1.51	1.05
1:F:265:ASN:N	1:H:276:ALA:HB1	1.48	1.05
1:A:274:GLY:H	1:C:266:LYS:CA	1.70	1.04
1:A:274:GLY:N	1:C:266:LYS:HA	1.73	1.04
1:E:266:LYS:N	1:G:273:GLU:N	2.04	1.02
1:A:266:LYS:HG3	1:C:273:GLU:N	1.74	1.02
1:B:265:ASN:O	1:B:267:LEU:HD13	1.59	1.02
1:B:267:LEU:CD1	1:D:271:ASN:O	2.08	1.01
1:A:266:LYS:CD	1:C:273:GLU:HB3	1.88	1.01
1:B:272:LEU:O	1:D:266:LYS:CD	2.08	1.01
1:G:74:SER:HB3	1:H:75:THR:HG22	1.42	1.01
1:A:276:ALA:O	1:C:265:ASN:N	1.94	1.01
1:A:266:LYS:HG2	1:C:273:GLU:C	1.66	1.00
1:F:265:ASN:HA	1:H:276:ALA:HB3	1.42	0.98
1:B:271:ASN:C	1:D:267:LEU:HD12	1.73	0.98
1:A:270:PHE:HB3	1:C:270:PHE:H	1.29	0.97
1:B:272:LEU:O	1:D:266:LYS:HD2	1.65	0.96
1:G:75:THR:HG23	1:H:75:THR:HG23	1.46	0.96
1:A:270:PHE:HB2	1:C:270:PHE:H	1.01	0.94
1:E:266:LYS:HA	1:G:275:LYS:N	1.81	0.94
1:E:266:LYS:H	1:G:273:GLU:N	1.29	0.94
1:E:75:THR:HG22	1:F:74:SER:HB3	1.49	0.94
1:F:266:LYS:CB	1:H:270:PHE:O	2.16	0.93
1:E:74:SER:HB3	1:F:75:THR:HG22	1.51	0.92
1:E:275:LYS:H	1:G:266:LYS:CA	1.80	0.92
1:E:272:LEU:N	1:G:266:LYS:O	1.93	0.92
1:C:74:SER:HB3	1:D:75:THR:HG22	1.49	0.92
1:B:266:LYS:CD	1:D:274:GLY:O	2.18	0.92
1:A:265:ASN:CB	1:C:276:ALA:HB3	2.00	0.91
1:A:265:ASN:HB3	1:C:276:ALA:CB	1.99	0.91
1:H:275:LYS:HZ2	1:H:275:LYS:HA	1.30	0.91
1:C:75:THR:CG2	1:D:74:SER:HB2	1.99	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:PHE:O	1:G:266:LYS:CB	2.19	0.90
1:F:266:LYS:HA	1:H:275:LYS:N	1.86	0.89
1:F:265:ASN:N	1:H:276:ALA:CB	0.73	0.88
1:A:270:PHE:HB2	1:C:269:ILE:C	1.95	0.86
1:C:272:LEU:HD23	1:C:276:ALA:HB3	1.57	0.86
1:A:266:LYS:HD3	1:C:273:GLU:CB	2.07	0.85
1:E:269:ILE:C	1:G:270:PHE:HB2	1.96	0.85
1:B:266:LYS:CG	1:D:274:GLY:O	2.20	0.85
1:C:75:THR:HG23	1:D:75:THR:HG23	1.59	0.85
1:A:74:SER:HB3	1:B:75:THR:HG22	1.59	0.84
1:B:274:GLY:O	1:D:266:LYS:CD	2.14	0.84
1:A:272:LEU:H	1:C:266:LYS:C	1.44	0.84
1:A:270:PHE:CA	1:C:269:ILE:N	2.35	0.83
1:A:266:LYS:HD3	1:C:273:GLU:HB3	1.61	0.83
1:B:265:ASN:O	1:B:267:LEU:CD1	2.21	0.82
1:F:268:ALA:HB2	1:H:270:PHE:CE2	1.38	0.82
1:B:272:LEU:O	1:D:266:LYS:HD3	1.77	0.82
1:B:68:LEU:HD12	1:B:124:LYS:HG2	1.61	0.82
1:E:269:ILE:O	1:E:269:ILE:HG12	1.78	0.82
1:E:75:THR:HG23	1:F:75:THR:HG23	1.61	0.81
1:E:275:LYS:N	1:G:266:LYS:CA	2.40	0.81
1:F:275:LYS:CE	1:F:275:LYS:HA	2.08	0.81
1:A:266:LYS:HA	1:C:274:GLY:N	1.96	0.80
1:E:270:PHE:H	1:G:270:PHE:HB2	0.64	0.80
1:B:266:LYS:HE3	1:D:274:GLY:O	1.83	0.79
1:E:265:ASN:N	1:G:272:LEU:O	2.09	0.78
1:G:75:THR:CG2	1:H:74:SER:HB3	2.06	0.78
1:A:266:LYS:CB	1:C:273:GLU:HB2	2.11	0.77
1:F:273:GLU:N	1:H:265:ASN:OD1	1.94	0.77
1:B:272:LEU:C	1:D:266:LYS:CD	2.53	0.76
1:B:271:ASN:O	1:D:267:LEU:HD12	1.85	0.76
1:H:275:LYS:HA	1:H:275:LYS:CE	2.15	0.76
1:A:270:PHE:HA	1:C:269:ILE:N	2.00	0.75
1:E:271:ASN:C	1:G:265:ASN:OD1	2.24	0.75
