



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 AM GMT

PDB ID : 2QEZ  
Title : Crystal structure of ethanolamine ammonia-lyase heavy chain (YP\_013784.1)  
from *Listeria monocytogenes* 4b F2365 at 2.15 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-06-26  
Resolution : 2.15 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

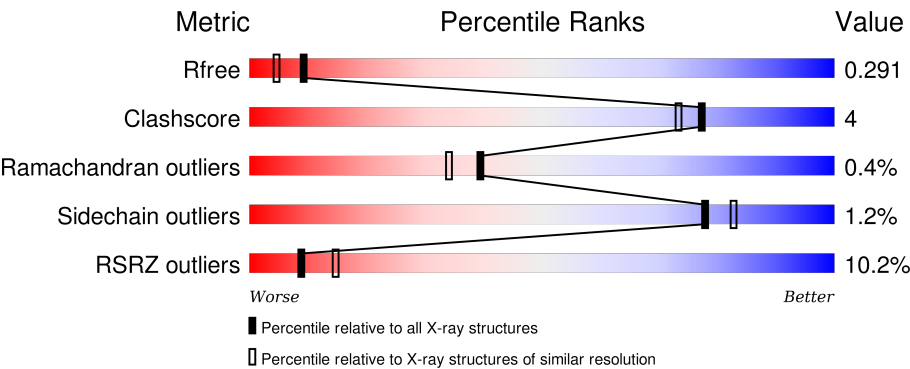
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.15 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 <sub>free</sub>	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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	455	
1	B	455	
1	C	455	
1	D	455	
1	E	455	

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Mol	Chain	Length	Quality of chain
1	F	455	

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	GOL	A	456	-	-	-	X
2	GOL	C	455	-	-	-	X
2	GOL	F	455	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20573 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 Ethanolamine ammonia-lyase heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	Se	0	3	0
			3346	2099	574	654	5	14			
1	B	437	Total	C	N	O	S	Se	0	3	0
			3306	2079	560	647	5	15			
1	C	437	Total	C	N	O	S	Se	0	1	0
			3228	2030	550	629	5	14			
1	D	438	Total	C	N	O	S	Se	0	3	0
			3325	2093	562	651	5	14			
1	E	434	Total	C	N	O	S	Se	0	2	0
			3261	2057	551	634	5	14			
1	F	443	Total	C	N	O	S	Se	0	1	0
			3317	2088	565	644	5	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q720Q3
B	0	GLY	-	LEADER SEQUENCE	UNP Q720Q3
C	0	GLY	-	LEADER SEQUENCE	UNP Q720Q3
D	0	GLY	-	LEADER SEQUENCE	UNP Q720Q3
E	0	GLY	-	LEADER SEQUENCE	UNP Q720Q3
F	0	GLY	-	LEADER SEQUENCE	UNP Q720Q3

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

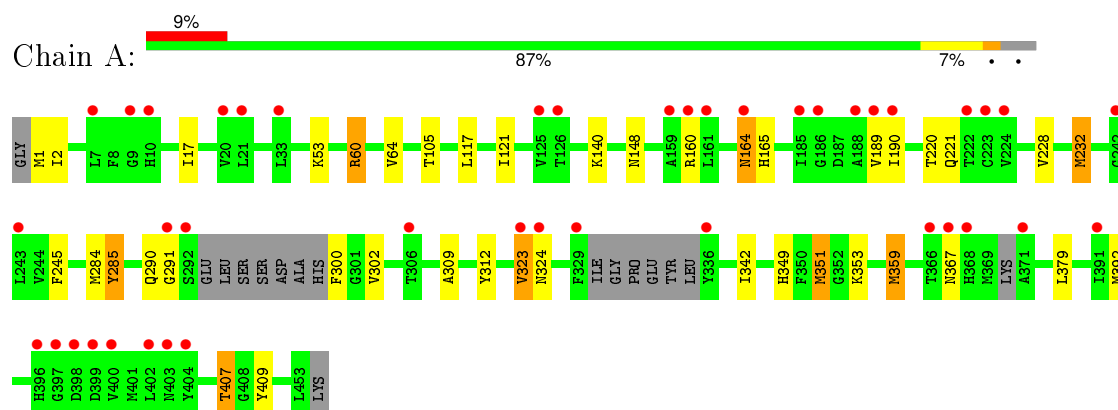
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	183	Total	O	0	0
			183	183		
3	B	97	Total	O	0	0
			97	97		
3	C	73	Total	O	0	0
			73	73		
3	D	168	Total	O	0	0
			168	168		
3	E	140	Total	O	0	0
			140	140		
3	F	93	Total	O	0	0
			93	93		

