



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:17 AM EDT

PDB ID : 2QEZ / pdb_00002qez
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

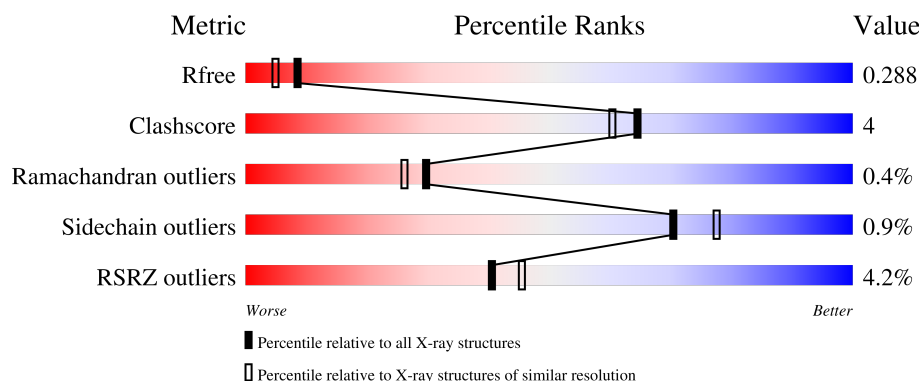
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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_{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	455	5% 85% 9% • •
1	B	455	3% 85% 10% •
1	C	455	4% 84% 11% • •
1	D	455	3% 85% 10% • •
1	E	455	4% 85% 10% • 5%

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Mol	Chain	Length	Quality of chain
1	F	455	4% 88% 8% . .

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	-	expression tag	UNP Q720Q3
B	0	GLY	-	expression tag	UNP Q720Q3
C	0	GLY	-	expression tag	UNP Q720Q3
D	0	GLY	-	expression tag	UNP Q720Q3
E	0	GLY	-	expression tag	UNP Q720Q3
F	0	GLY	-	expression tag	UNP Q720Q3

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

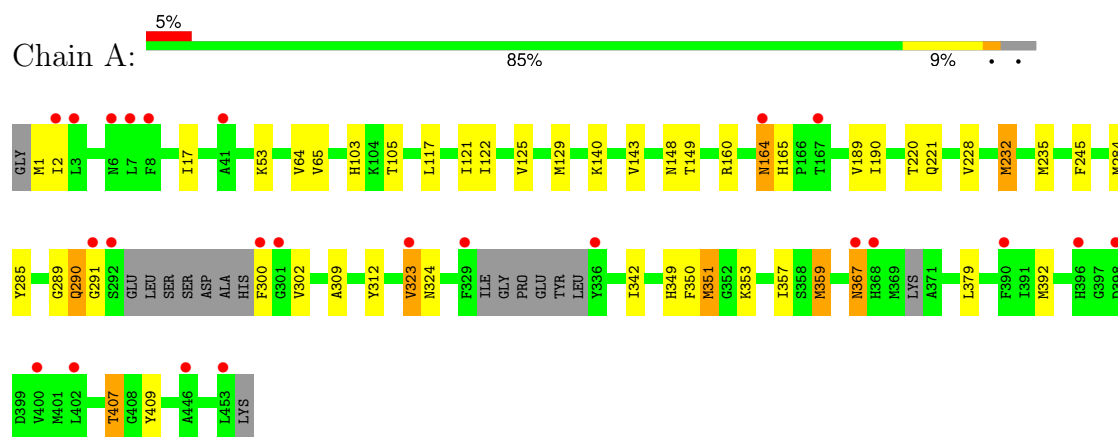
- Molecule 3 is water.