1:F:275:LYS:N	1:H:266:LYS:HA	2.02	0.75
1:E:270:PHE:H	1:G:270:PHE:HB3	1.41	0.75
1:E:265:ASN:OD1	1:G:271:ASN:C	2.25	0.74
1:C:272:LEU:CD2	1:C:276:ALA:HB3	2.17	0.74
1:F:276:ALA:H	1:H:265:ASN:C	1.91	0.74
1:F:270:PHE:CD2	1:H:267:LEU:O	2.41	0.74
1:F:275:LYS:HA	1:F:275:LYS:HZ2	1.49	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:ALA:CB	1:H:270:PHE:CZ	0.69	0.73
1:B:266:LYS:CE	1:D:274:GLY:O	2.37	0.73
1:F:268:ALA:HB1	1:H:270:PHE:CZ	0.76	0.73
1:F:268:ALA:HB1	1:H:270:PHE:CE1	1.92	0.72
1:G:75:THR:HG23	1:H:75:THR:CG2	2.18	0.72
1:A:270:PHE:HA	1:C:270:PHE:N	2.04	0.71
1:B:272:LEU:O	1:D:265:ASN:HA	1.87	0.71
1:D:266:LYS:N	1:D:266:LYS:HD2	2.06	0.71
1:F:266:LYS:HA	1:H:275:LYS:H	1.54	0.71
1:A:270:PHE:O	1:C:266:LYS:CB	2.08	0.71
1:E:266:LYS:HA	1:G:275:LYS:H	1.54	0.71
1:E:63:PRO:HB2	1:E:242:VAL:HB	1.73	0.71
1:E:267:LEU:O	1:G:267:LEU:HD12	1.91	0.71
1:F:265:ASN:CA	1:H:276:ALA:CB	2.08	0.70
1:A:75:THR:CG2	1:B:74:SER:HB2	2.21	0.69
1:F:268:ALA:CB	1:H:270:PHE:HE2	1.40	0.69
1:B:272:LEU:C	1:D:266:LYS:HD2	2.11	0.69
1:F:275:LYS:HZ2	1:F:275:LYS:CA	2.02	0.68
1:A:270:PHE:HA	1:C:269:ILE:CA	2.24	0.68
1:E:266:LYS:HD2	1:E:266:LYS:N	2.07	0.68
1:A:266:LYS:CB	1:C:274:GLY:H	2.06	0.68
1:F:270:PHE:HD2	1:H:267:LEU:O	1.76	0.68
1:D:97:ASN:HD22	1:D:184:ASN:HD22	1.42	0.67
1:F:268:ALA:HB2	1:H:270:PHE:CZ	1.51	0.67
1:C:75:THR:HG22	1:D:74:SER:CB	2.15	0.67
1:F:275:LYS:C	1:F:275:LYS:HZ2	1.97	0.67
1:E:270:PHE:HA	1:G:269:ILE:CA	2.25	0.67
1:A:270:PHE:HB2	1:C:269:ILE:CA	2.12	0.66
1:A:270:PHE:CA	1:C:269:ILE:C	2.64	0.66
1:A:274:GLY:N	1:C:266:LYS:CA	2.43	0.66
1:A:274:GLY:N	1:C:266:LYS:HG2	2.10	0.66
1:B:272:LEU:C	1:D:266:LYS:HD3	2.15	0.66
1:D:274:GLY:C	1:D:275:LYS:O	2.34	0.66
1:A:266:LYS:CA	1:C:274:GLY:N	2.44	0.66
1:E:270:PHE:O	1:G:266:LYS:HB3	1.95	0.65
1:B:271:ASN:O	1:D:267:LEU:CD1	2.45	0.65
1:E:269:ILE:C	1:G:270:PHE:CA	2.63	0.65
1:A:141:GLN:HB3	1:A:224:PRO:HD3	1.78	0.65
1:C:53:ARG:HG2	1:C:246:GLU:HG2	1.79	0.65
1:E:273:GLU:HG2	1:F:26:LEU:HD13	1.78	0.65
1:E:269:ILE:C	1:G:270:PHE:HA	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:LYS:HD2	1:G:266:LYS:H	1.62	0.65
1:E:267:LEU:HD12	1:G:267:LEU:O	1.97	0.64
1:E:54:ILE:HG22	1:E:69:GLY:HA3	1.79	0.64
1:F:268:ALA:HB3	1:H:270:PHE:CZ	0.85	0.64
1:G:53:ARG:HG2	1:G:246:GLU:HG2	1.78	0.64
1:B:270:PHE:HB3	1:D:267:LEU:O	1.98	0.63
1:E:269:ILE:N	1:G:270:PHE:CA	2.50	0.63
1:F:265:ASN:N	1:H:276:ALA:HB2	0.97	0.63
1:A:266:LYS:CB	1:C:274:GLY:N	2.62	0.62
1:A:274:GLY:N	1:C:266:LYS:CG	2.46	0.62
1:E:269:ILE:HD13	1:G:273:GLU:OE1	1.99	0.62
1:A:75:THR:HG22	1:B:74:SER:HB2	1.82	0.62
1:E:275:LYS:H	1:G:266:LYS:CB	2.11	0.62
1:A:270:PHE:C	1:C:268:ALA:N	2.50	0.62
1:F:275:LYS:NZ	1:F:275:LYS:O	2.32	0.62
1:C:44:ASP:HB3	1:C:56:LYS:HG3	1.82	0.62