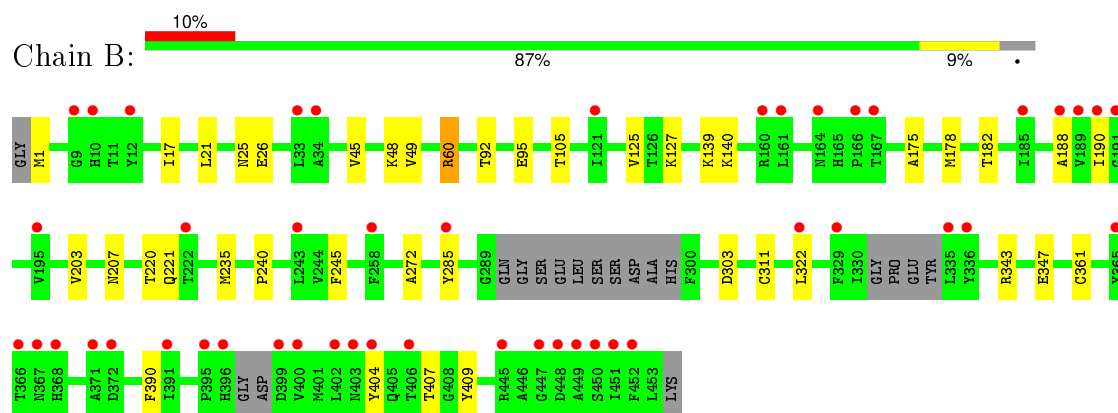
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

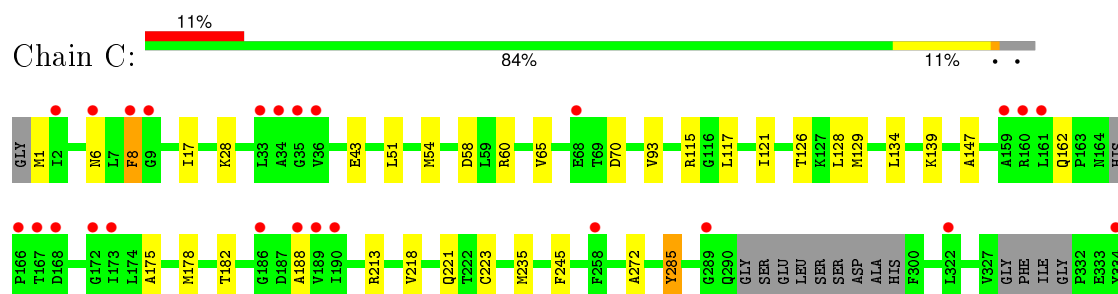
- Molecule 1: Ethanolamine ammonia-lyase heavy chain

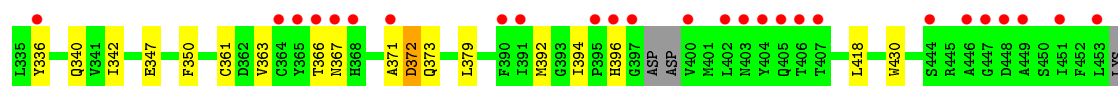


- Molecule 1: Ethanolamine ammonia-lyase heavy chain

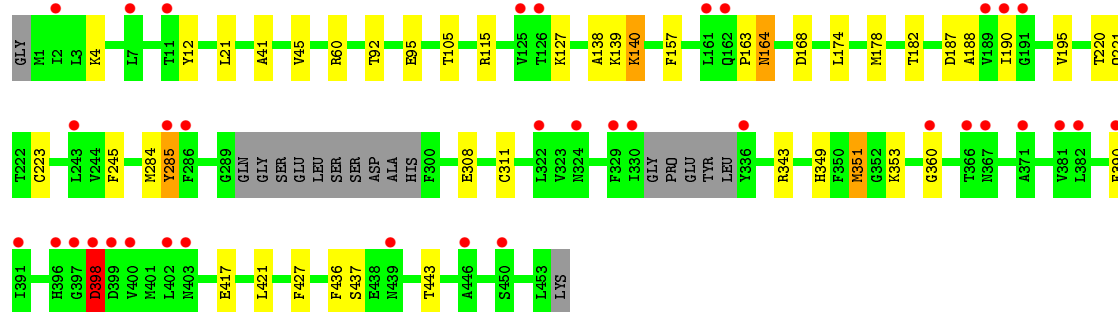
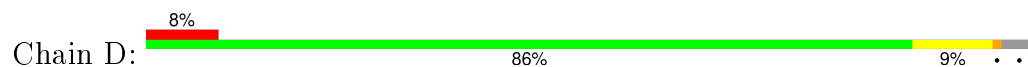


- Molecule 1: Ethanolamine ammonia-lyase heavy chain

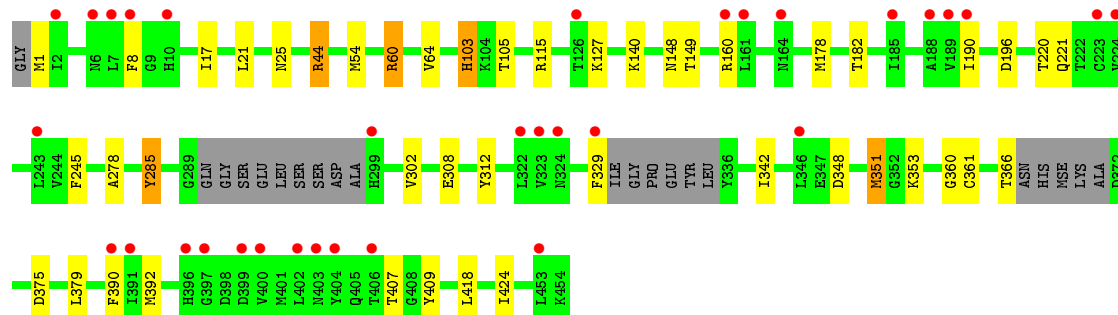
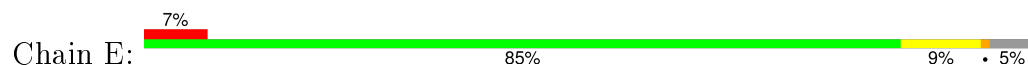