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		

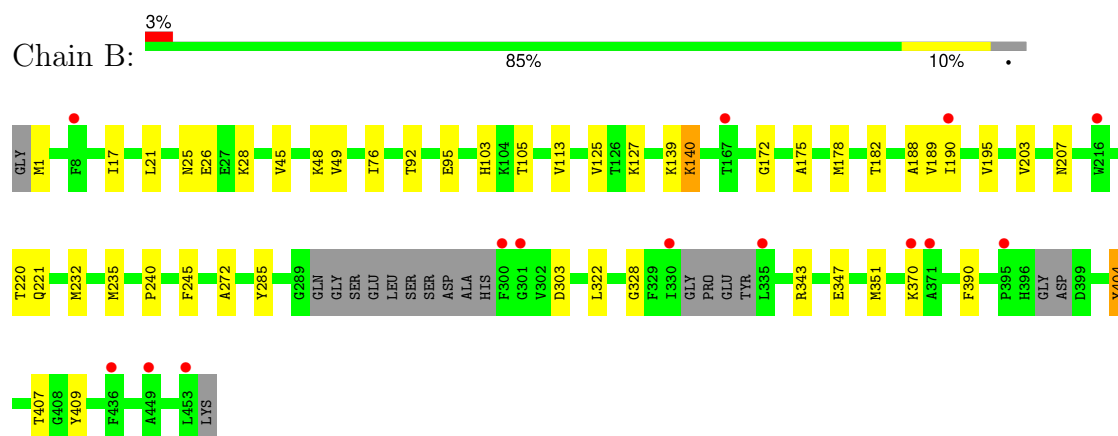
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

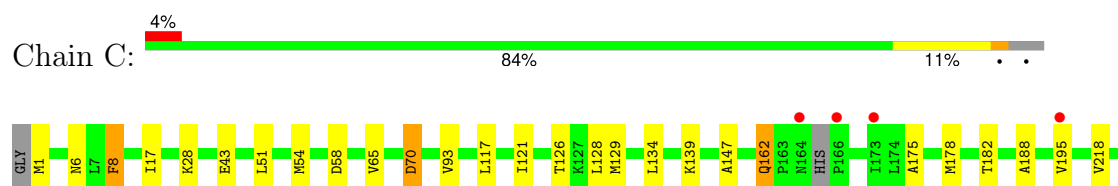
- Molecule 1: Ethanolamine ammonia-lyase heavy chain

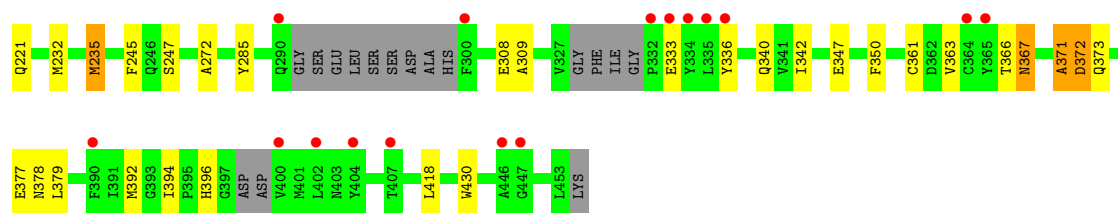


- Molecule 1: Ethanolamine ammonia-lyase heavy chain

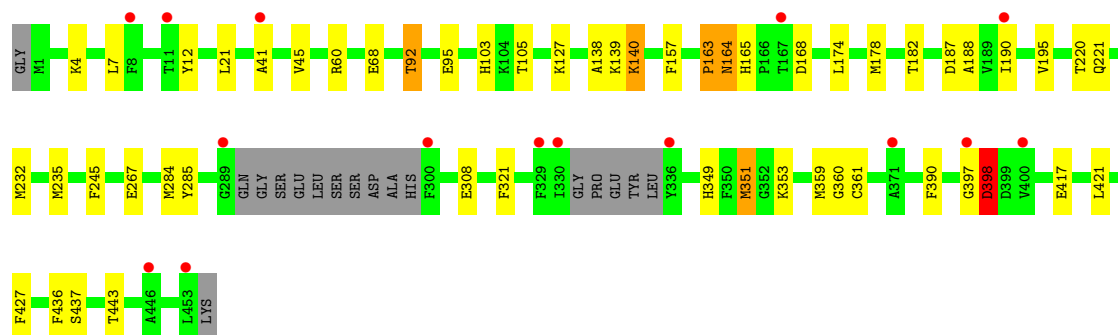
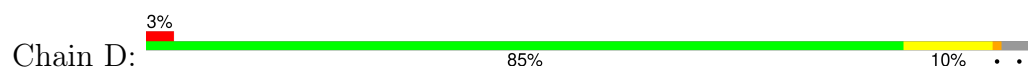