1:D:98:LEU:HD21	1:D:110:LEU:HD22	1.82	0.61
1:E:269:ILE:CA	1:G:270:PHE:HB2	2.20	0.61
1:E:68:LEU:HD12	1:E:124:LYS:HB3	1.82	0.60
1:H:63:PRO:HB2	1:H:242:VAL:HB	1.84	0.60
1:B:266:LYS:HD2	1:D:274:GLY:O	2.00	0.60
1:G:79:ILE:HD11	1:G:223:LEU:HB2	1.82	0.60
1:H:63:PRO:HG3	1:H:244:THR:HG23	1.83	0.60
1:A:177:TRP:HE1	1:A:204:HIS:HE1	1.48	0.60
1:E:267:LEU:O	1:G:267:LEU:CD1	2.48	0.60
1:A:54:ILE:HD11	1:A:247:VAL:HG23	1.83	0.59
1:B:270:PHE:HB3	1:D:271:ASN:N	2.17	0.59
1:G:266:LYS:HD2	1:G:266:LYS:N	2.17	0.59
1:A:270:PHE:HA	1:C:269:ILE:C	2.23	0.59
1:A:237:LEU:HD13	4:A:305:PGE:H42	1.85	0.58
1:F:266:LYS:CA	1:H:275:LYS:N	2.64	0.58
1:F:268:ALA:CB	1:H:270:PHE:HZ	1.24	0.58
1:E:273:GLU:N	1:G:266:LYS:N	2.39	0.58
1:A:271:ASN:C	1:C:266:LYS:CA	2.44	0.58
1:B:141:GLN:HB3	1:B:224:PRO:HD3	1.85	0.58
1:E:275:LYS:CA	1:G:266:LYS:HA	2.33	0.58
1:F:268:ALA:CB	1:H:270:PHE:CE2	0.86	0.57
1:E:266:LYS:H	1:G:273:GLU:CA	2.15	0.57
1:F:270:PHE:HA	1:H:269:ILE:CB	2.24	0.57
1:G:75:THR:CG2	1:H:75:THR:HG23	2.26	0.57
1:A:97:ASN:HD22	1:A:184:ASN:HD22	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LYS:HG2	1:C:274:GLY:CA	2.31	0.57
1:C:178:ASP:HB2	1:C:211:PHE:HZ	1.68	0.57
1:A:75:THR:HG23	1:B:74:SER:HB2	1.85	0.57
1:A:75:THR:HG23	1:B:75:THR:HG23	1.86	0.57
1:F:265:ASN:C	1:H:276:ALA:H	2.08	0.57
1:A:237:LEU:HD13	4:A:305:PGE:H52	1.87	0.56
1:E:269:ILE:CG1	1:E:269:ILE:O	2.49	0.56
1:G:177:TRP:HE1	1:G:204:HIS:CE1	2.24	0.56
1:E:268:ALA:N	1:G:270:PHE:O	2.39	0.56
1:F:275:LYS:C	1:F:275:LYS:NZ	2.53	0.56
1:B:270:PHE:HA	1:D:269:ILE:CB	2.36	0.55
1:E:30:THR:HG21	1:G:266:LYS:HG2	1.87	0.55
1:D:68:LEU:HD12	1:D:124:LYS:HB3	1.88	0.55
1:E:269:ILE:N	1:G:270:PHE:HA	2.20	0.55
1:F:270:PHE:C	1:H:268:ALA:N	2.57	0.55
1:B:271:ASN:C	1:D:267:LEU:CD1	2.62	0.55
1:G:175:THR:HG22	1:G:213:VAL:HG22	1.89	0.55
1:A:54:ILE:O	1:A:69:GLY:HA3	2.08	0.55
1:A:266:LYS:N	1:C:274:GLY:H	2.01	0.54
1:A:265:ASN:O	1:C:276:ALA:N	2.35	0.54
1:F:270:PHE:CD2	1:H:267:LEU:C	2.33	0.54
1:B:54:ILE:HD11	1:B:247:VAL:HG23	1.88	0.54
1:E:268:ALA:N	1:G:270:PHE:C	2.59	0.54
1:E:66:GLY:HA3	2:E:301:EDO:O1	2.08	0.54
1:F:275:LYS:H	1:H:266:LYS:HA	1.73	0.54
1:C:219:LEU:HD22	1:C:223:LEU:HD12	1.90	0.54
1:A:92:THR:HG22	1:A:189:ILE:HB	1.91	0.53
1:E:272:LEU:O	1:G:266:LYS:HD2	2.08	0.53
1:D:29:PHE:CZ	1:D:252:PHE:HB3	2.43	0.53
1:E:203:VAL:HG12	1:E:210:SER:HB3	1.89	0.53
1:A:63:PRO:HB2	1:A:242:VAL:HB	1.91	0.53
1:E:270:PHE:O	1:G:266:LYS:HB2	2.04	0.53
1:G:266:LYS:CD	1:G:266:LYS:H	2.21	0.53
1:B:274:GLY:O	1:B:275:LYS:O	2.26	0.53
1:B:115:VAL:HG22	1:B:116:PRO:HD2	1.91	0.52
1:F:268:ALA:HB1	1:H:270:PHE:HZ	1.03	0.52
1:E:75:THR:CG2	1:F:74:SER:HB3	2.32	0.52
1:B:271:ASN:N	1:D:270:PHE:HB3	2.24	0.52
1:E:275:LYS:CB	1:G:266:LYS:HA	2.40	0.52
1:H:178:ASP:HB2	1:H:211:PHE:CZ	2.45	0.52
