



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 PM UTC

PDB ID : 1PZ3 / pdb_00001pz3
Title : Crystal structure of a family 51 (GH51) alpha-L-arabinofuranosidase from *Geobacillus stearothermophilus* T6
Authors : Hoevel, K.; Shallom, D.; Niefind, K.; Belakhov, V.; Shoham, G.; Baasov, T.; Shoham, Y.; Schomburg, D.
Deposited on : 2003-07-09
Resolution : 1.75 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

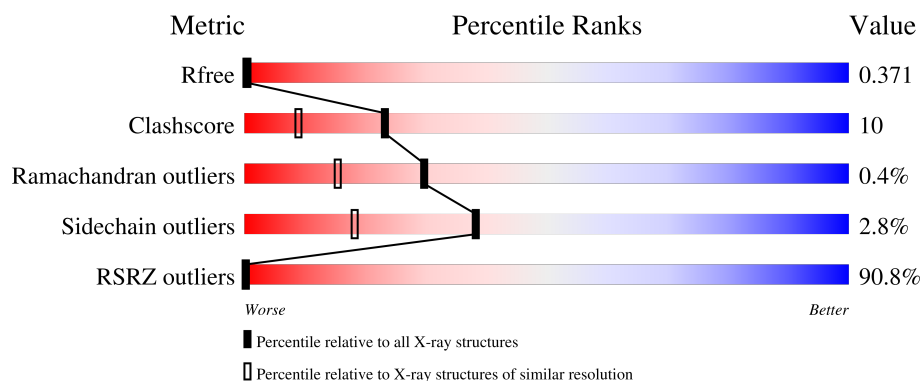
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	502	92% 81%16%..
1	B	502	88% 84%14%..

2 Entry composition [i](#)

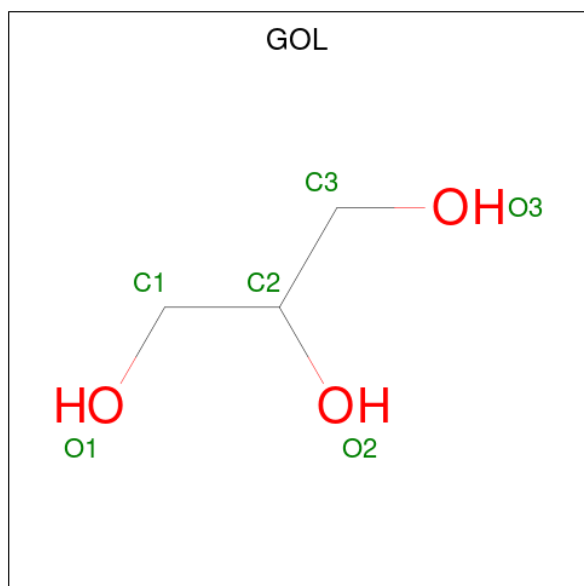
There are 3 unique types of molecules in this entry. The entry contains 9136 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3990	2542	680	748	20			
1	B	497	Total	C	N	O	S	0	0	0
			3990	2542	680	748	20			

- 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	B	1	Total	C	O	0	0
			6	3	3		

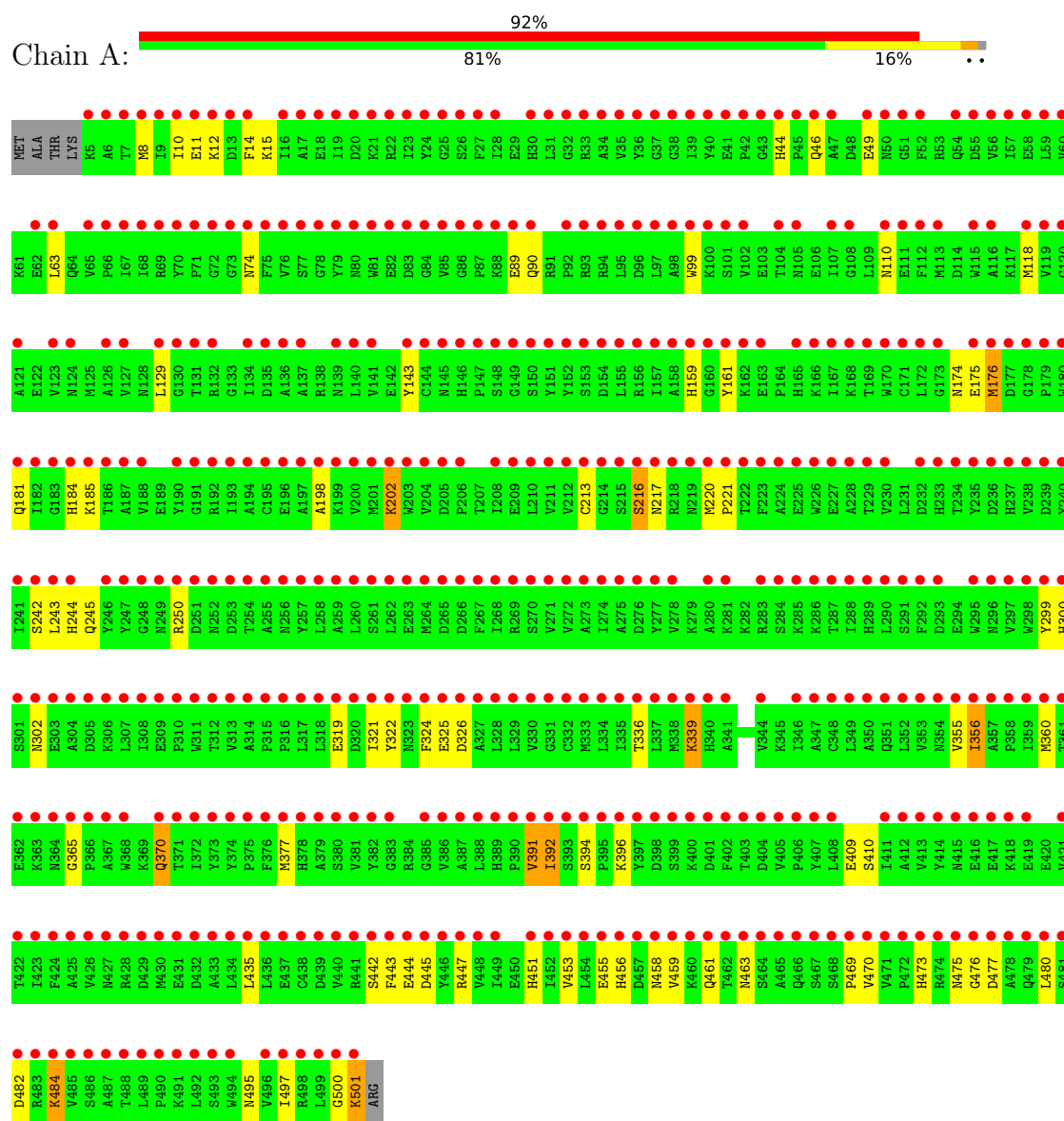
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	583	Total 583	O 583	0	0
3	B	561	Total 561	O 561	0	0

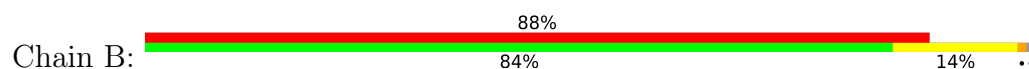
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Alpha-L-arabinofuranosidase