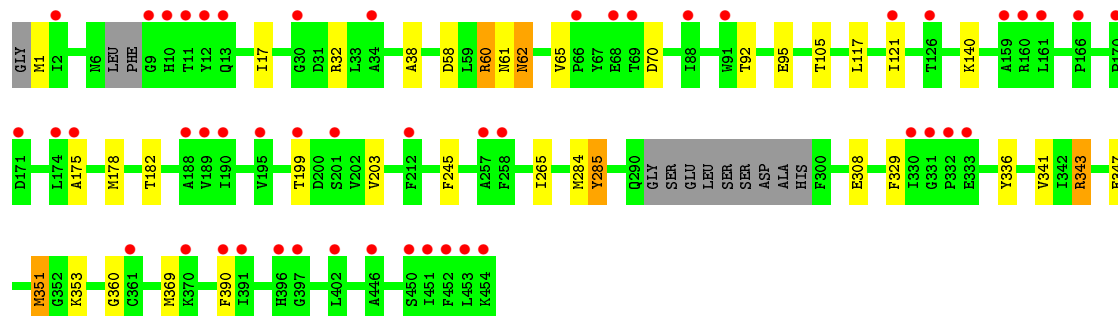
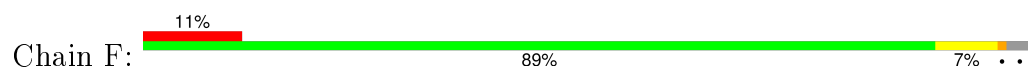
• Molecule 1: Ethanolamine ammonia-lyase heavy chain



• Molecule 1: Ethanolamine ammonia-lyase heavy chain



• Molecule 1: Ethanolamine ammonia-lyase heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	188.33 Å   223.70 Å   65.93 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	29.21 – 2.15 29.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.21-2.15) 99.6 (29.23-2.10)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.10 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.228   ,   0.279 0.245   ,   0.291	Depositor DCC
$R_{free}$ test set	7573 reflections (5.25%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 70.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 162421 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:  
GOL

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	0.80	9/3387 (0.3%)	0.84	6/4559 (0.1%)
1	B	0.63	2/3347 (0.1%)	0.77	2/4509 (0.0%)
1	C	0.65	2/3265 (0.1%)	0.79	3/4406 (0.1%)
1	D	0.68	4/3366 (0.1%)	0.81	5/4537 (0.1%)
1	E	0.70	2/3301 (0.1%)	0.80	4/4451 (0.1%)
1	F	0.64	1/3360 (0.0%)	0.79	1/4531 (0.0%)
All	All	0.69	20/20026 (0.1%)	0.80	21/26993 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	MSE	CG-SE	-10.82	1.58	1.95
1	A	359	MSE	CG-SE	-10.30	1.60	1.95
1	A	351	MSE	SE-CE	-9.47	1.39	1.95
1	A	323	VAL	C-O	8.32	1.39	1.23
1	D	351	MSE	SE-CE	8.23	2.44	1.95
1	A	359	MSE	SE-CE	-7.94	1.48	1.95
1	A	312	TYR	CE1-CZ	-7.30	1.29	1.38
1	E	351	MSE	SE-CE	7.29	2.38	1.95
1	C	361	CYS	CB-SG	-7.28	1.69	1.82
1	A	312	TYR	CG-CD2	5.96	1.46	1.39
1	A	232	MSE	SE-CE	-5.86	1.60	1.95
1	C	223	CYS	CB-SG	-5.71	1.72	1.81
1	F	351	MSE	SE-CE	5.64	2.28	1.95
1	B	361	CYS	CB-SG	-5.55	1.72	1.81
1	E	361	CYS	CB-SG	-5.47	1.73	1.81
1	D	284	MSE	SE-CE	-5.43	1.63	1.95
1	D	311	CYS	CB-SG	-5.31	1.73	1.81
1	D	223	CYS	CB-SG	-5.27	1.73	1.81
1	A	284	MSE	SE-CE	-5.18	1.64	1.95
1	B	311	CYS	CB-SG	-5.17	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	A	359	MSE	CG-SE-CE	-7.98	81.35	98.90
1	D	115	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	E	115	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	A	312	TYR	CE1-CZ-OH	-6.15	103.50	120.10
1	E	103	HIS	CB-CA-C	-6.08	98.24	110.40
1	E	115	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	E	60	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	115	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	60	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	115	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	312	TYR	OH-CZ-CE2	5.49	134.93	120.10
1	A	60	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	398	ASP	N-CA-C	5.41	125.62	111.00
1	A	60	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	F	343	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	140	LYS	CB-CA-C	-5.26	99.88	110.40
1	B	60	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	312	TYR	CB-CG-CD2	5.18	124.11	121.00
1	D	343	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	213	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3346	0	3223	20	0
1	B	3306	0	3145	21	0
1	C	3228	0	3051	27	0
1	D	3325	0	3192	23	0
1	E	3261	0	3136	29	0
1	F	3317	0	3167	25	0
2	A	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	6	0	8	0	0
2	D	12	0	16	0	0
2	F	6	0	8	0	0
3	A	183	0	0	4	0
3	B	97	0	0	1	0
3	C	73	0	0	1	0
3	D	168	0	0	0	0
3	E	140	0	0	3	0
3	F	93	0	0	1	0
All	All	20573	0	18962	142	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 4.