- Molecule 1: Ethanolamine ammonia-lyase heavy chain

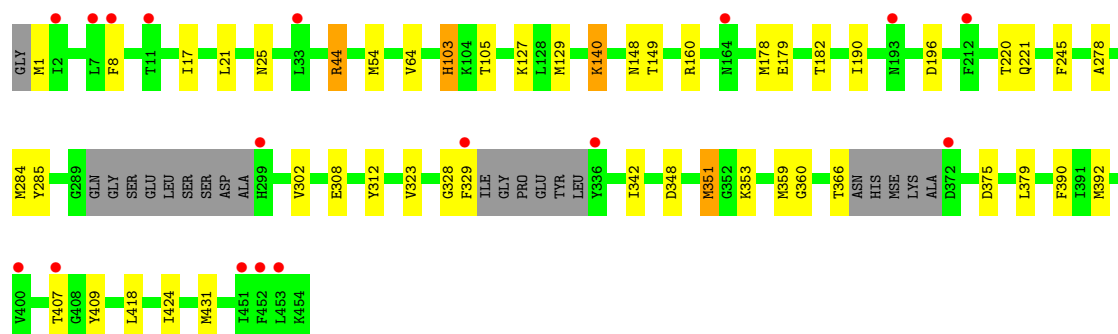
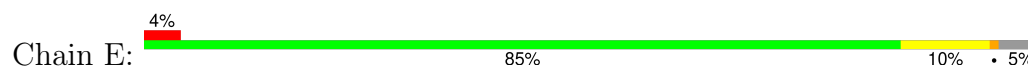




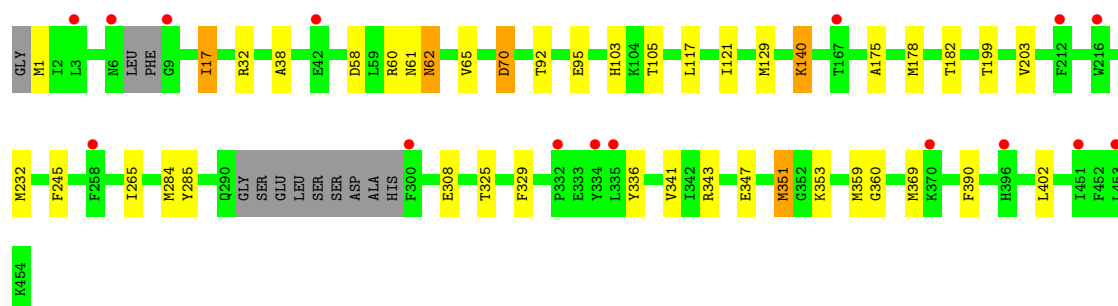
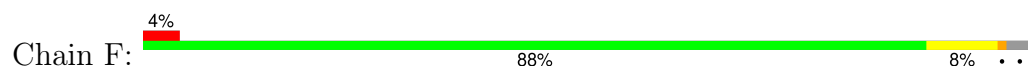
• Molecule 1: Ethanolamine ammonia-lyase heavy chain