• Molecule 1: Alpha-L-arabinofuranosidase



T488	A425	K363	N302	S242	I182	E122	K61
L489	V426	N364	E303	H244	G183	V123	E62
P490		G365	A304		A304	L243	L63
K491		P366	D305	Q245	K185	M125	Q64
L492	E431	A367	K306	Y246	T186	A126	V65
S493	A433	W368	L307	Y247	A187	V127	P66
W494	L434		I308		W188	M128	I67
N495	L435	A495	E309	N249	E189	L129	I68
L496	L436		P310	R250	V190	G130	R69
V497			W311	D251	G191	T131	Y70
R498	E437	Y373	T312	N252	R192	R132	P71
L499	C438	Y374	V313	D253	I193	G133	E71
	D439	P375	A314	T254	A194	D135	K12
G500	V440	F376	P315	A255	I193	G133	D13
K501	R441	K377	P316	N256	E195	A136	F14
ARG	S442	H378	L317	Y257	A197	A137	F75
	F443	A379	L318	L258	A198	R138	I16
	E444	S380	E319	A259	K199	M139	S77
	D445	V381	D320	L260	W200	L140	G78
	Y446	Y382	I321	L262	M201	V141	E18
	R447	G383	Y322	E263	K202	E142	N80
	V448	R384	N323	R269	W203	Y143	D21
	I449	G385	F324	E264	W204	C144	R22
	E450	V386	E325	D265	D205	M145	T23
	H451	A387	D326	D266	P206	H146	T24
	I452	L388	A327	F267	T207	P147	G86
	V453	H389	L328	L268	L208	S148	S26
	L454	P390	L329	E270	E209	G149	P87
	E455	V391	L329	R269	L210	S150	K88
	H456	T392	V330	S270	E209	S150	E89
	D457	S393	G331	V271	W211	Y151	F29
	M458	S394	C332	L371	V212	Y152	H30
	V459	P395	M333	A273	C213	S153	R91
	K460	K396	L334	I274	G214	D154	C32
	Q461		L335	A275	S215	L155	R33
	T462		T336	D276	S216	R156	L95
	M463	D398	L337	Y277	R217	I157	D96
	S464	S399	M338	V278	N218	A158	L97
	A465	D401	K339	K279	W219	H159	P98
	Q466	F402	H340	A280	W220	G160	A98
	S467	T403	S461	K281	P221	Y161	W99
	S468	D404	D342	K282	T222	K162	K100
	P469	V405	R343	R283	F223	E163	S101
	V470	P406	V344	S284	A224	P164	V40
	V471	Y407	K345	K285	E225	H165	F41
	P472	L408	L346	K286	W226	K166	E102
	H473	E409	A347	T287	E227	I167	E103
	R474		C348	L288	A228	K168	E104
	N475	S410	L349	H289	T229	T169	N105
	G476		A350	L290	V230	W170	I107
	D477	V413		S291	L231	Y170	G108
	A478	N415	V353	F292	D232	C171	L109
	Q479	E416	N354	D293	H233	L172	N110
	L480	E417	V355	E294	T234	G173	E111
	S481	K418	I356	W295	V235	M174	F52
	D482	E419	A357	N296	D236	E175	M113
	R483	E420	P358	V297	H237	M176	E53
	K484	V421	L359	W298	V238	G178	R53
	V485	T422	M360	Y299	D239	P179	F23
	S486	L423	T361	H300	Y240	W180	Q54
	A487	E424	E362	S301	I241	C121	W115
							D55
							D56
							V56
							I57
							E58
							L59
							W60

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	179.43Å 179.43Å 100.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.75 20.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.75) 98.6 (20.00-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 1.74Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.171 , 0.204 0.365 , 0.371	Depositor DCC
R_{free} test set	6001 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	9136	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.82	0/4091	0.89	1/5558 (0.0%)
1	B	0.78	1/4091 (0.0%)	0.87	0/5558
All	All	0.80	1/8182 (0.0%)	0.88	1/11116 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	176	MET	SD-CE	-8.40	1.58	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	CYS	CB-CA-C	-5.80	100.84	109.90

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	3990	0	3891	88	0
1	B	3990	0	3891	76	0
2	A	6	0	8	3	0
2	B	6	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	583	0	0	28	4
3	B	561	0	0	27	3
All	All	9136	0	7798	162	4