1:D:266:LYS:N	1:D:266:LYS:CD	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:PHE:HA	1:G:269:ILE:CB	2.39	0.52
1:C:98:LEU:HD21	1:C:110:LEU:HD22	1.92	0.52
1:F:229:VAL:HG12	1:F:250:TRP:HZ2	1.75	0.52
1:G:95:THR:OG1	1:G:186:GLU:HG2	2.09	0.51
1:F:275:LYS:HA	1:F:275:LYS:HZ3	0.59	0.51
1:E:272:LEU:C	1:G:266:LYS:HD2	2.31	0.51
1:B:143:VAL:H	1:B:223:LEU:HD21	1.75	0.51
1:F:270:PHE:HB3	1:H:267:LEU:O	2.11	0.51
1:D:265:ASN:O	1:D:267:LEU:CD1	2.59	0.51
1:D:97:ASN:HD22	1:D:184:ASN:ND2	2.09	0.50
1:E:266:LYS:O	1:G:272:LEU:N	2.44	0.50
1:D:56:LYS:NZ	3:D:302:PEG:H41	2.27	0.50
1:E:229:VAL:HG12	1:E:250:TRP:HZ2	1.77	0.50
1:A:270:PHE:CA	1:C:269:ILE:CA	2.88	0.50
1:D:152:ASN:C	1:D:154:GLY:H	2.14	0.50
1:A:219:LEU:HD22	1:A:223:LEU:HD12	1.94	0.50
1:F:268:ALA:HB2	1:H:270:PHE:HE2	1.24	0.49
1:D:267:LEU:O	1:D:271:ASN:CG	2.51	0.49
1:A:124:LYS:HA	1:A:234:THR:HG21	1.93	0.49
1:D:143:VAL:HG23	1:D:222:VAL:HG11	1.94	0.49
1:D:77:ILE:HD13	1:D:252:PHE:CE2	2.47	0.49
1:D:265:ASN:O	1:D:267:LEU:HD12	2.10	0.49
1:G:177:TRP:HE1	1:G:204:HIS:HE1	1.60	0.49
1:E:273:GLU:N	1:G:266:LYS:H	1.68	0.49
1:H:178:ASP:HB2	1:H:211:PHE:HZ	1.77	0.49
1:F:29:PHE:CZ	1:F:252:PHE:HB3	2.48	0.49
1:H:203:VAL:HG12	1:H:210:SER:HB3	1.94	0.49
1:E:177:TRP:HE1	1:E:204:HIS:HE1	1.61	0.48
1:E:266:LYS:HE3	1:G:274:GLY:O	2.14	0.48
1:F:107:ALA:O	1:F:243:GLU:HG2	2.14	0.48
1:A:68:LEU:HD12	1:A:124:LYS:HB3	1.96	0.48
1:E:29:PHE:CE2	1:E:252:PHE:HB3	2.49	0.48
1:E:270:PHE:C	1:G:267:LEU:C	2.73	0.48
1:E:269:ILE:C	1:G:270:PHE:CB	2.65	0.48
1:D:141:GLN:HB3	1:D:224:PRO:HD3	1.95	0.47
1:H:275:LYS:HZ3	1:H:275:LYS:N	2.06	0.47
1:A:97:ASN:HD22	1:A:184:ASN:ND2	2.13	0.47
1:F:267:LEU:O	1:H:267:LEU:O	2.32	0.47
1:A:162:ILE:HG13	1:A:177:TRP:HB2	1.96	0.47
1:E:106:PRO:HB2	1:E:243:GLU:OE1	2.15	0.47
1:E:269:ILE:CA	1:G:270:PHE:HA	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:ILE:HG22	1:E:254:SER:HB3	1.97	0.47
1:H:272:LEU:O	1:H:274:GLY:N	2.47	0.47
1:B:178:ASP:HB2	1:B:211:PHE:HZ	1.80	0.47
1:E:53:ARG:CZ	1:E:246:GLU:OE2	2.64	0.46
1:H:92:THR:HG22	1:H:189:ILE:HB	1.97	0.46
1:A:158:THR:HG23	1:A:159:GLU:H	1.80	0.46
1:B:272:LEU:O	1:D:265:ASN:CA	2.60	0.46
1:E:143:VAL:H	1:E:223:LEU:HD21	1.80	0.46
1:G:188:LEU:HD21	1:G:267:LEU:HD21	1.97	0.46
1:A:27:ILE:CG2	1:A:254:SER:HB3	2.46	0.46
1:G:151:TYR:HE1	1:G:156:ASP:O	1.98	0.46
1:D:107:ALA:HA	1:D:108:ASP:HA	1.71	0.46
1:C:189:ILE:HA	1:C:199:VAL:O	2.16	0.46
1:D:54:ILE:HG21	1:D:233:ALA:HB3	1.98	0.46
1:E:98:LEU:HD23	1:E:245:ASN:HA	1.98	0.46
1:A:75:THR:HG22	1:B:74:SER:CB	2.46	0.45
1:C:226:TRP:HB2	2:C:302:EDO:H11	1.99	0.45
1:C:177:TRP:HE1	1:C:204:HIS:HE1	1.64	0.45
1:B:264:GLU:HB2	1:D:275:LYS:C	2.36	0.45
1:E:107:ALA:HA	1:E:108:ASP:HA	1.80	0.45
1:E:152:ASN:H	1:E:156:ASP:HB2	1.80	0.45