All (142) 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:351:MSE:SE	1:F:351:MSE:CE	2.28	1.31
1:E:351:MSE:SE	1:E:351:MSE:CE	2.38	1.22
1:D:351:MSE:SE	1:D:351:MSE:CE	2.44	1.15
1:A:309:ALA:HB2	1:A:351:MSE:HE1	1.39	1.02
1:A:309:ALA:HB2	1:A:351:MSE:CE	1.90	1.01
1:E:1:MSE:SE	1:E:17:ILE:HD11	2.26	0.86
1:F:1:MSE:SE	1:F:17:ILE:HD11	2.33	0.78
1:B:105:THR:O	1:B:140:LYS:NZ	2.19	0.72
1:D:188:ALA:O	1:D:221:GLN:NE2	2.22	0.72
1:A:190:ILE:HD12	1:A:220:THR:HG21	1.77	0.66
1:E:149[A]:THR:HG21	3:E:473:HOH:O	1.95	0.66
1:E:105:THR:O	1:E:140:LYS:NZ	2.29	0.66
1:C:367:ASN:HA	1:C:372:ASP:N	2.12	0.63
1:F:265:ILE:HG23	1:F:284:MSE:HE2	1.80	0.63
3:A:631:HOH:O	1:F:369:MSE:HE3	2.00	0.62
1:A:323:VAL:O	1:A:359:MSE:SE	2.68	0.61
1:F:117:LEU:HD22	1:F:121:ILE:HG21	1.83	0.61
1:C:342:ILE:HA	1:C:379:LEU:HD13	1.83	0.60
1:C:117:LEU:HD22	1:C:121:ILE:HG21	1.84	0.60
1:A:160:ARG:HG2	1:A:189:VAL:HG12	1.84	0.60
1:C:126:THR:HG23	1:C:134:LEU:HD21	1.84	0.59
1:B:407:THR:OG1	1:B:409:TYR:CD2	2.55	0.59
1:C:175:ALA:HA	1:C:178:MSE:HE2	1.85	0.59
1:B:175:ALA:HA	1:B:178:MSE:HE2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:THR:O	1:F:140:LYS:NZ	2.36	0.59
1:F:62:ASN:HD22	1:F:62:ASN:N	2.01	0.59
1:D:105:THR:O	1:D:140:LYS:NZ	2.29	0.58
1:C:367:ASN:HA	1:C:372:ASP:H	1.67	0.58
1:B:407:THR:OG1	1:B:409:TYR:CE2	2.56	0.58
1:B:188:ALA:O	1:B:221:GLN:NE2	2.37	0.57
1:C:366:THR:HG22	1:C:396:HIS:HB2	1.87	0.57
1:B:25:ASN:ND2	1:B:303:ASP:OD2	2.35	0.55
1:D:190:ILE:HD12	1:D:220:THR:HG21	1.87	0.55
1:B:322:LEU:HD22	1:B:390:PHE:CE2	2.40	0.55
1:A:342:ILE:HA	1:A:379:LEU:HD13	1.89	0.55
1:D:163:PRO:HA	1:D:164:ASN:CB	2.37	0.55
1:C:373:GLN:NE2	3:C:525:HOH:O	2.39	0.55
1:A:309:ALA:CB	1:A:351:MSE:CE	2.76	0.54
1:A:407:THR:HG23	1:A:409:TYR:H	1.72	0.53
1:E:25:ASN:O	1:E:44:ARG:HD3	2.09	0.53
1:A:53:LYS:NZ	3:A:562:HOH:O	2.41	0.53
1:E:64:VAL:HG21	1:E:302:VAL:HG11	1.89	0.53
1:B:178:MSE:O	1:B:182:THR:HG23	2.07	0.53
1:C:65:VAL:HG12	1:C:70:ASP:HB2	1.90	0.53
1:F:199:THR:O	1:F:203:VAL:HG23	2.09	0.53
1:C:178:MSE:O	1:C:182:THR:HG23	2.08	0.53
1:B:26:GLU:OE2	1:B:48:LYS:NZ	2.37	0.53
1:E:21:LEU:O	1:E:127:LYS:HE3	2.08	0.53
1:C:336:TYR:HB3	1:C:340:GLN:OE1	2.09	0.53
1:C:235:MSE:HE1	1:C:272:ALA:HA	1.91	0.52
1:C:1:MSE:SE	1:C:17:ILE:HD11	2.59	0.52
1:A:117:LEU:HD22	1:A:121:ILE:HG21	1.89	0.52
1:F:32:ARG:CZ	1:F:38:ALA:O	2.58	0.52
1:B:203:VAL:O	1:B:207:ASN:ND2	2.34	0.52
1:D:349:HIS:NE2	1:D:353:LYS:NZ	2.57	0.51
1:F:353:LYS:NZ	3:F:459:HOH:O	2.43	0.51
1:D:182:THR:HG22	1:D:436:PHE:CE1	2.46	0.51
1:E:149[A]:THR:OG1	1:E:424:ILE:HG21	2.11	0.51
1:E:178:MSE:O	1:E:182:THR:HG23	2.11	0.51
1:A:349:HIS:NE2	1:A:353:LYS:NZ	2.55	0.51
1:E:360:GLY:HA3	1:E:390:PHE:CE2	2.46	0.50
1:B:407:THR:HG23	1:B:409:TYR:H	1.76	0.50
1:E:312:TYR:CE2	1:E:351:MSE:HE3	2.47	0.50
1:A:105:THR:O	1:A:140:LYS:NZ	2.33	0.50
1:A:392:MSE:HE2	3:A:582:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:360:GLY:HA3	1:F:390:PHE:CE2	2.47	0.49
1:A:245:PHE:HA	1:A:285:TYR:O	2.11	0.49
1:E:407:THR:OG1	1:E:409:TYR:CE2	2.66	0.49
1:C:162:GLN:OE1	1:C:392[B]:MSE:HE2	2.12	0.49
1:B:1:MSE:SE	1:B:17:ILE:HD11	2.63	0.49
1:B:21:LEU:O	1:B:127:LYS:HE3	2.13	0.49
1:C:93:VAL:HG12	1:C:128:LEU:HD12	1.95	0.49
1:F:58:ASP:O	1:F:62:ASN:ND2	2.44	0.48
1:E:245:PHE:HA	1:E:285:TYR:O	2.12	0.48