• 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, α , β , γ	188.33Å 223.70Å 65.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.21 – 2.15 29.21 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.21-2.15) 99.7 (29.21-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005, PHENIX	Depositor
R, R_{free}	0.228 , 0.279 0.238 , 0.288	Depositor DCC
R_{free} test set	8094 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20573	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	1.12	12/3387 (0.4%)	1.07	8/4559 (0.2%)
1	B	0.83	2/3347 (0.1%)	1.07	7/4509 (0.2%)
1	C	0.85	4/3265 (0.1%)	1.04	7/4406 (0.2%)
1	D	0.94	4/3366 (0.1%)	1.07	12/4537 (0.3%)
1	E	0.96	6/3301 (0.2%)	1.04	5/4451 (0.1%)
1	F	0.88	4/3360 (0.1%)	1.04	7/4531 (0.2%)
All	All	0.94	32/20026 (0.2%)	1.06	46/26993 (0.2%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	351	MSE	SE-CE	-18.63	1.39	1.95
1	D	351	MSE	SE-CE	16.20	2.44	1.95
1	A	359	MSE	SE-CE	-15.61	1.48	1.95
1	E	351	MSE	SE-CE	14.33	2.38	1.95
1	A	323	VAL	C-O	12.69	1.39	1.24
1	A	351	MSE	CG-SE	-12.27	1.58	1.95
1	A	359	MSE	CG-SE	-11.68	1.60	1.95
1	A	232	MSE	SE-CE	-11.53	1.60	1.95
1	F	351	MSE	SE-CE	11.09	2.28	1.95
1	D	284	MSE	SE-CE	-10.69	1.63	1.95
1	A	284	MSE	SE-CE	-10.19	1.64	1.95
1	D	235	MSE	SE-CE	-8.08	1.71	1.95
1	D	359	MSE	SE-CE	-7.72	1.72	1.95
1	E	359	MSE	SE-CE	-6.90	1.74	1.95
1	E	129	MSE	SE-CE	-6.31	1.76	1.95
1	E	284	MSE	SE-CE	-6.27	1.76	1.95
1	B	351	MSE	SE-CE	6.21	2.14	1.95
1	A	129	MSE	SE-CE	-6.15	1.76	1.95
1	E	431	MSE	SE-CE	-6.09	1.77	1.95
1	F	359	MSE	SE-CE	-5.97	1.77	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	MSE	SE-CE	-5.96	1.77	1.95
1	C	367	ASN	N-CA	5.80	1.53	1.46
1	F	232	MSE	SE-CE	-5.44	1.79	1.95
1	C	235	MSE	SE-CE	-5.42	1.79	1.95
1	E	351	MSE	CG-SE	-5.33	1.79	1.95
1	C	367	ASN	CA-C	5.26	1.59	1.52
1	A	149	THR	CA-CB	-5.17	1.45	1.53
1	B	232	MSE	SE-CE	-5.17	1.79	1.95
1	A	367	ASN	N-CA	5.15	1.52	1.46
1	F	129	MSE	SE-CE	-5.14	1.80	1.95