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (162) 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:A:319:GLU:CD	3:A:1038:HOH:O	1.67	1.27
1:B:392:ILE:HG21	3:B:1027:HOH:O	1.52	1.09
1:B:118:MET:CG	3:B:1026:HOH:O	2.06	1.03
1:B:118:MET:SD	3:B:1026:HOH:O	2.15	1.01
1:B:118:MET:HG3	3:B:1026:HOH:O	1.59	1.00
1:A:244:HIS:HE1	3:A:1069:HOH:O	1.45	1.00
1:B:175:GLU:OE1	3:B:959:HOH:O	1.83	0.96
1:A:451:HIS:CD2	1:A:497:ILE:HG12	2.01	0.94
1:B:354:ASN:HD21	1:B:361:THR:H	1.22	0.88
1:A:244:HIS:CE1	3:A:1069:HOH:O	2.21	0.86
1:A:220:MET:SD	3:A:997:HOH:O	2.35	0.85
1:A:451:HIS:HD2	1:A:497:ILE:HG12	1.40	0.83
1:A:319:GLU:OE1	3:A:1038:HOH:O	1.75	0.81
1:A:14:PHE:CZ	1:B:391:VAL:HG21	2.15	0.80
1:A:44:HIS:HD2	1:A:46:GLN:H	1.29	0.80
1:A:220:MET:HE2	3:A:1079:HOH:O	1.80	0.80
1:A:451:HIS:ND1	1:A:476:GLY:HA3	1.96	0.79
1:B:175:GLU:HG3	1:B:216:SER:HB3	1.63	0.78
1:A:451:HIS:CE1	1:A:495:ASN:HD22	2.03	0.77
1:A:463:ASN:HD21	1:A:470:VAL:H	1.34	0.75
1:A:175:GLU:CG	1:A:216:SER:HB3	2.18	0.74
1:B:216:SER:OG	3:B:1017:HOH:O	2.06	0.73
1:B:480:LEU:HD22	1:B:485:VAL:HG22	1.70	0.73
1:A:220:MET:SD	3:A:1079:HOH:O	2.46	0.73
1:B:166:LYS:HG2	3:B:789:HOH:O	1.89	0.71
1:B:11:GLU:HG2	1:B:14:PHE:HD1	1.54	0.70
1:A:220:MET:CE	3:A:1079:HOH:O	2.37	0.70
1:A:250:ARG:HH21	1:A:302:ASN:HD21	1.36	0.70
1:A:143:TYR:OH	1:A:159:HIS:HD2	1.75	0.70
1:B:175:GLU:CG	1:B:216:SER:HB3	2.22	0.69
1:B:117:LYS:NZ	1:B:118:MET:HE3	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:HIS:CE1	1:B:461:GLN:HG2	2.29	0.68
1:B:220:MET:SD	3:B:1017:HOH:O	2.52	0.68
1:B:300:HIS:HD2	1:B:321:ILE:O	1.77	0.67
1:A:175:GLU:OE1	3:A:793:HOH:O	2.12	0.67
2:B:503:GOL:H2	3:B:505:HOH:O	1.94	0.66
1:A:451:HIS:HE1	1:A:495:ASN:HD22	1.41	0.66
1:A:14:PHE:CE2	1:B:391:VAL:HG21	2.30	0.65
1:B:456:HIS:HE1	1:B:461:GLN:HG2	1.63	0.64
1:A:184:HIS:HE1	3:A:676:HOH:O	1.81	0.64
1:A:360:MET:HE2	3:A:669:HOH:O	1.97	0.64
1:B:250:ARG:HH21	1:B:302:ASN:HD21	1.45	0.63
1:A:360:MET:CE	3:A:669:HOH:O	2.47	0.63
1:A:44:HIS:CD2	1:A:46:GLN:H	2.16	0.63
1:B:11:GLU:CG	1:B:14:PHE:HD1	2.12	0.63
2:A:503:GOL:H2	3:A:546:HOH:O	1.98	0.62
1:A:300:HIS:HE1	1:A:326:ASP:OD2	1.82	0.62
1:B:299:TYR:CE1	1:B:300:HIS:CE1	2.88	0.61
1:B:217:ASN:CB	3:B:1017:HOH:O	2.48	0.61
1:A:175:GLU:CD	1:A:216:SER:HB3	2.26	0.60
1:B:389:HIS:HD2	3:B:803:HOH:O	1.83	0.59
1:B:44:HIS:ND1	1:B:45:PRO:HD2	2.18	0.59
1:A:391:VAL:HB	1:B:14:PHE:CZ	2.37	0.59
1:A:473:HIS:HD2	1:A:475:ASN:H	1.50	0.58
1:B:174:ASN:HD22	1:B:181:GLN:HE22	1.51	0.58
1:A:220:MET:HE3	1:A:221:PRO:HD2	1.86	0.57
1:B:143:TYR:OH	1:B:159:HIS:HD2	1.87	0.57
1:B:8:MET:HG3	1:B:392:ILE:HG22	1.87	0.57
1:B:500:GLY:O	1:B:501:LYS:HB2	2.04	0.57
1:B:300:HIS:CD2	1:B:321:ILE:O	2.57	0.57
1:B:64:GLN:NE2	3:B:600:HOH:O	2.38	0.57
1:B:11:GLU:HG2	1:B:14:PHE:CD1	2.39	0.56
1:B:146:HIS:HD2	3:B:611:HOH:O	1.88	0.56
1:B:100:LYS:NZ	3:B:797:HOH:O	2.39	0.56
1:B:299:TYR:CZ	1:B:300:HIS:CE1	2.94	0.56
1:A:10:ILE:O	1:A:442:SER:OG	2.22	0.55
1:A:300:HIS:HD2	3:A:656:HOH:O	1.89	0.55
1:A:49:GLU:HG2	3:A:768:HOH:O	2.05	0.55
1:A:175:GLU:HG2	1:A:216:SER:HB3	1.87	0.55
1:B:217:ASN:HB3	3:B:1017:HOH:O	2.06	0.54
1:B:174:ASN:HD22	1:B:181:GLN:NE2	2.05	0.54
1:B:167:ILE:HB	1:B:170:TRP:CZ2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLU:HB3	1:A:459:VAL:HB	1.90	0.54
1:B:480:LEU:HD22	1:B:485:VAL:CG2	2.36	0.53
1:A:216:SER:HB2	3:A:997:HOH:O	2.07	0.53
1:B:164:PRO:HG2	1:B:166:LYS:HE2	1.88	0.53
1:A:74:ASN:HA	1:A:181:GLN:HE22	1.73	0.53
1:A:174:ASN:HD22	1:A:181:GLN:NE2	2.07	0.53
1:A:129:LEU:O	1:A:185:LYS:HE3	2.09	0.52
1:A:410:SER:HB3	3:A:1086:HOH:O	2.09	0.52
1:A:174:ASN:HD22	1:A:181:GLN:HE22	1.56	0.52
1:B:74:ASN:HA	1:B:181:GLN:HE22	1.75	0.52
1:B:456:HIS:HD2	3:B:921:HOH:O	1.92	0.52
1:A:14:PHE:CE2	1:B:391:VAL:CG2	2.93	0.52
1:A:198:ALA:O	1:A:202:LYS:HE3	2.10	0.51
1:B:354:ASN:ND2	1:B:361:THR:H	2.00	0.51
1:A:99:TRP:CH2	2:A:503:GOL:H31	2.45	0.51
1:A:217:ASN:ND2	3:A:997:HOH:O	2.43	0.51
1:A:435:LEU:HD22	1:A:435:LEU:N	2.25	0.51
1:B:176:MET:HA	1:B:176:MET:HE2	1.92	0.51
1:A:89:GLU:HG2	1:A:90:GLN:NE2	2.25	0.51
1:A:456:HIS:CE1	1:A:461:GLN:HG2	2.46	0.51
1:B:409:GLU:OE1	3:B:1025:HOH:O	2.19	0.50
1:A:11:GLU:CG	1:A:14:PHE:HD1	2.24	0.50
1:A:216:SER:CB	3:A:997:HOH:O	2.59	0.50
1:A:391:VAL:HG12	1:A:391:VAL:O	2.12	0.50
1:B:453:VAL:HB	1:B:473:HIS:CD2	2.47	0.50
1:A:159:HIS:HE1	3:A:574:HOH:O	1.94	0.50
1:B:389:HIS:CD2	3:B:803:HOH:O	2.61	0.49
1:B:44:HIS:CD2	1:B:53:ARG:CZ	2.95	0.49
1:A:322:TYR:H	1:A:370:GLN:HE22	1.61	0.49
1:A:220:MET:CG	3:A:997:HOH:O	2.57	0.49
1:A:322:TYR:H	1:A:370:GLN:NE2	2.11	0.49
1:A:455:GLU:OE2	1:A:473:HIS:HE1	1.96	0.48
1:B:269:ARG:HG3	1:B:340:HIS:HE1	1.78	0.48
1:B:218:ARG:O	3:B:1018:HOH:O	2.20	0.48
1:A:451:HIS:CE1	1:A:453:VAL:HG22	2.49	0.48
1:A:44:HIS:HE1	1:A:365:GLY:O	1.95	0.48
1:B:109:LEU:O	1:B:113:MET:HG2	2.13	0.48
1:A:12:LYS:O	1:A:15:LYS:NZ	2.30	0.48
1:B:125:MET:HB3	1:B:170:TRP:CE3	2.49	0.48
1:B:325:GLU:HB3	1:B:459:VAL:HB	1.96	0.48
1:A:447:ARG:HD2	3:A:1042:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASN:HB2	3:B:1017:HOH:O	2.13	0.48
1:A:482:ASP:OD1	3:A:955:HOH:O	2.20	0.47
1:A:110:ASN:HB3	1:A:161:TYR:CZ	2.50	0.47
1:B:32:GLY:HA2	1:B:315:PRO:O	2.15	0.47
1:B:125:MET:HG2	1:B:170:TRP:CZ3	2.50	0.47
1:A:324:PHE:CZ	1:A:455:GLU:HA	2.50	0.46
1:A:339:LYS:HE3	1:A:409:GLU:OE2	2.15	0.46
1:A:245:GLN:NE2	3:A:685:HOH:O	2.48	0.46
1:A:11:GLU:HG2	1:A:14:PHE:HD1	1.81	0.46
1:B:299:TYR:CE1	1:B:300:HIS:HE1	2.33	0.46
1:B:242:SER:HA	1:B:291:SER:O	2.17	0.45
1:A:336:THR:HA	1:A:339:LYS:HG2	1.98	0.45
1:B:177:ASP:OD1	1:B:220:MET:HE2	2.17	0.45
1:B:453:VAL:HB	1:B:473:HIS:NE2	2.31	0.45
1:A:339:LYS:HD2	3:A:993:HOH:O	2.17	0.45
1:B:159:HIS:HE1	3:B:612:HOH:O	2.00	0.45
1:B:99:TRP:CH2	2:B:503:GOL:H31	2.52	0.44
1:B:117:LYS:HZ3	1:B:118:MET:HE3	1.82	0.43
1:B:252:ASN:HD21	1:B:460:LYS:HE3	1.81	0.43
1:A:463:ASN:ND2	1:A:470:VAL:H	2.10	0.43
1:A:456:HIS:HE1	1:A:469:PRO:HB2	1.83	0.43
1:A:11:GLU:HG2	1:A:14:PHE:CD1	2.54	0.43
1:A:484:LYS:HB2	1:A:484:LYS:NZ	2.33	0.43
1:A:321:ILE:HA	1:A:370:GLN:HE22	1.84	0.43
1:B:220:MET:CG	3:B:1017:HOH:O	2.66	0.42
1:A:63:LEU:HD23	1:A:377:MET:HG3	2.02	0.42
1:B:146:HIS:HE1	3:B:687:HOH:O	2.02	0.42
1:B:473:HIS:CE1	3:B:988:HOH:O	2.72	0.42
1:A:392:ILE:CD1	1:A:394:SER:HB3	2.49	0.42
1:A:10:ILE:HG22	1:A:443:PHE:CE1	2.55	0.42
1:A:500:GLY:O	1:A:501:LYS:HB2	2.20	0.42
1:B:110:ASN:HB3	1:B:161:TYR:CZ	2.55	0.42
1:A:243:LEU:HD12	1:A:243:LEU:N	2.35	0.42
1:B:289:HIS:HE1	3:B:839:HOH:O	2.03	0.42
1:A:242:SER:C	1:A:243:LEU:HD12	2.44	0.41
1:B:237:HIS:HD2	3:B:867:HOH:O	2.03	0.41
1:B:479:GLN:NE2	3:B:820:HOH:O	2.53	0.41
1:A:355:VAL:O	1:A:356:ILE:C	2.62	0.41
1:A:456:HIS:HD2	1:A:458:ASN:H	1.67	0.41
1:B:473:HIS:CE1	1:B:475:ASN:HB2	2.56	0.41
1:A:99:TRP:CZ2	2:A:503:GOL:H31	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ARG:NE	3:A:1018:HOH:O	2.53	0.41
1:A:175:GLU:HB2	3:A:1069:HOH:O	2.20	0.41
1:A:10:ILE:HG22	1:A:443:PHE:HE1	1.86	0.41
1:A:176:MET:O	1:A:184:HIS:HD2	2.04	0.41
1:B:324:PHE:CZ	1:B:455:GLU:HA	2.55	0.40
1:B:451:HIS:CG	1:B:476:GLY:HA3	2.57	0.40
1:A:10:ILE:HA	3:A:834:HOH:O	2.22	0.40
1:A:477:ASP:C	1:A:477:ASP:OD1	2.65	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:763:HOH:O	3:B:511:HOH:O[6_554]	2.07	0.13
3:A:1063:HOH:O	3:B:992:HOH:O[1_554]	2.13	0.07
3:A:1041:HOH:O	3:B:688:HOH:O[1_554]	2.16	0.04
3:A:507:HOH:O	3:A:564:HOH:O[2_655]	2.17	0.03