1:E:312:TYR:HE2	1:E:351:MSE:HE3	1.78	0.48
1:C:28:LYS:NZ	1:C:347:GLU:OE1	2.28	0.48
1:A:290:GLN:HA	1:A:291:GLY:HA2	1.67	0.47
1:D:157:PHE:HB2	1:D:421:LEU:HD13	1.96	0.47
1:B:45:VAL:O	1:B:49:VAL:HG23	2.15	0.47
1:D:138:ALA:HB1	1:D:349:HIS:CE1	2.50	0.47
1:B:240:PRO:HA	3:B:522:HOH:O	2.14	0.47
1:B:139:LYS:HD2	1:C:418:LEU:HD12	1.97	0.46
1:D:21:LEU:O	1:D:127:LYS:HE3	2.16	0.46
1:D:168:ASP:OD2	1:D:195:VAL:HG23	2.16	0.46
1:D:360:GLY:HA3	1:D:390:PHE:CE2	2.50	0.46
1:B:235:MSE:HE1	1:B:272:ALA:HA	1.99	0.45
1:D:92:THR:HG22	1:D:95:GLU:CG	2.47	0.45
1:F:62:ASN:ND2	1:F:62:ASN:N	2.65	0.45
1:E:196:ASP:OD2	3:E:568:HOH:O	2.21	0.45
1:E:190:ILE:HD12	1:E:220:THR:HG21	1.97	0.45
1:D:437:SER:HA	1:D:443:THR:HG23	1.99	0.45
1:A:148:ASN:HB2	1:A:221:GLN:OE1	2.17	0.45
1:F:92:THR:HG22	1:F:95:GLU:CG	2.47	0.45
1:C:1:MSE:HE2	1:C:58:ASP:HB3	1.99	0.45
1:A:64:VAL:HG21	1:A:302:VAL:HG11	1.97	0.45
1:C:129:MSE:HE1	1:C:350:PHE:CE1	2.51	0.45
1:F:60:ARG:HD3	1:F:60:ARG:C	2.38	0.44
1:E:353:LYS:NZ	3:E:476:HOH:O	2.41	0.44
1:C:367:ASN:HA	1:C:372:ASP:HA	1.98	0.44
1:B:190:ILE:HD12	1:B:220:THR:HG21	2.00	0.44
1:C:218:VAL:HG22	1:C:430:TRP:CZ2	2.53	0.44
1:D:417:GLU:OE1	1:E:103:HIS:NE2	2.49	0.44
1:C:363:VAL:O	1:C:394:ILE:N	2.49	0.44
1:F:245:PHE:HA	1:F:285:TYR:O	2.17	0.44
1:F:65:VAL:HG12	1:F:70:ASP:HB2	1.99	0.44
1:C:188:ALA:O	1:C:221:GLN:NE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:GLU:HB3	1:F:351:MSE:HE1	1.99	0.43
1:B:92:THR:HG22	1:B:95:GLU:CG	2.48	0.43
1:C:245:PHE:HA	1:C:285:TYR:O	2.19	0.43
1:D:245:PHE:HA	1:D:285:TYR:O	2.19	0.43
1:F:329:PHE:CE1	1:F:341:VAL:HB	2.54	0.43
1:E:329:PHE:CZ	1:E:375:ASP:HB3	2.54	0.43
1:E:348:ASP:HA	1:E:351:MSE:HE2	2.00	0.42
1:E:149[A]:THR:HG22	1:E:221:GLN:OE1	2.20	0.42
1:D:163:PRO:HA	1:D:164:ASN:HB3	2.01	0.42
1:A:324[A]:ASN:CG	3:A:544:HOH:O	2.56	0.42
1:F:61:ASN:C	1:F:62:ASN:HD22	2.22	0.42
1:E:407:THR:HG23	1:E:409:TYR:H	1.83	0.42
1:D:308:GLU:HB3	1:D:351:MSE:HE1	2.02	0.42
1:B:343:ARG:HD2	1:B:347:GLU:OE2	2.20	0.42
1:C:51:LEU:HA	1:C:54:MSE:HE3	2.01	0.42
1:A:228:VAL:O	1:A:232:MSE:HG3	2.20	0.42
1:B:245:PHE:HA	1:B:285:TYR:O	2.20	0.42
1:D:174:LEU:HG	1:D:178:MSE:HE2	2.01	0.42
1:E:342:ILE:HA	1:E:379:LEU:HD13	2.01	0.42
1:C:6:ASN:O	1:C:8:PHE:N	2.53	0.42
1:D:187:ASP:HB3	1:D:427:PHE:CD1	2.55	0.42
1:D:139:LYS:HD2	1:E:418:LEU:HD12	2.02	0.41
1:E:64:VAL:HG21	1:E:302:VAL:CG1	2.50	0.41
1:A:1:MSE:SE	1:A:17:ILE:HD11	2.71	0.41
1:E:148:ASN:OD1	1:E:278:ALA:HA	2.20	0.41
1:F:265:ILE:CG2	1:F:284:MSE:HE2	2.48	0.41
1:F:360:GLY:HA3	1:F:390:PHE:CD2	2.56	0.41
1:D:41:ALA:O	1:D:45:VAL:HG23	2.21	0.41
1:F:343:ARG:HD2	1:F:347:GLU:CD	2.41	0.41
1:E:54:MSE:HB2	1:E:54:MSE:HE3	1.98	0.41
1:F:175:ALA:HA	1:F:178:MSE:HE2	2.03	0.41
1:C:147:ALA:HB3	1:C:221:GLN:HG2	2.04	0.40
1:F:178:MSE:O	1:F:182:THR:HG23	2.21	0.40
1:E:160:ARG:O	1:E:392:MSE:HE3	2.21	0.40
1:E:308:GLU:HB3	1:E:351:MSE:HE1	2.04	0.40
1:D:4:LYS:HA	1:D:12:TYR:O	2.21	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	434/455 (95%)	417 (96%)	13 (3%)	4 (1%)	21	13
1	B	432/455 (95%)	417 (96%)	15 (4%)	0	100	100
1	C	428/455 (94%)	407 (95%)	18 (4%)	3 (1%)	26	18
1	D	435/455 (96%)	416 (96%)	17 (4%)	2 (0%)	34	26
1	E	428/455 (94%)	414 (97%)	13 (3%)	1 (0%)	52	51
1	F	438/455 (96%)	416 (95%)	22 (5%)	0	100	100
All	All	2595/2730 (95%)	2487 (96%)	98 (4%)	10 (0%)	39	34