1:F:265:ASN:N	1:H:276:ALA:N	2.61	0.45
1:E:42:GLN:OE1	1:E:70:ARG:HD3	2.16	0.45
1:F:98:LEU:HD21	1:F:110:LEU:HD22	1.98	0.45
1:A:107:ALA:HA	1:A:108:ASP:HA	1.70	0.45
1:B:107:ALA:HA	1:B:108:ASP:HA	1.66	0.45
1:B:147:PHE:HZ	1:B:187:VAL:HG11	1.80	0.45
1:A:98:LEU:HD23	1:A:245:ASN:HA	1.98	0.45
1:G:54:ILE:O	1:G:69:GLY:HA3	2.17	0.45
1:H:53:ARG:HG2	1:H:246:GLU:HG2	1.99	0.45
1:B:269:ILE:CB	1:D:270:PHE:HA	2.45	0.45
1:E:162:ILE:HG13	1:E:177:TRP:HB2	1.98	0.45
1:A:53:ARG:HG2	1:A:246:GLU:HG2	1.99	0.44
1:D:31:PHE:N	1:D:250:TRP:O	2.48	0.44
1:F:272:LEU:HD23	1:H:265:ASN:HB3	0.82	0.44
1:D:269:ILE:O	1:D:273:GLU:HG3	2.17	0.44
1:H:186:GLU:HB2	1:H:203:VAL:HG23	2.00	0.44
1:E:270:PHE:C	1:G:267:LEU:CA	2.55	0.44
1:C:79:ILE:CD1	1:C:223:LEU:HB2	2.47	0.44
1:E:186:GLU:HB2	1:E:203:VAL:HG23	1.99	0.44
1:E:269:ILE:HG21	1:G:273:GLU:OE1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLU:HG3	1:C:266:LYS:HB2	1.70	0.44
1:H:141:GLN:HB3	1:H:224:PRO:HD3	2.00	0.44
1:B:266:LYS:HG3	1:D:274:GLY:O	1.59	0.44
1:D:43:ARG:HG3	1:D:68:LEU:HD22	2.00	0.44
1:F:189:ILE:HA	1:F:199:VAL:O	2.18	0.44
1:G:75:THR:HG22	1:H:74:SER:CB	2.09	0.44
1:G:147:PHE:HZ	1:G:187:VAL:HG11	1.83	0.43
1:E:112:PHE:CE1	1:E:229:VAL:HG13	2.53	0.43
1:E:53:ARG:HG2	1:E:246:GLU:OE2	2.18	0.43
1:C:75:THR:HG21	1:D:73:TYR:CZ	2.53	0.43
1:G:92:THR:HB	1:G:252:PHE:HD1	1.84	0.43
1:H:272:LEU:O	1:H:273:GLU:C	2.56	0.43
1:B:43:ARG:HD2	1:B:68:LEU:HB3	2.01	0.43
1:F:107:ALA:HA	1:F:108:ASP:HA	1.67	0.43
1:F:178:ASP:HB2	1:F:211:PHE:HZ	1.84	0.43
1:F:276:ALA:N	1:H:265:ASN:O	2.30	0.43
1:B:63:PRO:HB2	1:B:242:VAL:HB	2.00	0.43
1:D:54:ILE:CG2	1:D:233:ALA:HB3	2.49	0.43
1:D:53:ARG:HG2	1:D:246:GLU:HG2	2.00	0.43
1:G:68:LEU:HD12	1:G:124:LYS:HA	2.01	0.43
1:A:93:SER:HA	1:A:187:VAL:O	2.18	0.43
1:G:147:PHE:CZ	1:G:187:VAL:HG11	2.54	0.43
1:C:70:ARG:NH1	1:C:121:PRO:HA	2.34	0.42
1:B:273:GLU:HA	1:D:266:LYS:HD3	1.27	0.42
1:G:175:THR:CG2	1:G:213:VAL:HG22	2.49	0.42
1:G:266:LYS:CD	1:G:266:LYS:N	2.82	0.42
1:D:33:LYS:HA	1:D:33:LYS:HD3	1.85	0.42
1:A:186:GLU:HB2	1:A:203:VAL:HG23	2.01	0.42
1:A:269:ILE:CB	1:C:270:PHE:HA	2.48	0.42
1:C:116:PRO:HB2	1:C:119:SER:HB2	2.01	0.42
1:E:105:SER:N	1:E:106:PRO:HD3	2.34	0.42
1:F:114:LEU:HD23	1:F:227:VAL:HG21	2.01	0.42
1:G:26:LEU:HB2	1:H:30:THR:HB	2.01	0.42
1:B:178:ASP:HB2	1:B:211:PHE:CZ	2.55	0.42
1:C:138:SER:HA	1:C:167:ASN:CG	2.40	0.42
1:C:32:LYS:HZ2	1:D:24:ALA:N	2.18	0.42
1:E:54:ILE:O	1:E:69:GLY:HA3	2.20	0.42
1:G:98:LEU:HD21	1:G:110:LEU:HD22	2.02	0.42
1:A:157:PRO:HD2	1:A:161:HIS:CE1	2.54	0.42
1:D:160:ARG:HB2	1:D:177:TRP:O	2.20	0.42
1:E:110:LEU:HD23	1:E:147:PHE:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:269:ILE:CG2	1:G:270:PHE:HA	2.50	0.42
1:E:271:ASN:H	1:G:267:LEU:HA	1.15	0.42
