



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:24 AM UTC

PDB ID : 4AMW / pdb_00004amw
Title : CRYSTAL STRUCTURE OF THE GRACILARIOPSIS LEMANEIFORMIS
ALPHA-1,4- GLUCAN LYASE Covalent Intermediate Complex with 5-fluoro-
idosyl- fluoride
Authors : Rozeboom, H.J.; Yu, S.; Madrid, S.; Kalk, K.H.; Dijkstra, B.W.
Deposited on : 2012-03-14
Resolution : 1.90 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

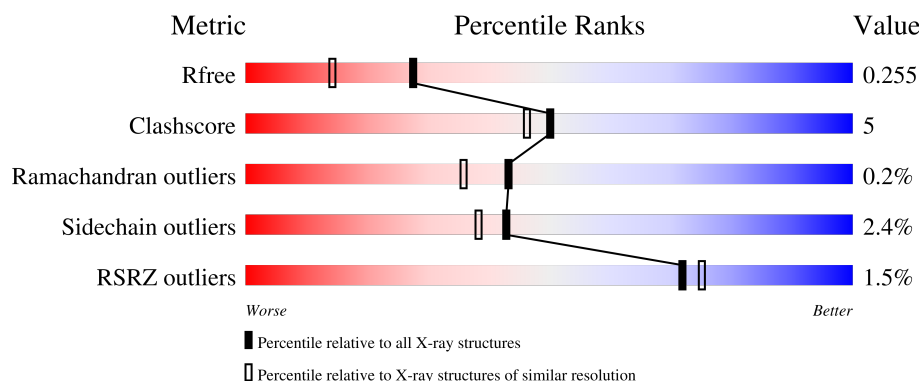
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1027	% 88%12%
1	B	1027	2% 88%11%
1	C	1027	2% 87%12%
1	D	1027	% 86%13%

2 Entry composition [i](#)

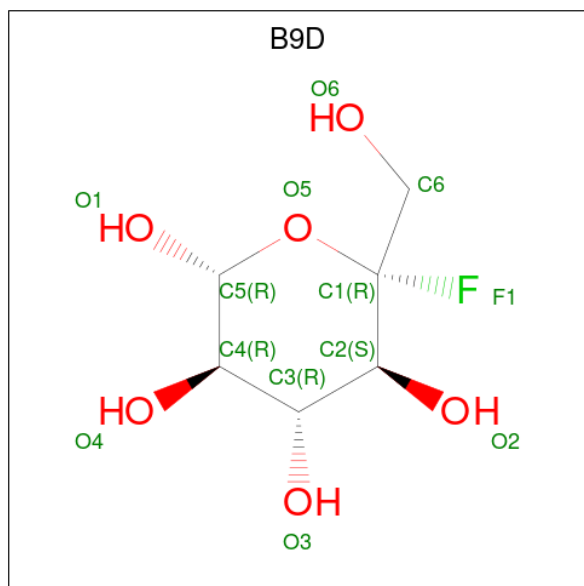
There are 5 unique types of molecules in this entry. The entry contains 35670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-1,4-GLUCAN LYASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1025	Total	C	N	O	S	0	1	0
			8170	5140	1386	1596	48			
1	B	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	C	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	D	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			

- Molecule 2 is 5-fluoro-alpha-L-idopyranose (CCD ID: B9D) (formula: C₆H₁₁FO₆).



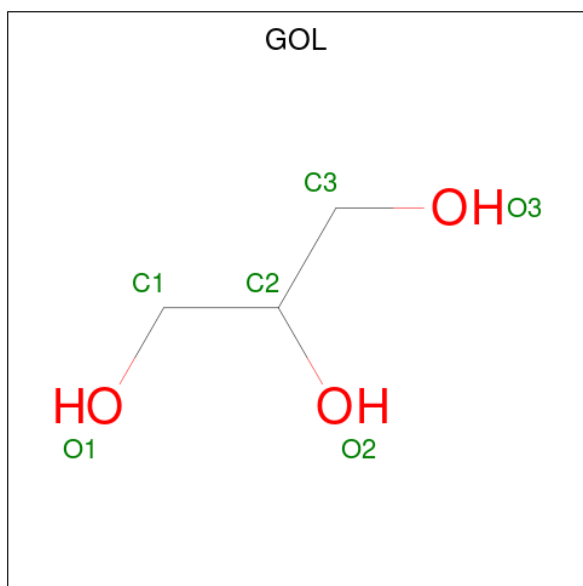
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			12	6	1	5		
2	B	1	Total	C	F	O	0	0
			12	6	1	5		