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	495/502 (99%)	471 (95%)	22 (4%)	2 (0%)	30	15
1	B	495/502 (99%)	477 (96%)	16 (3%)	2 (0%)	30	15
All	All	990/1004 (99%)	948 (96%)	38 (4%)	4 (0%)	30	15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	TYR
1	B	299	TYR

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Mol	Chain	Res	Type
1	A	356	ILE
1	B	356	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	430/434 (99%)	415 (96%)	15 (4%)	32	12
1	B	430/434 (99%)	421 (98%)	9 (2%)	47	27
All	All	860/868 (99%)	836 (97%)	24 (3%)	38	18

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	118	MET
1	A	176	MET
1	A	202	LYS
1	A	216	SER
1	A	339	LYS
1	A	370	GLN
1	A	391	VAL
1	A	392	ILE
1	A	396	LYS
1	A	444	GLU
1	A	445	ASP
1	A	480	LEU
1	A	484	LYS
1	A	501	LYS
1	B	5	LYS
1	B	46	GLN
1	B	117	LYS
1	B	176	MET
1	B	285	LYS
1	B	392	ILE

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Mol	Chain	Res	Type
1	B	466	GLN
1	B	480	LEU
1	B	501	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	64	GLN
1	A	105	ASN
1	A	159	HIS
1	A	181	GLN
1	A	184	HIS
1	A	219	ASN
1	A	237	HIS
1	A	245	GLN
1	A	300	HIS
1	A	302	ASN
1	A	370	GLN
1	A	451	HIS
1	A	456	HIS
1	A	463	ASN
1	A	473	HIS
1	A	479	GLN
1	A	495	ASN
1	B	64	GLN
1	B	105	ASN
1	B	146	HIS
1	B	159	HIS
1	B	181	GLN
1	B	184	HIS
1	B	245	GLN
1	B	252	ASN
1	B	300	HIS
1	B	302	ASN
1	B	354	ASN
1	B	364	ASN
1	B	389	HIS
1	B	461	GLN
1	B	475	ASN
1	B	479	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 ⓘ

2 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	B	503	-	5,5,5	0.67	0	5,5,5	0.90	0
2	GOL	A	503	-	5,5,5	0.68	0	5,5,5	1.07	1 (20%)

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	B	503	-	-	2/4/4/4	-
2	GOL	A	503	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	503	GOL	O2-C2-C1	2.26	118.55	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	C1-C2-C3-O3
2	B	503	GOL	C1-C2-C3-O3
2	A	503	GOL	O2-C2-C3-O3
2	B	503	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	GOL	2	0
2	A	503	GOL	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	497/502 (99%)	3.42	460 (92%) 0 0	13, 23, 40, 56	0
1	B	497/502 (99%)	3.22	443 (89%) 0 0	16, 23, 37, 47	0
All	All	994/1004 (99%)	3.32	903 (90%) 0 0	13, 23, 39, 56	0