1:F:272:LEU:HD22	1:H:265:ASN:HB2	1.30	0.42
1:F:160:ARG:HB2	1:F:177:TRP:O	2.19	0.41
1:G:183:GLU:HG3	1:G:207:GLN:HE22	1.84	0.41
1:H:107:ALA:HA	1:H:108:ASP:HA	1.75	0.41
1:H:275:LYS:HZ2	1:H:275:LYS:CA	2.03	0.41
1:A:199:VAL:HG13	1:A:214:SER:HB3	2.01	0.41
1:C:97:ASN:HD22	1:C:184:ASN:HD22	1.68	0.41
1:A:92:THR:CG2	1:A:189:ILE:HB	2.49	0.41
1:C:107:ALA:HA	1:C:108:ASP:HA	1.73	0.41
1:D:267:LEU:H	1:D:267:LEU:CD1	2.25	0.41
1:D:146:GLU:HG2	1:D:163:GLY:O	2.20	0.41
1:E:199:VAL:HG21	1:G:203:VAL:HG11	2.03	0.41
1:C:75:THR:CG2	1:D:75:THR:HG23	2.41	0.41
1:E:93:SER:HA	1:E:187:VAL:O	2.21	0.41
1:E:27:ILE:CG2	1:E:254:SER:HB3	2.50	0.41
1:G:105:SER:N	1:G:106:PRO:HD3	2.35	0.41
1:D:105:SER:O	1:D:241:TYR:HA	2.20	0.41
1:C:178:ASP:HB2	1:C:211:PHE:CZ	2.53	0.41
1:A:72:PHE:HA	1:A:230:GLY:HA3	2.03	0.41
1:A:265:ASN:CB	1:C:276:ALA:CB	2.80	0.41
1:C:116:PRO:O	1:C:119:SER:HB3	2.21	0.41
1:A:266:LYS:CB	1:C:273:GLU:CB	2.82	0.41
1:H:274:GLY:O	1:H:275:LYS:C	2.58	0.41
1:B:238:SER:HB2	1:B:241:TYR:HD1	1.86	0.40
1:G:273:GLU:HG2	1:H:26:LEU:HD13	2.04	0.40
1:F:271:ASN:HA	1:H:268:ALA:H	1.72	0.40
1:A:266:LYS:CG	1:C:273:GLU:N	2.39	0.40
1:B:68:LEU:HA	1:B:234:THR:HG22	2.03	0.40
1:E:100:ALA:HA	1:E:101:PRO:HD3	1.96	0.40
1:E:44:ASP:HB3	1:E:56:LYS:HG3	2.02	0.40
1:F:271:ASN:OD1	1:F:272:LEU:HG	2.21	0.40
1:G:116:PRO:HD3	1:G:141:GLN:O	2.21	0.40
1:H:28:SER:HA	1:H:252:PHE:O	2.21	0.40
1:B:98:LEU:HD21	1:B:110:LEU:HD22	2.03	0.40
1:G:115:VAL:HG12	1:G:142:THR:HG23	2.03	0.40
1:C:43:ARG:HG3	1:C:68:LEU:HD22	2.03	0.40
1:C:77:ILE:HD13	1:C:252:PHE:CE2	2.56	0.40
1:F:53:ARG:HA	1:F:246:GLU:HG2	2.04	0.40

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	245/281 (87%)	227 (93%)	16 (6%)	2 (1%)	22	62
1	B	245/281 (87%)	230 (94%)	15 (6%)	0	100	100
1	C	243/281 (86%)	226 (93%)	16 (7%)	1 (0%)	38	75
1	D	244/281 (87%)	230 (94%)	13 (5%)	1 (0%)	38	75
1	E	243/281 (86%)	224 (92%)	15 (6%)	4 (2%)	11	43
1	F	243/281 (86%)	223 (92%)	19 (8%)	1 (0%)	38	75
1	G	243/281 (86%)	231 (95%)	11 (4%)	1 (0%)	38	75
1	H	246/281 (88%)	231 (94%)	14 (6%)	1 (0%)	38	75
All	All	1952/2248 (87%)	1822 (93%)	119 (6%)	11 (1%)	28	67

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	TYR
1	E	106	PRO
1	H	273	GLU
1	C	106	PRO
1	E	117	VAL
1	E	167	ASN
1	A	106	PRO
1	F	266	LYS
1	G	106	PRO
1	E	153	GLY
1	D	106	PRO

### 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	203/237 (86%)	202 (100%)	1 (0%)	91	96
1	B	203/237 (86%)	201 (99%)	2 (1%)	80	92
1	C	201/237 (85%)	199 (99%)	2 (1%)	80	92
1	D	203/237 (86%)	201 (99%)	2 (1%)	80	92
1	E	203/237 (86%)	198 (98%)	5 (2%)	53	83
1	F	198/237 (84%)	196 (99%)	2 (1%)	80	92
1	G	202/237 (85%)	201 (100%)	1 (0%)	91	96
1	H	203/237 (86%)	197 (97%)	6 (3%)	46	79
All	All	1616/1896 (85%)	1595 (99%)	21 (1%)	73	91