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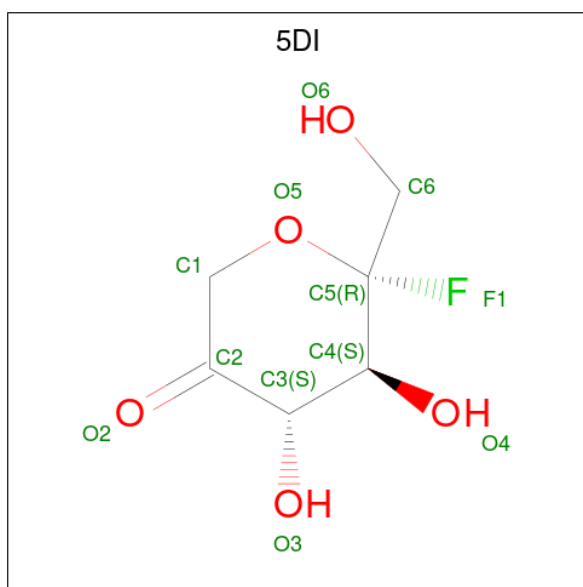
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is alpha-D-threo-hexo-2,5-diulo-2,6-pyranosyl fluoride (CCD ID: 5DI) (formula: $C_6H_9FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	F	O	0	0
			12	6	1	5		

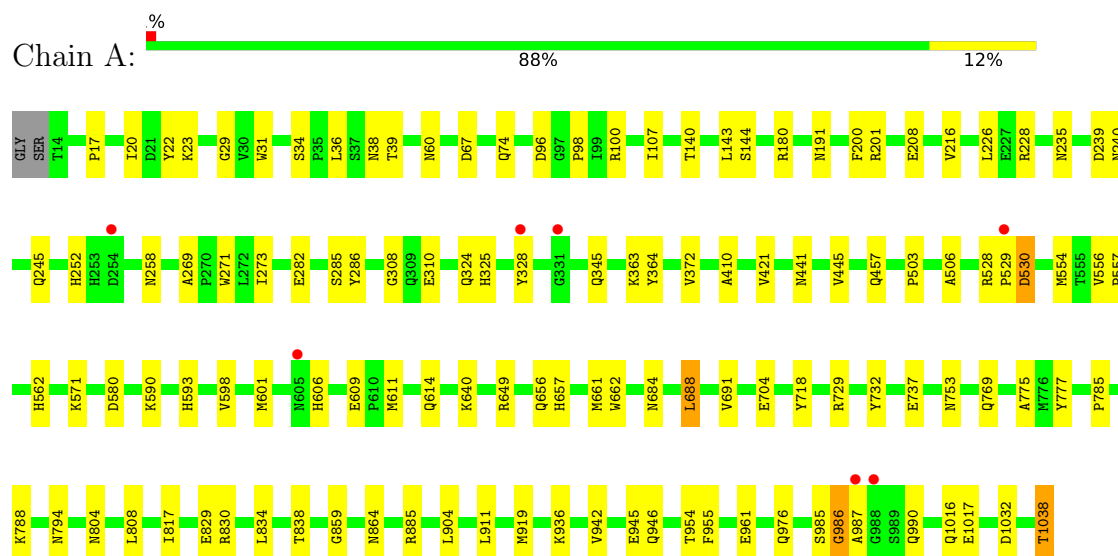
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	901	Total	O	0	0
			901	901		
5	B	548	Total	O	0	0
			548	548		
5	C	581	Total	O	0	0
			581	581		
5	D	894	Total	O	0	0
			894	894		

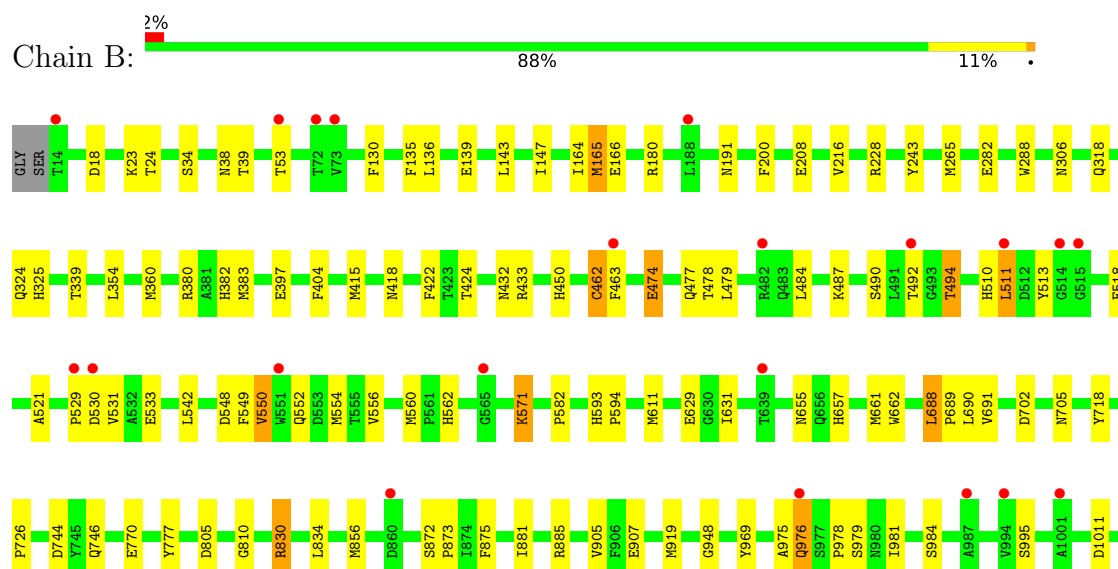
3 Residue-property plots [i](#)