All (903) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	307	LEU	9.5
1	B	170	TRP	9.3
1	A	402	PHE	9.2
1	B	180	TRP	7.7
1	B	307	LEU	7.6
1	A	180	TRP	6.9
1	A	251	ASP	6.9
1	A	151	TYR	6.8
1	A	314	ALA	6.8
1	A	252	ASN	6.8
1	B	311	TRP	6.5
1	A	459	VAL	6.5
1	A	435	LEU	6.4
1	A	479	GLN	6.3
1	A	313	VAL	6.2
1	A	457	ASP	6.2
1	A	259	ALA	6.2
1	A	218	ARG	6.2
1	A	115	TRP	6.1
1	A	403	THR	6.0
1	B	473	HIS	6.0
1	B	308	ILE	6.0
1	B	214	GLY	5.9
1	A	304	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	187	ALA	5.8
1	B	47	ALA	5.8
1	A	442	SER	5.8
1	B	81	TRP	5.8
1	B	51	GLY	5.7
1	A	255	ALA	5.7
1	A	440	VAL	5.7
1	B	141	VAL	5.7
1	A	441	ARG	5.6
1	B	129	LEU	5.6
1	B	203	TRP	5.5
1	B	312	THR	5.5
1	A	448	VAL	5.5
1	B	151	TYR	5.5
1	B	217	ASN	5.4
1	B	157	ILE	5.4
1	B	480	LEU	5.4
1	B	403	THR	5.4
1	A	436	LEU	5.4
1	B	397	TYR	5.4
1	A	449	ILE	5.4
1	A	7	THR	5.3
1	A	406	PRO	5.3
1	A	471	VAL	5.3
1	B	456	HIS	5.3
1	A	241	ILE	5.2
1	B	85	VAL	5.2
1	B	471	VAL	5.2
1	A	434	LEU	5.2
1	B	467	SER	5.2
1	A	99	TRP	5.1
1	B	392	ILE	5.1
1	B	440	VAL	5.1
1	B	459	VAL	5.1
1	B	178	GLY	5.1
1	A	481	SER	5.1
1	A	486	SER	5.1
1	A	188	VAL	5.1
1	B	313	VAL	5.1
1	B	481	SER	5.0
1	B	44	HIS	5.0
1	A	312	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	392	ILE	5.0
1	B	9	ILE	5.0
1	B	287	THR	5.0
1	B	188	VAL	5.0
1	A	220	MET	5.0
1	B	213	CYS	5.0
1	A	327	ALA	5.0
1	A	423	ILE	5.0
1	A	480	LEU	5.0
1	B	76	VAL	5.0
1	B	99	TRP	5.0
1	A	136	ALA	4.9
1	A	443	PHE	4.9
1	A	311	TRP	4.9
1	B	172	LEU	4.9
1	A	446	TYR	4.8
1	B	158	ALA	4.8
1	B	314	ALA	4.8
1	B	465	ALA	4.8
1	A	150	SER	4.8
1	A	215	SER	4.8
1	A	365	GLY	4.8
1	A	405	VAL	4.8
1	B	212	VAL	4.8
1	A	407	TYR	4.8
1	A	332	CYS	4.8
1	B	438	CYS	4.8
1	A	298	TRP	4.8
1	A	319	GLU	4.8
1	B	191	GLY	4.8
1	A	308	ILE	4.8
1	A	411	ILE	4.8
1	B	167	ILE	4.8
1	A	315	PRO	4.8
1	B	316	PRO	4.8
1	B	255	ALA	4.8
1	A	242	SER	4.8
1	A	267	PHE	4.8
1	B	402	PHE	4.8
1	B	405	VAL	4.8
1	A	397	TYR	4.7
1	A	310	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	215	SER	4.7
1	B	228	ALA	4.7
1	A	248	GLY	4.7
1	B	78	GLY	4.7
1	B	86	GLY	4.7
1	B	31	LEU	4.7
1	A	157	ILE	4.7
1	A	81	TRP	4.7
1	A	75	PHE	4.7
1	A	200	VAL	4.7
1	A	43	GLY	4.7
1	A	288	ILE	4.6
1	B	321	ILE	4.6
1	B	365	GLY	4.6
1	A	217	ASN	4.6
1	A	36	TYR	4.6
1	B	246	TYR	4.6
1	B	299	TYR	4.6
1	B	413	VAL	4.6
1	B	396	LYS	4.6
1	B	223	PHE	4.6
1	A	320	ASP	4.6
1	A	212	VAL	4.5
1	A	246	TYR	4.5
1	B	49	GLU	4.5
1	B	391	VAL	4.5
1	B	226	TRP	4.5
1	A	247	TYR	4.5
1	A	258	LEU	4.5
1	B	368	TRP	4.5
1	A	9	ILE	4.5
1	B	357	ALA	4.5
1	A	173	GLY	4.5
1	B	75	PHE	4.5
1	B	466	GLN	4.5
1	A	356	ILE	4.5
1	B	107	ILE	4.5
1	A	482	ASP	4.5
1	B	222	THR	4.5
1	B	206	PRO	4.4
1	A	257	TYR	4.4
1	B	119	VAL	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	283	ARG	4.4
1	A	72	GLY	4.4
1	A	70	TYR	4.4
1	A	299	TYR	4.4
1	A	112	PHE	4.4
1	A	456	HIS	4.4
1	B	146	HIS	4.4
1	A	438	CYS	4.4
1	A	316	PRO	4.4
1	B	220	MET	4.4
1	A	244	HIS	4.4
1	A	47	ALA	4.3
1	A	367	ALA	4.3
1	B	194	ALA	4.3
1	B	447	ARG	4.3
1	A	39	ILE	4.3
1	A	268	ILE	4.3
1	A	395	PRO	4.3
1	A	469	PRO	4.3
1	A	295	TRP	4.3
1	B	131	THR	4.3
1	A	445	ASP	4.3
1	A	50	ASN	4.3
1	B	195	CYS	4.3
1	B	244	HIS	4.3
1	B	269	ARG	4.3
1	A	27	PHE	4.3
1	B	252	ASN	4.3
1	A	102	VAL	4.3
1	A	426	VAL	4.3
1	B	10	ILE	4.3
1	B	300	HIS	4.3
1	B	356	ILE	4.3
1	A	213	CYS	4.3
1	A	104	THR	4.2
1	A	275	ALA	4.2
1	A	329	LEU	4.2
1	A	52	PHE	4.2
1	A	431	GLU	4.2
1	A	404	ASP	4.2
1	B	84	GLY	4.2
1	B	145	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	275	ALA	4.2
1	A	146	HIS	4.2
1	B	317	LEU	4.2
1	A	376	PHE	4.2
1	A	278	VAL	4.2
1	A	413	VAL	4.2
1	A	256	ASN	4.2
1	A	222	THR	4.2
1	B	431	GLU	4.2
1	A	228	ALA	4.2
1	A	492	LEU	4.2
1	B	161	TYR	4.2
1	B	27	PHE	4.2
1	A	355	VAL	4.2
1	A	485	VAL	4.2
1	B	218	ARG	4.2
1	A	368	TRP	4.2
1	A	335	ILE	4.2
1	B	241	ILE	4.2
1	A	493	SER	4.1
1	B	116	ALA	4.1
1	B	136	ALA	4.1
1	B	367	ALA	4.1
1	A	13	ASP	4.1
1	A	140	LEU	4.1
1	A	44	HIS	4.1
1	A	10	ILE	4.1
1	A	216	SER	4.1
1	B	150	SER	4.1
1	A	17	ALA	4.1
1	A	447	ARG	4.1
1	A	262	LEU	4.1
1	A	161	TYR	4.1
1	B	40	TYR	4.1
1	B	322	TYR	4.1