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	ASN
1	C	8	PHE
1	C	371	ALA
1	D	164	ASN
1	A	164	ASN
1	C	372	ASP
1	D	398	ASP
1	A	165	HIS
1	E	8	PHE
1	A	2	ILE

### 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	345/362 (95%)	340 (99%)	5 (1%)	74	80
1	B	335/362 (92%)	332 (99%)	3 (1%)	84	89
1	C	320/362 (88%)	316 (99%)	4 (1%)	76	82
1	D	340/362 (94%)	337 (99%)	3 (1%)	84	89
1	E	332/362 (92%)	328 (99%)	4 (1%)	78	83
1	F	336/362 (93%)	332 (99%)	4 (1%)	78	83
All	All	2008/2172 (92%)	1985 (99%)	23 (1%)	78	85

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	A	164	ASN
1	A	285	TYR
1	A	300	PHE
1	A	407	THR
1	B	60	ARG
1	B	125	VAL
1	B	404	TYR
1	C	43	GLU
1	C	60	ARG
1	C	139	LYS
1	C	285	TYR
1	D	60	ARG
1	D	285	TYR
1	D	398	ASP
1	E	44	ARG
1	E	60	ARG
1	E	285	TYR
1	E	366	THR
1	F	60	ARG
1	F	62	ASN
1	F	285	TYR
1	F	336	TYR

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

Mol	Chain	Res	Type
1	B	373	GLN
1	F	62	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	$\# Z  > 2$
2	GOL	A	455	-	5,5,5	0.33	0	5,5,5	0.46	0
2	GOL	A	456	-	5,5,5	0.40	0	5,5,5	0.76	0
2	GOL	C	455	-	5,5,5	0.51	0	5,5,5	0.58	0
2	GOL	D	455	-	5,5,5	0.36	0	5,5,5	0.17	0
2	GOL	D	456	-	5,5,5	0.41	0	5,5,5	0.50	0
2	GOL	F	455	-	5,5,5	0.43	0	5,5,5	0.24	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	GOL	A	455	-	-	0/4/4/4	0/0/0/0
2	GOL	A	456	-	-	0/4/4/4	0/0/0/0
2	GOL	C	455	-	-	0/4/4/4	0/0/0/0
2	GOL	D	455	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	456	-	-	0/4/4/4	0/0/0/0
2	GOL	F	455	-	-	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.