1	C	232	MSE	SE-CE	-5.05	1.80	1.95
1	A	65	VAL	CA-CB	-5.00	1.50	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	359	MSE	CG-SE-CE	-7.99	81.35	98.92
1	E	103	HIS	CB-CA-C	-7.32	98.24	110.68
1	C	195	VAL	N-CA-C	-6.57	104.36	110.53
1	E	328	GLY	N-CA-C	6.50	122.84	111.14
1	D	103	HIS	CB-CA-C	-6.48	100.45	110.81
1	C	371	ALA	CA-C-N	6.43	133.27	121.70
1	C	371	ALA	C-N-CA	6.43	133.27	121.70
1	D	163	PRO	CA-C-N	6.39	133.20	121.70
1	D	163	PRO	C-N-CA	6.39	133.20	121.70
1	B	103	HIS	CB-CA-C	-6.29	100.74	110.81
1	F	70	ASP	N-CA-C	6.25	118.70	108.52
1	D	397	GLY	CA-C-N	6.23	132.91	121.70
1	D	397	GLY	C-N-CA	6.23	132.91	121.70
1	B	189	VAL	CB-CA-C	-6.20	103.18	111.80
1	E	323	VAL	N-CA-C	-6.01	99.40	108.17
1	D	165	HIS	CA-C-N	5.85	125.33	119.24
1	D	165	HIS	C-N-CA	5.85	125.33	119.24
1	B	328	GLY	N-CA-C	5.81	120.74	110.80
1	B	140	LYS	CB-CA-C	-5.81	100.80	110.68
1	C	333	GLU	N-CA-C	5.81	119.19	111.75
1	F	359	MSE	N-CA-C	5.80	117.97	108.52
1	A	122	ILE	N-CA-C	-5.75	104.90	110.42
1	C	247	SER	N-CA-C	-5.57	101.39	110.20
1	A	312	TYR	CE1-CZ-OH	-5.46	103.50	119.90
1	D	140	LYS	CB-CA-C	-5.46	99.88	110.46
1	B	370	LYS	N-CA-C	-5.45	99.20	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361	CYS	N-CA-C	5.39	117.40	108.13
1	A	290	GLN	N-CA-C	5.35	117.96	109.24
1	F	140	LYS	CB-CA-C	-5.35	100.73	110.63
1	A	289	GLY	N-CA-C	-5.33	104.74	111.72
1	D	321	PHE	N-CA-C	-5.24	105.63	112.23
1	E	359	MSE	N-CA-C	5.23	117.77	109.24
1	D	398	ASP	N-CA-C	5.22	125.62	111.00
1	E	140	LYS	CB-CA-C	-5.19	101.02	110.63
1	A	367	ASN	N-CA-CB	5.18	119.24	110.49
1	D	92	THR	CB-CA-C	5.17	118.88	109.83
1	A	103	HIS	CB-CA-C	-5.12	102.62	110.81
1	B	195	VAL	N-CA-C	-5.09	105.88	110.82
1	F	402	LEU	N-CA-C	-5.08	105.82	111.36
1	F	103	HIS	CB-CA-C	-5.07	102.69	110.81
1	F	325	THR	N-CA-C	-5.07	103.98	110.53
1	F	17	ILE	N-CA-C	-5.03	105.64	110.72
1	B	76	ILE	CB-CA-C	-5.02	105.54	111.97
1	A	312	TYR	OH-CZ-CE2	5.01	134.93	119.90
1	C	70	ASP	N-CA-C	5.01	117.13	109.07
1	C	361	CYS	N-CA-C	5.01	116.19	107.93