1	B	173	GLY	4.1
1	B	52	PHE	4.1
1	A	254	THR	4.1
1	A	421	VAL	4.1
1	A	28	ILE	4.1
1	A	346	ILE	4.1
1	A	429	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	251	ASP	4.1
1	A	158	ALA	4.1
1	A	465	ALA	4.1
1	B	327	ALA	4.1
1	A	322	TYR	4.1
1	B	234	THR	4.1
1	A	470	VAL	4.1
1	B	42	PRO	4.0
1	B	32	GLY	4.0
1	A	97	LEU	4.0
1	B	70	TYR	4.0
1	A	223	PHE	4.0
1	B	16	ILE	4.0
1	A	487	ALA	4.0
1	B	187	ALA	4.0
1	B	224	ALA	4.0
1	A	86	GLY	4.0
1	B	399	SER	4.0
1	A	96	ASP	4.0
1	A	31	LEU	4.0
1	B	453	VAL	4.0
1	A	452	ILE	4.0
1	B	248	GLY	4.0
1	A	454	LEU	4.0
1	A	90	GLN	4.0
1	A	466	GLN	4.0
1	A	306	LYS	4.0
1	A	391	VAL	4.0
1	B	457	ASP	4.0
1	B	133	GLY	4.0
1	A	444	GLU	3.9
1	A	184	HIS	3.9
1	A	300	HIS	3.9
1	A	484	LYS	3.9
1	B	298	TRP	3.9
1	A	433	ALA	3.9
1	A	85	VAL	3.9
1	A	141	VAL	3.9
1	A	204	VAL	3.9
1	A	297	VAL	3.9
1	B	230	VAL	3.9
1	B	208	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	388	LEU	3.9
1	B	112	PHE	3.9
1	B	443	PHE	3.9
1	A	107	ILE	3.9
1	A	496	VAL	3.9
1	B	57	ILE	3.9
1	A	261	SER	3.9
1	A	51	GLY	3.9
1	A	430	MET	3.9
1	B	407	TYR	3.9
1	A	366	PRO	3.9
1	A	14	PHE	3.9
1	B	14	PHE	3.9
1	A	336	THR	3.8
1	B	272	VAL	3.8
1	B	344	VAL	3.8
1	A	305	ASP	3.8
1	B	242	SER	3.8
1	A	108	GLY	3.8
1	B	63	LEU	3.8
1	B	155	LEU	3.8
1	A	194	ALA	3.8
1	B	240	TYR	3.8
1	B	164	PRO	3.8
1	B	331	GLY	3.8
1	A	260	LEU	3.8
1	A	303	GLU	3.8
1	A	437	GLU	3.8
1	A	135	ASP	3.8
1	B	373	TYR	3.8
1	B	421	VAL	3.8
1	A	130	GLY	3.8
1	A	451	HIS	3.8
1	A	349	LEU	3.8
1	B	435	LEU	3.8
1	B	482	ASP	3.8
1	A	379	ALA	3.8
1	B	137	ALA	3.8
1	A	427	ASN	3.8
1	B	186	THR	3.8
1	A	362	GLU	3.8
1	B	5	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	423	ILE	3.7
1	A	76	VAL	3.7
1	B	204	VAL	3.7
1	A	393	SER	3.7
1	A	328	LEU	3.7
1	A	458	ASN	3.7
1	A	6	ALA	3.7
1	A	42	PRO	3.7
1	B	198	ALA	3.7
1	A	186	THR	3.7
1	B	144	CYS	3.7
1	A	214	GLY	3.7
1	A	123	VAL	3.7
1	A	272	VAL	3.7
1	B	254	THR	3.7
1	A	32	GLY	3.7
1	A	398	ASP	3.7
1	A	360	MET	3.7
1	A	193	ILE	3.7
1	A	263	GLU	3.7
1	A	309	GLU	3.7
1	B	483	ARG	3.7
1	A	229	THR	3.7
1	B	152	TYR	3.7
1	B	235	TYR	3.7
1	B	284	SER	3.7
1	B	292	PHE	3.6
1	A	60	VAL	3.6
1	B	200	VAL	3.6
1	B	71	PRO	3.6
1	B	366	PRO	3.6
1	A	408	LEU	3.6
1	A	499	LEU	3.6
1	A	354	ASN	3.6
1	A	463	ASN	3.6
1	A	269	ARG	3.6
1	A	40	TYR	3.6
1	A	68	ILE	3.6
1	B	268	ILE	3.6
1	B	424	PHE	3.6
1	B	163	GLU	3.6
1	B	169	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	ALA	3.6
1	A	273	ALA	3.6
1	A	425	ALA	3.6
1	B	123	VAL	3.6
1	B	197	ALA	3.6
1	A	191	GLY	3.6
1	A	317	LEU	3.6
1	B	262	LEU	3.6
1	A	143	TYR	3.6
1	A	87	PRO	3.6
1	A	179	PRO	3.6
1	A	321	ILE	3.6
1	B	87	PRO	3.6
1	A	183	GLY	3.6
1	A	301	SER	3.6
1	A	399	SER	3.6
1	A	478	ALA	3.6
1	B	381	VAL	3.6
1	A	59	LEU	3.6
1	A	318	LEU	3.6
1	A	389	HIS	3.6
1	B	414	TYR	3.6
1	A	491	LYS	3.5
1	B	484	LYS	3.5
1	B	494	TRP	3.5
1	B	278	VAL	3.5
1	B	348	CYS	3.5
1	A	364	ASN	3.5
1	A	414	TYR	3.5
1	A	462	THR	3.5
1	A	71	PRO	3.5
1	A	221	PRO	3.5
1	B	43	GLY	3.5
1	A	16	ILE	3.5
1	B	193	ILE	3.5
1	B	288	ILE	3.5
1	B	346	ILE	3.5
1	B	267	PHE	3.5
1	B	184	HIS	3.5
1	A	432	ASP	3.5
1	B	46	GLN	3.5
1	B	323	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	464	SER	3.5
1	A	468	SER	3.5
1	B	442	SER	3.5
1	A	417	GLU	3.5
1	B	419	GLU	3.5
1	B	79	TYR	3.5
1	A	176	MET	3.5
1	A	224	ALA	3.5
1	A	280	ALA	3.5
1	B	280	ALA	3.5
1	B	404	ASP	3.5
1	A	292	PHE	3.5
1	A	400	LYS	3.5
1	A	290	LEU	3.5
1	B	260	LEU	3.5
1	B	65	VAL	3.5
1	B	102	VAL	3.5
1	B	448	VAL	3.5
1	B	444	GLU	3.5
1	A	38	GLY	3.5
1	B	72	GLY	3.5
1	A	418	LYS	3.4
1	A	116	ALA	3.4
1	A	197	ALA	3.4
1	B	362	GLU	3.4
1	A	172	LEU	3.4
1	B	492	LEU	3.4
1	A	250	ARG	3.4
1	A	488	THR	3.4
1	A	45	PRO	3.4
1	B	190	TYR	3.4
1	A	302	ASN	3.4
1	B	487	ALA	3.4
1	A	101	SER	3.4
1	B	258	LEU	3.4
1	B	127	VAL	3.4
1	B	104	THR	3.4
1	B	147	PRO	3.4
1	B	50	ASN	3.4
1	B	304	ALA	3.4
1	A	380	SER	3.4
1	B	250	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	441	ARG	3.4
1	A	167	ILE	3.4
1	B	109	LEU	3.4
1	A	144	CYS	3.4
1	A	341	ALA	3.3
1	A	378	HIS	3.3
1	A	243	LEU	3.3
1	A	361	THR	3.3
1	A	371	THR	3.3
1	B	361	THR	3.3
1	B	395	PRO	3.3