No monomer is involved in short contacts.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	424/455 (93%)	0.71	42 (9%) 9 15	21, 47, 79, 99	0
1	B	422/455 (92%)	0.72	47 (11%) 7 12	35, 51, 82, 104	0
1	C	422/455 (92%)	0.80	51 (12%) 6 9	36, 52, 82, 94	0
1	D	423/455 (92%)	0.60	36 (8%) 13 19	32, 48, 80, 93	0
1	E	420/455 (92%)	0.58	33 (7%) 15 22	30, 48, 81, 88	0
1	F	428/455 (94%)	0.75	49 (11%) 7 11	35, 51, 81, 89	0
All	All	2539/2730 (93%)	0.70	258 (10%) 9 15	21, 50, 81, 104	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	SER	9.3
1	C	400	VAL	9.1
1	A	329	PHE	8.5
1	E	329	PHE	8.0
1	C	167	THR	8.0
1	E	400	VAL	7.3
1	C	402	LEU	7.3
1	C	334	TYR	7.3
1	C	404	TYR	6.3
1	B	166	PRO	6.2
1	C	447	GLY	6.1
1	B	329	PHE	5.9
1	B	195	VAL	5.9
1	D	330	ILE	5.7
1	B	400	VAL	5.7
1	C	336	TYR	5.7
1	A	397	GLY	5.6
1	B	449	ALA	5.6
1	C	173	ILE	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	189	VAL	5.1
1	D	397	GLY	4.9
1	A	402	LEU	4.8
1	E	453	LEU	4.7
1	C	397	GLY	4.6
1	C	9	GLY	4.6
1	D	336	TYR	4.5
1	D	398	ASP	4.4
1	C	166	PRO	4.4
1	B	403	ASN	4.4
1	B	404	TYR	4.4
1	E	189	VAL	4.4
1	F	189	VAL	4.4
1	F	396	HIS	4.4
1	F	159	ALA	4.3
1	F	451	ILE	4.3
1	F	258	PHE	4.3
1	B	167	THR	4.3
1	B	402	LEU	4.2
1	F	453	LEU	4.2
1	C	366	THR	4.2
1	C	448	ASP	4.1
1	F	2	ILE	4.1
1	C	396	HIS	4.1
1	B	371	ALA	4.1
1	A	190	ILE	4.1
1	C	289	GLY	4.1
1	B	368	HIS	4.1
1	E	8	PHE	4.1
1	F	452	PHE	4.0
1	C	364	CYS	3.9
1	A	336	TYR	3.9
1	B	396	HIS	3.9
1	B	33[A]	LEU	3.9
1	D	285	TYR	3.8
1	D	399	ASP	3.8
1	C	453	LEU	3.8
1	C	449	ALA	3.7
1	F	332	PRO	3.7
1	C	390	PHE	3.7
1	B	190	ILE	3.7
1	F	397	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	159	ALA	3.7
1	A	189	VAL	3.6
1	D	11	THR	3.6
1	C	168	ASP	3.6
1	A	399	ASP	3.6
1	A	161	LEU	3.6
1	B	336	TYR	3.6
1	B	372	ASP	3.5
1	D	446	ALA	3.5
1	C	189	VAL	3.5
1	D	402	LEU	3.5
1	D	400	VAL	3.4
1	D	243	LEU	3.4
1	B	12	TYR	3.4
1	A	367	ASN	3.4
1	F	333	GLU	3.4
1	A	366	THR	3.4
1	C	34	ALA	3.4
1	C	406	THR	3.3
1	C	8	PHE	3.3
1	B	445	ARG	3.3
1	A	33	LEU	3.3
1	F	160	ARG	3.3
1	B	164	ASN	3.3
1	D	371	ALA	3.3
1	C	391	ILE	3.3
1	C	403	ASN	3.3
1	A	400	VAL	3.3
1	F	34	ALA	3.2
1	B	161	LEU	3.2
1	D	324[A]	ASN	3.2
1	F	391	ILE	3.2
1	A	21	LEU	3.2
1	C	446	ALA	3.2
1	B	365	TYR	3.2
1	C	160	ARG	3.2
1	B	367	ASN	3.2
1	E	403	ASN	3.2
1	D	396	HIS	3.1
1	F	9	GLY	3.1
1	F	30	GLY	3.1
1	C	36	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	366	THR	3.1
1	D	189	VAL	3.1
1	F	195	VAL	3.1
1	A	398	ASP	3.0
1	C	365	TYR	3.0
1	A	159	ALA	3.0
1	C	33	LEU	3.0
1	B	395	PRO	3.0
1	E	190	ILE	3.0
1	D	366	THR	3.0
1	C	451	ILE	2.9
1	F	174	LEU	2.9
1	D	367	ASN	2.9
1	E	7	LEU	2.9
1	C	405	GLN	2.9
1	D	390	PHE	2.9
1	F	212	PHE	2.9
1	A	242	GLY	2.9
1	F	331	GLY	2.9
1	F	12	TYR	2.9
1	B	448	ASP	2.9
1	E	243	LEU	2.9