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	22	0
1	B	3306	0	3145	25	0
1	C	3228	0	3051	29	0
1	D	3325	0	3192	24	0
1	E	3261	0	3136	30	0
1	F	3317	0	3167	26	0
2	A	12	0	16	0	0
2	C	6	0	8	0	0
2	D	12	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	153	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 (153) 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:CE	1:D:351:MSE:SE	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:342:ILE:HA	1:A:379:LEU:HD13	1.89	0.55
1:B:322:LEU:HD22	1:B:390:PHE:CE2	2.40	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:349:HIS:NE2	1:A:353:LYS:NZ	2.55	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:C:336:TYR:HB3	1:C:340:GLN:OE1	2.09	0.53
1:E:21:LEU:O	1:E:127:LYS:HE3	2.08	0.53
1:C:1:MSE:SE	1:C:17:ILE:HD11	2.59	0.52
1:C:235:MSE:HE1	1:C:272:ALA:HA	1.91	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:C:28:LYS:NZ	1:C:347:GLU:OE1	2.28	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: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:A:105:THR:O	1:A:140:LYS:NZ	2.33	0.50
1:E:312:TYR:CE2	1:E:351:MSE:HE3	2.47	0.50
1:A:392:MSE:HE2	3:A:582:HOH:O	2.12	0.49
1:F:360:GLY:HA3	1:F:390:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:60:ARG:HD3	1:F:60:ARG:C	2.38	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: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:A:324[A]:ASN:CG	3:A:544:HOH:O	2.56	0.47
1:B:45:VAL:O	1:B:49:VAL:HG23	2.15	0.47
1:F:61:ASN:C	1:F:62:ASN:HD22	2.22	0.47
1:B:240:PRO:HA	3:B:522:HOH:O	2.14	0.47
1:D:138:ALA:HB1	1:D:349:HIS:CE1	2.50	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:E:196:ASP:OD2	3:E:568:HOH:O	2.21	0.45
1:F:62:ASN:N	1:F:62:ASN:ND2	2.65	0.45
1:E:190:ILE:HD12	1:E:220:THR:HG21	1.97	0.45
1:A:148:ASN:HB2	1:A:221:GLN:OE1	2.17	0.45
1:D:437:SER:HA	1:D:443:THR:HG23	1.99	0.45
1:F:92:THR:HG22	1:F:95:GLU:CG	2.47	0.45
1:A:64:VAL:HG21	1:A:302:VAL:HG11	1.97	0.45
1:C:1:MSE:HE2	1:C:58:ASP:HB3	1.99	0.45
1:C:129:MSE:HE1	1:C:350:PHE:CE1	2.51	0.45
1:F:343:ARG:HD2	1:F:347:GLU:CD	2.41	0.44
1:E:353:LYS:NZ	3:E:476:HOH:O	2.41	0.44
1:B:190:ILE:HD12	1:B:220:THR:HG21	2.00	0.44
1:C:367:ASN:HA	1:C:372:ASP:HA	1.98	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:A:143:VAL:HG11	1:A:357:ILE:C	2.43	0.44
1:F:245:PHE:HA	1:F:285:TYR:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:VAL:HG12	1:F:70:ASP:HB2	1.99	0.44
1:B:92:THR:HG22	1:B:95:GLU:CD	2.43	0.43
1:C:188:ALA:O	1:C:221:GLN:NE2	2.51	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:F:308:GLU:HB3	1:F:351:MSE:HE1	1.99	0.43
1:B:172:GLY:O	1:B:404:TYR:OH	2.32	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:B:404:TYR:CD1	1:B:404:TYR:C	2.96	0.43
1:E:329:PHE:CZ	1:E:375:ASP:HB3	2.54	0.43
1:A:350:PHE:O	1:A:351:MSE:C	2.61	0.43
1:E:348:ASP:HA	1:E:351:MSE:HE2	2.00	0.42
1:D:163:PRO:HA	1:D:164:ASN:HB3	2.01	0.42
1:E:149[A]:THR:HG22	1:E:221:GLN:OE1	2.20	0.42
1:B:28:LYS:NZ	1:B:347:GLU:OE1	2.43	0.42
1:E:407:THR:HG23	1:E:409:TYR:H	1.83	0.42
1:B:343:ARG:HD2	1:B:347:GLU:OE2	2.20	0.42
1:D:308:GLU:HB3	1:D:351:MSE:HE1	2.02	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:C:51:LEU:HA	1:C:54:MSE:HE3	2.01	0.42
1:D:174:LEU:HG	1:D:178:MSE:HE2	2.01	0.42
1:E:179:GLU:O	1:E:182:THR:OG1	2.35	0.42
1:C:6:ASN:O	1:C:8:PHE:N	2.53	0.42
1:E:342:ILE:HA	1:E:379:LEU:HD13	2.01	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:A:1:MSE:SE	1:A:17:ILE:HD11	2.71	0.41
1:E:64:VAL:HG21	1:E:302:VAL:CG1	2.50	0.41
1:E:148:ASN:OD1	1:E:278:ALA:HA	2.20	0.41
1:C:308:GLU:O	1:C:309:ALA:C	2.64	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:C:377:GLU:O	1:C:378:ASN:C	2.64	0.41
1:D:41:ALA:O	1:D:45:VAL:HG23	2.21	0.41
1:E:54:MSE:HE3	1:E:54:MSE:HB2	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:D:232:MSE:HE1	1:D:267:GLU:CD	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:ARG:O	1:E:392:MSE:HE3	2.21	0.40
1:D:4:LYS:HA	1:D:12:TYR:O	2.21	0.40
1:E:308:GLU:HB3	1:E:351:MSE:HE1	2.04	0.40
1:F:61:ASN:C	1:F:62:ASN:ND2	2.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/455 (95%)	417 (96%)	13 (3%)	4 (1%)	14	9
1	B	432/455 (95%)	417 (96%)	15 (4%)	0	100	100
1	C	428/455 (94%)	407 (95%)	18 (4%)	3 (1%)	18	13
1	D	435/455 (96%)	416 (96%)	17 (4%)	2 (0%)	24	20
1	E	428/455 (94%)	414 (97%)	13 (3%)	1 (0%)	43	44
1	F	438/455 (96%)	416 (95%)	22 (5%)	0	100	100
All	All	2595/2730 (95%)	2487 (96%)	98 (4%)	10 (0%)	30	26