1	B	271	VAL	3.3
1	B	355	VAL	3.3
1	A	181	GLN	3.3
1	B	115	TRP	3.3
1	A	331	GLY	3.3
1	B	39	ILE	3.3
1	B	134	ILE	3.3
1	B	372	ILE	3.3
1	A	155	LEU	3.3
1	A	337	LEU	3.3
1	A	370	GLN	3.3
1	A	236	ASP	3.3
1	B	48	ASP	3.3
1	B	445	ASP	3.3
1	B	17	ALA	3.3
1	A	483	ARG	3.3
1	A	37	GLY	3.3
1	A	149	GLY	3.3
1	B	354	ASN	3.3
1	B	486	SER	3.3
1	B	45	PRO	3.3
1	A	195	CYS	3.3
1	A	230	VAL	3.3
1	B	238	VAL	3.3
1	A	249	ASN	3.3
1	A	460	LYS	3.2
1	A	501	LYS	3.2
1	B	394	SER	3.2
1	B	464	SER	3.2
1	A	494	TRP	3.2
1	B	30	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	135	ASP	3.2
1	B	179	PRO	3.2
1	A	95	LEU	3.2
1	A	283	ARG	3.2
1	A	323	ASN	3.2
1	A	8	MET	3.2
1	B	6	ALA	3.2
1	B	433	ALA	3.2
1	B	301	SER	3.2
1	A	253	ASP	3.2
1	A	340	HIS	3.2
1	A	19	ILE	3.2
1	B	418	LYS	3.2
1	A	394	SER	3.2
1	A	453	VAL	3.2
1	B	359	ILE	3.2
1	A	210	LEU	3.2
1	A	226	TRP	3.2
1	A	467	SER	3.2
1	B	171	CYS	3.2
1	B	389	HIS	3.2
1	A	422	THR	3.2
1	A	333	MET	3.1
1	A	339	LYS	3.1
1	A	396	LYS	3.1
1	A	182	ILE	3.1
1	A	153	SER	3.1
1	B	243	LEU	3.1
1	B	318	LEU	3.1
1	A	476	GLY	3.1
1	A	41	GLU	3.1
1	A	56	VAL	3.1
1	B	199	LYS	3.1
1	A	92	PRO	3.1
1	B	154	ASP	3.1
1	B	210	LEU	3.1
1	A	12	LYS	3.1
1	B	462	THR	3.1
1	A	203	TRP	3.1
1	B	330	VAL	3.1
1	A	416	GLU	3.1
1	A	401	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	305	ASP	3.1
1	A	240	TYR	3.1
1	B	247	TYR	3.1
1	B	374	TYR	3.1
1	A	67	ILE	3.1
1	B	282	LYS	3.1
1	B	98	ALA	3.1
1	B	273	ALA	3.1
1	A	287	THR	3.1
1	A	324	PHE	3.1
1	B	393	SER	3.1
1	A	390	PRO	3.0
1	B	56	VAL	3.0
1	B	143	TYR	3.0
1	B	174	ASN	3.0
1	B	328	LEU	3.0
1	B	335	ILE	3.0
1	B	434	LEU	3.0
1	B	259	ALA	3.0
1	A	377	MET	3.0
1	B	281	LYS	3.0
1	B	196	GLU	3.0
1	A	208	ILE	3.0
1	A	489	LEU	3.0
1	B	34	ALA	3.0
1	B	290	LEU	3.0
1	B	452	ILE	3.0
1	B	501	LYS	3.0
1	B	73	GLY	3.0
1	B	458	ASN	3.0
1	A	35	VAL	3.0
1	B	35	VAL	3.0
1	B	297	VAL	3.0
1	B	426	VAL	3.0
1	B	55	ASP	3.0
1	B	181	GLN	3.0
1	B	425	ALA	3.0
1	A	372	ILE	3.0
1	B	23	ILE	3.0
1	B	59	LEU	3.0
1	B	118	MET	3.0
1	B	388	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	489	LEU	3.0
1	B	175	GLU	3.0
1	A	145	ASN	3.0
1	B	183	GLY	3.0
1	B	221	PRO	3.0
1	B	310	PRO	3.0
1	A	65	VAL	2.9
1	A	119	VAL	2.9
1	B	253	ASP	2.9
1	B	165	HIS	2.9
1	A	100	LYS	2.9
1	A	126	ALA	2.9
1	A	129	LEU	2.9
1	A	134	ILE	2.9
1	B	80	ASN	2.9
1	B	37	GLY	2.9
1	B	406	PRO	2.9
1	A	265	ASP	2.9
1	A	266	ASP	2.9
1	B	177	ASP	2.9
1	B	205	ASP	2.9
1	B	113	MET	2.9
1	B	153	SER	2.9
1	A	5	LYS	2.9
1	A	202	LYS	2.9
1	B	294	GLU	2.9
1	B	347	ALA	2.9
1	B	140	LEU	2.9
1	A	490	PRO	2.9
1	A	94	ARG	2.9
1	B	326	ASP	2.9
1	B	306	LYS	2.9
1	B	18	GLU	2.9
1	A	211	VAL	2.9
1	A	330	VAL	2.9
1	A	353	VAL	2.9
1	A	374	TYR	2.9
1	B	90	GLN	2.9
1	B	337	LEU	2.9
1	A	439	ASP	2.9
1	B	293	ASP	2.9
1	A	473	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	415	ASN	2.9
1	B	376	PHE	2.8
1	B	156	ARG	2.8
1	B	60	VAL	2.8
1	A	178	GLY	2.8
1	A	385	GLY	2.8
1	B	130	GLY	2.8
1	B	61	LYS	2.8
1	A	63	LEU	2.8
1	A	289	HIS	2.8
1	B	329	LEU	2.8
1	A	171	CYS	2.8
1	B	207	THR	2.8
1	A	20	ASP	2.8
1	B	38	GLY	2.8
1	A	386	VAL	2.8
1	B	496	VAL	2.8
1	A	147	PRO	2.8
1	B	446	TYR	2.8
1	B	124	ASN	2.8
1	B	302	ASN	2.8
1	B	192	ARG	2.8
1	B	360	MET	2.8
1	B	398	ASP	2.8
1	B	295	TRP	2.8
1	B	216	SER	2.8
1	A	381	VAL	2.8
1	B	296	ASN	2.8
1	A	23	ILE	2.8
1	A	497	ILE	2.8
1	B	19	ILE	2.8
1	B	185	LYS	2.8
1	B	363	LYS	2.8
1	B	233	HIS	2.8
1	B	160	GLY	2.8
1	B	126	ALA	2.7
1	B	350	ALA	2.7
1	A	424	PHE	2.7
1	B	74	ASN	2.7
1	B	324	PHE	2.7
1	B	315	PRO	2.7
1	B	469	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	TYR	2.7
1	A	205	ASP	2.7
1	B	432	ASP	2.7
1	B	449	ILE	2.7
1	A	233	HIS	2.7
1	B	336	THR	2.7
1	A	84	GLY	2.7
1	A	383	GLY	2.7
1	B	110	ASN	2.7
1	A	347	ALA	2.7
1	A	350	ALA	2.7
1	A	118	MET	2.7
1	A	206	PRO	2.7
1	B	92	PRO	2.7
1	B	375	PRO	2.7
1	A	271	VAL	2.7
1	A	24	TYR	2.7
1	A	373	TYR	2.7
1	B	289	HIS	2.7
1	A	131	THR	2.7
1	A	169	THR	2.7
1	B	229	THR	2.7
1	B	41	GLU	2.7
1	B	263	GLU	2.7
1	A	80	ASN	2.7
1	B	128	ASN	2.7
1	B	219	ASN	2.7
1	B	333	MET	2.7
1	B	491	LYS	2.7
1	B	474	ARG	2.7
1	B	101	SER	2.7
1	B	332	CYS	2.7
1	B	382	TYR	2.7