1	D	439[A]	ASN	2.9
1	B	10	HIS	2.8
1	C	186	GLY	2.8
1	D	190	ILE	2.8
1	B	335	LEU	2.8
1	E	6	ASN	2.8
1	C	68	GLU	2.8
1	A	164	ASN	2.8
1	B	188	ALA	2.8
1	B	399	ASP	2.8
1	C	368	HIS	2.7
1	A	291	GLY	2.7
1	F	161	LEU	2.7
1	F	188	ALA	2.7
1	A	223	CYS	2.7
1	E	324	ASN	2.7
1	A	20	VAL	2.7
1	A	324[A]	ASN	2.7
1	E	391	ILE	2.7
1	C	188	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	390	PHE	2.7
1	E	397	GLY	2.7
1	E	2	ILE	2.6
1	E	396	HIS	2.6
1	A	188	ALA	2.6
1	B	406	THR	2.6
1	E	223	CYS	2.6
1	B	258	PHE	2.6
1	E	10	HIS	2.6
1	C	407	THR	2.6
1	F	69	THR	2.6
1	B	285	TYR	2.6
1	A	9	GLY	2.6
1	B	322	LEU	2.6
1	A	396	HIS	2.6
1	A	7	LEU	2.6
1	E	188	ALA	2.6
1	E	299	HIS	2.6
1	D	329	PHE	2.5
1	C	190	ILE	2.5
1	F	166	PRO	2.5
1	C	258	PHE	2.5
1	D	126	THR	2.5
1	A	368	HIS	2.5
1	D	7	LEU	2.5
1	E	399	ASP	2.5
1	B	391	ILE	2.5
1	F	454	LYS	2.5
1	F	201	SER	2.5
1	E	406	THR	2.5
1	D	391	ILE	2.5
1	A	371	ALA	2.5
1	E	160	ARG	2.5
1	A	404	TYR	2.5
1	F	390	PHE	2.5
1	E	402	LEU	2.5
1	A	185	ILE	2.5
1	C	35	GLY	2.4
1	F	402	LEU	2.4
1	E	164	ASN	2.4
1	F	330	ILE	2.4
1	C	322	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	450	SER	2.4
1	F	175	ALA	2.4
1	E	404	TYR	2.4
1	A	160	ARG	2.4
1	A	125	VAL	2.4
1	F	446	ALA	2.4
1	B	121	ILE	2.4
1	B	452	PHE	2.4
1	D	286	PHE	2.4
1	A	10	HIS	2.3
1	E	323	VAL	2.3
1	F	370	LYS	2.3
1	D	191	GLY	2.3
1	F	450	SER	2.3
1	A	403	ASN	2.3
1	F	11	THR	2.3
1	F	190	ILE	2.3
1	D	382	LEU	2.3
1	E	224	VAL	2.3
1	F	91	TRP	2.3
1	B	451	ILE	2.3
1	A	126	THR	2.3
1	B	222	THR	2.3
1	F	257	ALA	2.3
1	B	160	ARG	2.3
1	C	161	LEU	2.3
1	E	346	LEU	2.3
1	F	13	GLN	2.2
1	F	361	CYS	2.2
1	E	185	ILE	2.2
1	B	191	GLY	2.2
1	C	371	ALA	2.2
1	F	10	HIS	2.2
1	F	170	PRO	2.2
1	E	126	THR	2.2
1	B	9	GLY	2.2
1	C	395	PRO	2.2
1	A	306	THR	2.2
1	D	161	LEU	2.2
1	F	199	THR	2.2
1	F	66	PRO	2.2
1	D	360	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	185	ILE	2.2
1	E	322	LEU	2.1
1	B	450	SER	2.1
1	C	172	GLY	2.1
1	F	68	GLU	2.1
1	A	323	VAL	2.1
1	B	34	ALA	2.1
1	C	2	ILE	2.1
1	F	126	THR	2.1
1	A	224	VAL	2.1
1	A	222	THR	2.1
1	D	125	VAL	2.1
1	D	381	VAL	2.1
1	C	367	ASN	2.1
1	A	391	ILE	2.1
1	F	88	ILE	2.1
1	B	243	LEU	2.1
1	F	171	ASP	2.1
1	B	447	GLY	2.1
1	D	2	ILE	2.0
1	A	243	LEU	2.0
1	D	403	ASN	2.0
1	A	186	GLY	2.0
1	F	121	ILE	2.0
1	C	444	SER	2.0
1	D	322	LEU	2.0
1	E	161	LEU	2.0
1	D	162	GLN	2.0
1	C	6	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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	GOL	F	455	6/6	0.87	0.18	2.78	55,60,62,70	0
2	GOL	A	456	6/6	0.91	0.23	2.68	46,48,59,61	0
2	GOL	C	455	6/6	0.93	0.25	2.11	48,57,68,76	0
2	GOL	D	455	6/6	0.85	0.18	1.33	48,54,59,67	0
2	GOL	D	456	6/6	0.89	0.19	0.73	45,50,52,56	0
2	GOL	A	455	6/6	0.86	0.14	0.40	47,58,64,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.