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

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Mol	Chain	Res	Type
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%)	341 (99%)	4 (1%)	63	70
1	B	335/362 (92%)	332 (99%)	3 (1%)	70	77
1	C	320/362 (88%)	317 (99%)	3 (1%)	70	77
1	D	340/362 (94%)	336 (99%)	4 (1%)	63	70
1	E	332/362 (92%)	330 (99%)	2 (1%)	78	84
1	F	336/362 (93%)	334 (99%)	2 (1%)	78	84
All	All	2008/2172 (92%)	1990 (99%)	18 (1%)	70	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	A	164	ASN
1	A	300	PHE
1	A	407	THR
1	B	113	VAL
1	B	125	VAL
1	B	404	TYR
1	C	43	GLU
1	C	139	LYS
1	C	162	GLN
1	D	7	LEU
1	D	60	ARG
1	D	68	GLU
1	D	398	ASP
1	E	44	ARG
1	E	366	THR

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Mol	Chain	Res	Type
1	F	62	ASN
1	F	336	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	290	GLN
1	A	367	ASN
1	B	13	GLN
1	B	90	ASN
1	B	304	GLN
1	B	373	GLN
1	C	324	ASN
1	C	374	ASN
1	C	389	ASN
1	C	403	ASN
1	D	162	GLN
1	D	221	GLN
1	D	304	GLN
1	D	389	ASN
1	E	274	GLN
1	F	10	HIS
1	F	62	ASN
1	F	79	GLN
1	F	274	GLN