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	B	115	VAL
1	B	267	LEU
1	C	79	ILE
1	C	158	THR
1	D	37	THR
1	D	117	VAL
1	E	28	SER
1	E	108	ASP
1	E	110	LEU
1	E	158	THR
1	E	247	VAL
1	F	203	VAL
1	F	275	LYS
1	G	108	ASP
1	H	54	ILE
1	H	108	ASP
1	H	123	ASP
1	H	159	GLU
1	H	251	SER
1	H	275	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	184	ASN
1	A	204	HIS
1	B	184	ASN
1	C	102	ASN
1	C	184	ASN
1	C	204	HIS
1	C	245	ASN
1	D	102	ASN
1	D	184	ASN
1	E	97	ASN
1	E	102	ASN
1	E	184	ASN
1	E	196	ASN
1	E	204	HIS
1	F	184	ASN
1	F	196	ASN
1	F	204	HIS
1	G	204	HIS
1	G	207	GLN
1	G	245	ASN
1	H	97	ASN
1	H	184	ASN
1	H	204	HIS
1	H	245	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 carbohydrates in this entry.

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

Of 35 ligands modelled in this entry, 16 are monoatomic - leaving 19 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
2	EDO	A	301	-	3,3,3	0.43	0	2,2,2	0.43	0
2	EDO	A	302	-	3,3,3	0.47	0	2,2,2	0.37	0
3	PEG	A	303	-	6,6,6	0.49	0	5,5,5	0.42	0
3	PEG	A	304	-	6,6,6	0.47	0	5,5,5	0.28	0
4	PGE	A	305	-	9,9,9	0.50	0	8,8,8	0.19	0
2	EDO	B	301	-	3,3,3	0.47	0	2,2,2	0.33	0
3	PEG	B	302	-	6,6,6	0.49	0	5,5,5	0.32	0
2	EDO	C	301	-	3,3,3	0.44	0	2,2,2	0.43	0
2	EDO	C	302	-	3,3,3	0.48	0	2,2,2	0.30	0
3	PEG	C	303	-	6,6,6	0.47	0	5,5,5	0.28	0
2	EDO	D	301	-	3,3,3	0.45	0	2,2,2	0.32	0
3	PEG	D	302	-	6,6,6	0.47	0	5,5,5	0.28	0
2	EDO	E	301	-	3,3,3	0.45	0	2,2,2	0.48	0
3	PEG	E	302	-	6,6,6	0.47	0	5,5,5	0.27	0
2	EDO	F	301	-	3,3,3	0.49	0	2,2,2	0.35	0
2	EDO	F	302	-	3,3,3	0.47	0	2,2,2	0.37	0
2	EDO	G	301	-	3,3,3	0.47	0	2,2,2	0.29	0
2	EDO	G	302	-	3,3,3	0.45	0	2,2,2	0.36	0
3	PEG	G	303	-	6,6,6	0.54	0	5,5,5	0.23	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	EDO	A	301	-	-	0/1/1/1	0/0/0/0
2	EDO	A	302	-	-	0/1/1/1	0/0/0/0
3	PEG	A	303	-	-	0/4/4/4	0/0/0/0
3	PEG	A	304	-	-	0/4/4/4	0/0/0/0
4	PGE	A	305	-	-	0/7/7/7	0/0/0/0
2	EDO	B	301	-	-	0/1/1/1	0/0/0/0
3	PEG	B	302	-	-	0/4/4/4	0/0/0/0
2	EDO	C	301	-	-	0/1/1/1	0/0/0/0
2	EDO	C	302	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	C	303	-	-	0/4/4/4	0/0/0/0
2	EDO	D	301	-	-	0/1/1/1	0/0/0/0
3	PEG	D	302	-	-	0/4/4/4	0/0/0/0
2	EDO	E	301	-	-	0/1/1/1	0/0/0/0
3	PEG	E	302	-	-	0/4/4/4	0/0/0/0
2	EDO	F	301	-	-	0/1/1/1	0/0/0/0
2	EDO	F	302	-	-	0/1/1/1	0/0/0/0
2	EDO	G	301	-	-	0/1/1/1	0/0/0/0
2	EDO	G	302	-	-	0/1/1/1	0/0/0/0
3	PEG	G	303	-	-	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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	305	PGE	2	0
2	C	302	EDO	1	0
3	D	302	PEG	1	0
2	E	301	EDO	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, 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	249/281 (88%)	-0.19	6 (2%)	59	38	24, 42, 72, 83	13 (5%)
1	B	249/281 (88%)	-0.09	6 (2%)	59	38	25, 50, 84, 103	14 (5%)
1	C	247/281 (87%)	-0.23	8 (3%)	48	25	20, 39, 67, 69	12 (4%)
1	D	248/281 (88%)	-0.21	8 (3%)	48	25	22, 42, 66, 81	11 (4%)
1	E	247/281 (87%)	-0.27	6 (2%)	59	38	20, 41, 67, 78	11 (4%)
1	F	247/281 (87%)	0.20	18 (7%)	16	6	29, 69, 122, 159	13 (5%)
1	G	247/281 (87%)	-0.16	9 (3%)	43	21	18, 43, 72, 92	11 (4%)
1	H	250/281 (88%)	0.03	10 (4%)	39	19	26, 59, 90, 102	12 (4%)
All	All	1984/2248 (88%)	-0.12	71 (3%)	43	21	18, 46, 88, 159	97 (4%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	236	GLY	6.7