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: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

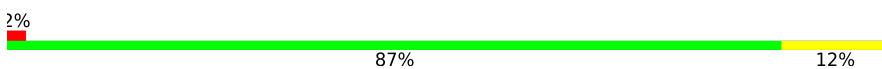


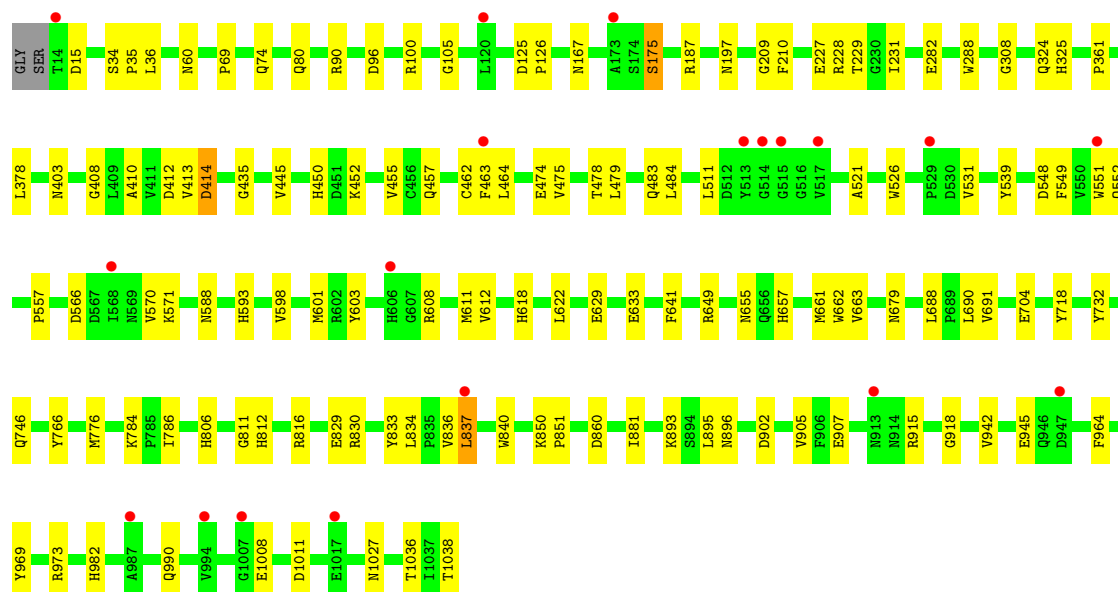
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1



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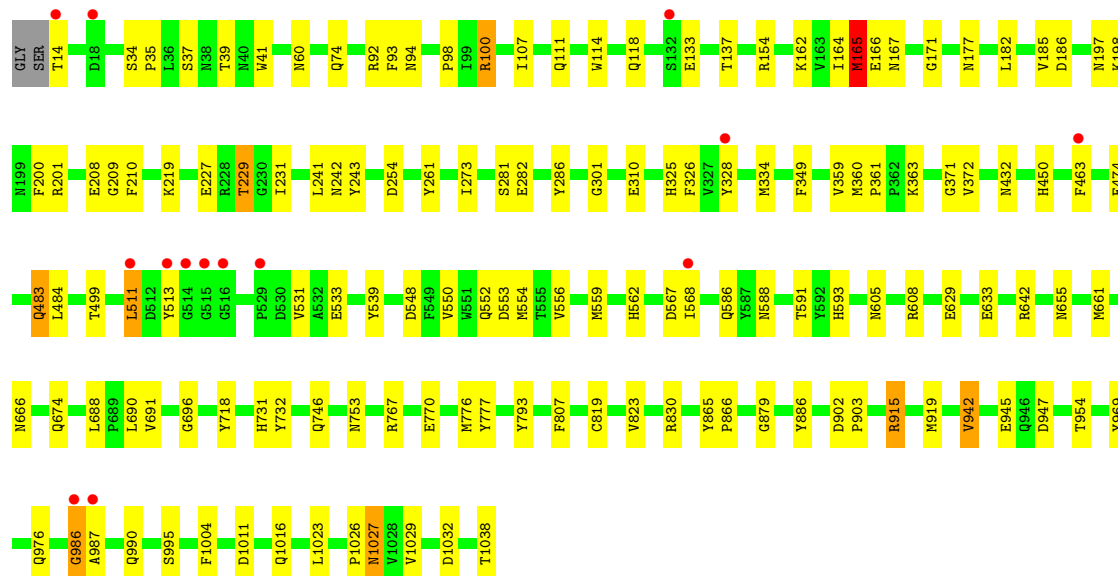
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