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 oligosaccharides 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	D	455	-	5,5,5	0.42	0	5,5,5	0.16	0
2	GOL	A	455	-	5,5,5	0.40	0	5,5,5	0.44	0
2	GOL	C	455	-	5,5,5	0.52	0	5,5,5	0.66	0
2	GOL	F	455	-	5,5,5	0.45	0	5,5,5	0.24	0
2	GOL	A	456	-	5,5,5	0.42	0	5,5,5	0.85	0
2	GOL	D	456	-	5,5,5	0.42	0	5,5,5	0.59	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	D	455	-	-	1/4/4/4	-
2	GOL	A	455	-	-	0/4/4/4	-
2	GOL	C	455	-	-	2/4/4/4	-
2	GOL	F	455	-	-	0/4/4/4	-
2	GOL	A	456	-	-	3/4/4/4	-
2	GOL	D	456	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	455	GOL	C1-C2-C3-O3
2	A	456	GOL	C1-C2-C3-O3
2	C	455	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	456	GOL	O2-C2-C3-O3
2	D	455	GOL	O1-C1-C2-O2
2	A	456	GOL	O1-C1-C2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	424/455 (93%)	0.49	24 (5%)	29	33	11, 47, 79, 99	3 (0%)
1	B	422/455 (92%)	0.44	14 (3%)	49	53	23, 51, 82, 104	3 (0%)
1	C	422/455 (92%)	0.54	20 (4%)	36	41	36, 52, 82, 94	0
1	D	423/455 (92%)	0.43	15 (3%)	47	51	20, 48, 80, 93	3 (0%)
1	E	420/455 (92%)	0.43	17 (4%)	42	47	15, 48, 81, 88	2 (0%)
1	F	428/455 (94%)	0.55	16 (3%)	45	49	24, 51, 81, 89	1 (0%)
All	All	2539/2730 (93%)	0.48	106 (4%)	40	45	11, 50, 81, 104	12 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	300	PHE	5.1
1	E	329	PHE	5.0
1	A	329	PHE	4.6
1	B	371	ALA	4.3
1	D	371	ALA	4.2
1	F	300	PHE	4.0
1	B	300	PHE	3.9
1	E	8	PHE	3.9
1	A	400	VAL	3.8
1	B	335	LEU	3.7
1	F	6	ASN	3.6
1	A	7	LEU	3.6
1	F	453	LEU	3.6
1	A	300	PHE	3.4
1	B	330	ILE	3.3
1	F	335	LEU	3.3
1	C	332	PRO	3.3
1	C	173	ILE	3.3
1	A	3	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	SER	3.2
1	F	334	TYR	3.1
1	F	9	GLY	3.0
1	A	402	LEU	3.0
1	A	2	ILE	3.0
1	C	336	TYR	3.0
1	C	334	TYR	3.0
1	C	404	TYR	3.0
1	E	336	TYR	3.0
1	F	370	LYS	3.0
1	A	301	GLY	2.9
1	A	8	PHE	2.9
1	C	400	VAL	2.8
1	D	453	LEU	2.8
1	C	166	PRO	2.8
1	F	212	PHE	2.8
1	B	449	ALA	2.8
1	D	11	THR	2.8
1	C	300	PHE	2.7
1	C	390	PHE	2.7
1	A	167	THR	2.7
1	C	407	THR	2.7
1	D	397	GLY	2.6
1	D	446	ALA	2.6
1	E	299	HIS	2.6
1	E	453	LEU	2.6
1	E	400	VAL	2.6
1	A	446	ALA	2.6
1	E	407	THR	2.6
1	C	335	LEU	2.6
1	D	8	PHE	2.6
1	A	164	ASN	2.5
1	E	451	ILE	2.5
1	B	370	LYS	2.5
1	D	289	GLY	2.5
1	C	446	ALA	2.4
1	B	453	LEU	2.4
1	A	6	ASN	2.4
1	A	41	ALA	2.4
1	C	164	ASN	2.4
1	E	164	ASN	2.3
1	A	398	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	193	ASN	2.3
1	D	330	ILE	2.3
1	D	167	THR	2.3
1	F	332	PRO	2.3
1	D	400	VAL	2.3
1	C	402	LEU	2.3
1	B	8	PHE	2.2
1	D	41	ALA	2.2
1	D	336	TYR	2.2
1	A	368	HIS	2.2
1	A	396	HIS	2.2
1	C	290	GLN	2.2
1	A	390	PHE	2.2
1	C	447	GLY	2.2
1	C	333	GLU	2.1
1	D	329	PHE	2.1
1	C	195	VAL	2.1
1	A	291	GLY	2.1
1	B	436	PHE	2.1
1	E	212	PHE	2.1
1	F	258	PHE	2.1
1	F	3	LEU	2.1
1	A	336	TYR	2.1
1	F	396	HIS	2.1
1	B	190	ILE	2.1
1	D	190	ILE	2.1
1	E	2	ILE	2.1
1	F	451	ILE	2.1
1	E	452	PHE	2.1
1	F	42	GLU	2.1
1	B	395	PRO	2.1
1	F	167	THR	2.1
1	B	301	GLY	2.1
1	B	216	TRP	2.1
1	A	453	LEU	2.0
1	E	33	LEU	2.0
1	A	367	ASN	2.0
1	E	372	ASP	2.0
1	B	167	THR	2.0
1	E	11	THR	2.0
1	A	323	VAL	2.0
1	F	216	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	7	LEU	2.0
1	C	364	CYS	2.0
1	C	365	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	D	455	6/6	0.80	0.15	48,54,59,67	0
2	GOL	A	456	6/6	0.83	0.17	46,48,59,61	0
2	GOL	F	455	6/6	0.83	0.16	55,60,62,70	0
2	GOL	D	456	6/6	0.84	0.12	45,50,52,56	0
2	GOL	A	455	6/6	0.84	0.14	47,58,64,70	0
2	GOL	C	455	6/6	0.87	0.17	48,57,68,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.