1	H	153	GLY	6.2
1	D	153	GLY	5.2
1	A	259	ASN	5.0
1	H	154	GLY	4.9
1	F	276	ALA	4.8
1	C	276	ALA	4.6
1	B	60	ASN	4.5
1	F	237	LEU	4.2
1	G	153	GLY	4.2
1	A	271	ASN	4.2
1	C	269	ILE	4.1
1	F	58	ALA	4.0
1	A	275	LYS	4.0
1	A	260	LYS	3.9
1	G	259	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	H	273	GLU	3.6
1	C	154	GLY	3.6
1	C	273	GLU	3.6
1	F	136	TYR	3.6
1	H	271	ASN	3.5
1	F	275	LYS	3.2
1	F	273	GLU	3.2
1	E	273	GLU	3.2
1	E	153	GLY	3.1
1	D	271	ASN	2.9
1	E	271	ASN	2.8
1	B	154	GLY	2.8
1	F	153	GLY	2.8
1	D	275	LYS	2.8
1	E	259	ASN	2.7
1	D	265	ASN	2.7
1	B	273	GLU	2.7
1	H	275	LYS	2.7
1	F	234	THR	2.7
1	G	154	GLY	2.6
1	F	154	GLY	2.6
1	D	154	GLY	2.6
1	D	259	ASN	2.6
1	B	259	ASN	2.6
1	F	122	LYS	2.4
1	H	123	ASP	2.4
1	F	60	ASN	2.4
1	G	275	LYS	2.4
1	C	271	ASN	2.4
1	F	109	GLY	2.4
1	B	100	ALA	2.4
1	C	265	ASN	2.3
1	F	158	THR	2.3
1	H	274	GLY	2.3
1	F	265	ASN	2.3
1	F	135	ASN	2.3
1	H	155	TRP	2.2
1	C	136	TYR	2.2
1	D	274	GLY	2.2
1	E	275	LYS	2.2
1	G	273	GLU	2.2
1	G	274	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	274	GLY	2.2
1	G	265	ASN	2.1
1	H	276	ALA	2.1
1	G	135	ASN	2.1
1	A	273	GLU	2.1
1	E	136	TYR	2.1
1	A	132	ASP	2.1
1	B	153	GLY	2.1
1	F	57	ALA	2.0
1	C	153	GLY	2.0
1	G	176	SER	2.0
1	H	261	GLU	2.0
1	D	239	LYS	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 carbohydrates 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. 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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EDO	F	301	4/4	0.79	0.36	6.50	38,38,38,38	4
2	EDO	C	301	4/4	0.91	0.27	5.99	46,46,46,47	0
2	EDO	G	301	4/4	0.90	0.46	5.59	50,50,50,50	4
2	EDO	D	301	4/4	0.84	0.34	2.83	37,38,38,38	4
2	EDO	A	302	4/4	0.88	0.38	1.94	39,39,39,39	4
2	EDO	B	301	4/4	0.90	0.30	1.20	35,35,36,36	4
2	EDO	G	302	4/4	0.96	0.19	0.89	41,42,42,42	0
2	EDO	A	301	4/4	0.94	0.28	0.71	21,21,22,23	4

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	F	302	4/4	0.90	0.24	0.46	41,41,41,41	4
2	EDO	E	301	4/4	0.85	0.21	-0.12	31,32,32,32	0
5	CA	E	303	1/1	0.95	0.19	-0.61	47,47,47,47	0
6	MN	E	304	1/1	0.97	0.13	-0.85	56,56,56,56	0
6	MN	C	305	1/1	0.97	0.13	-1.12	35,35,35,35	0
5	CA	A	306	1/1	0.82	0.13	-1.46	45,45,45,45	0
6	MN	A	307	1/1	0.98	0.13	-1.54	49,49,49,49	0
6	MN	F	304	1/1	0.89	0.13	-1.58	73,73,73,73	0
5	CA	D	303	1/1	0.75	0.15	-1.60	56,56,56,56	0
6	MN	D	304	1/1	0.92	0.06	-1.61	48,48,48,48	0
5	CA	B	303	1/1	0.87	0.14	-1.74	48,48,48,48	0
6	MN	H	302	1/1	0.85	0.06	-1.90	64,64,64,64	0
5	CA	H	301	1/1	0.93	0.11	-2.07	30,30,30,30	0
6	MN	B	304	1/1	0.95	0.07	-2.31	40,40,40,40	0
6	MN	G	305	1/1	0.98	0.08	-2.33	32,32,32,32	0
5	CA	F	303	1/1	0.81	0.08	-2.61	86,86,86,86	0
5	CA	C	304	1/1	0.92	0.10	-2.84	34,34,34,34	0
5	CA	G	304	1/1	0.98	0.05	-2.92	30,30,30,30	0
3	PEG	A	304	7/7	0.89	0.27	-	49,49,49,50	7
3	PEG	A	303	7/7	0.80	0.22	-	50,50,50,50	7
3	PEG	D	302	7/7	0.91	0.11	-	42,43,43,43	7
2	EDO	C	302	4/4	0.94	0.15	-	39,40,40,40	0
3	PEG	B	302	7/7	0.63	0.17	-	53,53,53,53	7
3	PEG	G	303	7/7	0.75	0.23	-	46,47,47,48	0
3	PEG	C	303	7/7	0.68	0.22	-	54,55,55,55	7
4	PGE	A	305	10/10	0.85	0.31	-	40,41,41,41	10
3	PEG	E	302	7/7	0.90	0.13	-	49,49,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.