1	B	279	LYS	2.7
1	B	121	ALA	2.7
1	B	340	HIS	2.6
1	A	291	SER	2.6
1	A	124	ASN	2.6
1	A	235	TYR	2.6
1	A	57	ILE	2.6
1	A	498	ARG	2.6
1	B	33	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	91	ARG	2.6
1	B	132	ARG	2.6
1	B	303	GLU	2.6
1	A	270	SER	2.6
1	A	74	ASN	2.6
1	B	125	MET	2.6
1	B	139	ASN	2.6
1	B	176	MET	2.6
1	A	78	GLY	2.6
1	A	55	ASP	2.6
1	A	83	ASP	2.6
1	A	352	LEU	2.6
1	B	53	ARG	2.6
1	B	89	GLU	2.6
1	A	382	TYR	2.6
1	B	353	VAL	2.6
1	B	470	VAL	2.6
1	A	284	SER	2.6
1	B	168	LYS	2.6
1	A	105	ASN	2.6
1	A	219	ASN	2.6
1	A	25	GLY	2.6
1	A	73	GLY	2.6
1	B	498	ARG	2.6
1	B	83	ASP	2.6
1	A	351	GLN	2.6
1	B	97	LEU	2.6
1	A	238	VAL	2.6
1	A	344	VAL	2.6
1	A	168	LYS	2.6
1	B	182	ILE	2.6
1	B	400	LYS	2.6
1	A	11	GLU	2.6
1	A	89	GLU	2.6
1	B	209	GLU	2.6
1	B	25	GLY	2.5
1	B	54	GLN	2.5
1	A	139	ASN	2.5
1	A	225	GLU	2.5
1	A	419	GLU	2.5
1	A	274	ILE	2.5
1	B	67	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	68	ILE	2.5
1	A	461	GLN	2.5
1	B	422	THR	2.5
1	B	159	HIS	2.5
1	B	237	HIS	2.5
1	A	363	LYS	2.5
1	A	175	GLU	2.5
1	B	437	GLU	2.5
1	A	357	ALA	2.5
1	A	412	ALA	2.5
1	B	274	ILE	2.5
1	B	120	GLY	2.5
1	A	201	MET	2.5
1	A	455	GLU	2.5
1	A	170	TRP	2.5
1	A	276	ASP	2.5
1	A	198	ALA	2.5
1	B	36	TYR	2.5
1	B	341	ALA	2.5
1	A	30	HIS	2.5
1	A	120	GLY	2.5
1	B	108	GLY	2.5
1	A	359	ILE	2.5
1	B	117	LYS	2.5
1	A	474	ARG	2.5
1	B	309	GLU	2.5
1	B	439	ASP	2.4
1	B	95	LEU	2.4
1	B	417	GLU	2.4
1	A	338	MET	2.4
1	A	358	PRO	2.4
1	B	26	SER	2.4
1	B	211	VAL	2.4
1	B	468	SER	2.4
1	A	110	ASN	2.4
1	A	296	ASN	2.4
1	B	401	ASP	2.4
1	B	189	GLU	2.4
1	B	202	LYS	2.4
1	B	369	LYS	2.4
1	A	472	PRO	2.4
1	B	349	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	472	PRO	2.4
1	B	490	PRO	2.4
1	A	77	SER	2.4
1	A	148	SER	2.4
1	B	261	SER	2.4
1	A	232	ASP	2.4
1	B	82	GLU	2.4
1	A	33	ARG	2.4
1	B	100	LYS	2.4
1	B	384	ARG	2.4
1	A	165	HIS	2.4
1	A	237	HIS	2.4
1	B	476	GLY	2.4
1	A	46	GLN	2.4
1	B	270	SER	2.4
1	A	334	LEU	2.4
1	B	454	LEU	2.4
1	B	488	THR	2.4
1	A	239	ASP	2.4
1	B	265	ASP	2.4
1	B	21	LYS	2.4
1	B	386	VAL	2.4
1	A	54	GLN	2.3
1	B	410	SER	2.3
1	B	415	ASN	2.3
1	A	375	PRO	2.3
1	A	18	GLU	2.3
1	B	96	ASP	2.3
1	B	232	ASP	2.3
1	B	477	ASP	2.3
1	A	166	LYS	2.3
1	A	49	GLU	2.3
1	A	66	PRO	2.3
1	B	264	MET	2.3
1	B	479	GLN	2.3
1	A	277	TYR	2.3
1	A	196	GLU	2.3
1	A	69	ARG	2.3
1	A	93	ARG	2.3
1	A	477	ASP	2.3
1	A	234	THR	2.3
1	A	121	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	231	LEU	2.3
1	A	62	GLU	2.3
1	B	455	GLU	2.3
1	B	105	ASN	2.3
1	A	152	TYR	2.3
1	A	199	LYS	2.3
1	A	286	LYS	2.3
1	B	24	TYR	2.3
1	A	500	GLY	2.3
1	B	266	ASP	2.3
1	B	377	MET	2.3
1	B	66	PRO	2.2
1	B	387	ALA	2.2
1	B	239	ASP	2.2
1	A	79	TYR	2.2
1	A	190	TYR	2.2
1	B	257	TYR	2.2
1	B	62	GLU	2.2
1	B	227	GLU	2.2
1	B	358	PRO	2.2
1	B	390	PRO	2.2
1	B	7	THR	2.2
1	B	69	ARG	2.2
1	A	475	ASN	2.2
1	A	177	ASP	2.2
1	B	385	GLY	2.2
1	A	209	GLU	2.2
1	A	22	ARG	2.2
1	A	132	ARG	2.2
1	A	156	ARG	2.2
1	B	22	ARG	2.2
1	A	21	LYS	2.2
1	A	127	VAL	2.2
1	A	113	MET	2.2
1	A	137	ALA	2.2
1	A	387	ALA	2.2
1	B	379	ALA	2.2
1	A	82	GLU	2.2
1	A	111	GLU	2.2
1	A	163	GLU	2.2
1	B	499	LEU	2.2
1	A	264	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	114	ASP	2.1
1	B	236	ASP	2.1
1	B	11	GLU	2.1
1	A	34	ALA	2.1
1	B	478	ALA	2.1
1	B	249	ASN	2.1
1	B	485	VAL	2.1
1	A	185	LYS	2.1
1	B	162	LYS	2.1
1	B	256	ASN	2.1
1	A	154	ASP	2.1
1	A	326	ASP	2.1
1	B	20	ASP	2.1
1	B	343	ARG	2.1
1	A	285	LYS	2.1
1	B	339	LYS	2.1
1	A	58	GLU	2.1
1	A	26	SER	2.1
1	B	13	ASP	2.1
1	A	159	HIS	2.1
1	A	88	LYS	2.1
1	A	281	LYS	2.1
1	A	160	GLY	2.0
1	B	149	GLY	2.0
1	A	325	GLU	2.0
1	B	122	GLU	2.0
1	A	293	ASP	2.0
1	A	192	ARG	2.0
1	B	436	LEU	2.0
1	A	227	GLU	2.0
1	B	475	ASN	2.0
1	A	428	ARG	2.0
1	B	28	ILE	2.0
1	B	138	ARG	2.0
1	B	320	ASP	2.0
1	B	342	ASP	2.0
1	A	348	CYS	2.0
1	A	162	LYS	2.0
1	B	12	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 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($\text{\AA}^2$)	Q<0.9
2	GOL	A	503	6/6	0.75	0.17	24,27,31,32	0
2	GOL	B	503	6/6	0.78	0.20	25,28,32,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.