Chain C:  87% 12%



• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

Chain D:  86% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.10Å 97.30Å 136.28Å 80.31° 83.29° 85.21°	Depositor
Resolution (Å)	43.57 – 1.90 43.57 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.5 (43.57-1.90) 93.5 (43.57-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.207 , 0.254 0.208 , 0.255	Depositor DCC
R_{free} test set	17168 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35670	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.61% 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, CSO, B9D, 5DI

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	0.97	4/8382 (0.0%)	1.01	8/11399 (0.1%)
1	B	0.75	3/8374 (0.0%)	0.90	11/11389 (0.1%)
1	C	0.73	1/8374 (0.0%)	0.89	6/11389 (0.1%)
1	D	0.93	3/8374 (0.0%)	1.00	7/11389 (0.1%)
All	All	0.86	11/33504 (0.0%)	0.95	32/45566 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	976	GLN	CA-C	13.99	1.71	1.52
1	B	556	VAL	CA-CB	11.64	1.59	1.54
1	B	975	ALA	C-N	-7.88	1.22	1.33
1	A	273	ILE	N-CA	-6.84	1.38	1.46
1	D	556	VAL	CA-CB	6.18	1.58	1.53
1	A	421	VAL	CA-CB	5.93	1.60	1.54
1	C	435	GLY	N-CA	5.74	1.49	1.44
1	D	567	ASP	C-N	-5.42	1.27	1.34
1	A	271	TRP	N-CA	-5.21	1.39	1.46
1	A	285	SER	CA-C	-5.12	1.46	1.52
1	D	767	ARG	N-CA	-5.02	1.40	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	556	VAL	N-CA-CB	7.85	115.45	110.50
1	B	571	LYS	CA-C-N	-5.95	114.63	120.52
1	B	571	LYS	C-N-CA	-5.95	114.63	120.52
1	C	784	LYS	CA-C-N	-5.87	113.92	119.85
1	C	784	LYS	C-N-CA	-5.87	113.92	119.85
1	B	631	ILE	N-CA-C	5.83	116.48	110.82
1	C	902	ASP	CA-C-N	5.60	125.92	119.93
1	C	902	ASP	C-N-CA	5.60	125.92	119.93
1	B	810	GLY	N-CA-C	5.59	119.24	112.48
1	B	556	VAL	N-CA-CB	5.50	114.21	110.52
1	A	258	ASN	CA-C-N	-5.46	114.13	119.76
1	A	258	ASN	C-N-CA	-5.46	114.13	119.76
1	A	528	ARG	CA-C-N	-5.43	114.37	119.85
1	A	528	ARG	C-N-CA	-5.43	114.37	119.85
1	A	240	ASN	N-CA-C	5.36	117.27	109.71
1	D	34	SER	CA-C-N	5.25	125.06	119.28
1	D	34	SER	C-N-CA	5.25	125.06	119.28
1	B	404	PHE	CA-C-N	-5.21	114.43	119.90
1	B	404	PHE	C-N-CA	-5.21	114.43	119.90
1	A	775	ALA	N-CA-C	-5.20	105.69	111.36
1	B	34	SER	CA-C-N	5.19	124.99	119.28
1	B	34	SER	C-N-CA	5.19	124.99	119.28
1	D	879	GLY	N-CA-C	-5.17	107.67	115.32
1	A	34	SER	CA-C-N	5.09	124.70	119.05
1	A	34	SER	C-N-CA	5.09	124.70	119.05
1	B	834	LEU	CA-C-N	5.08	124.99	119.76
1	B	834	LEU	C-N-CA	5.08	124.99	119.76
1	D	94	ASN	CA-C-N	-5.07	114.82	120.45
1	D	94	ASN	C-N-CA	-5.07	114.82	120.45
1	C	105	GLY	CA-C-N	5.04	124.83	119.28
1	C	105	GLY	C-N-CA	5.04	124.83	119.28
1	D	165	MET	CG-SD-CE	-5.02	89.85	100.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	529	PRO	Peptide

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	8170	0	7614	82	0
1	B	8162	0	7606	73	0
1	C	8162	0	7606	79	0
1	D	8162	0	7606	101	0
2	A	12	0	9	1	0
2	B	12	0	9	2	0
2	C	12	0	8	0	0
3	A	24	0	32	1	0
3	B	6	0	8	1	0
3	D	12	0	16	1	0
4	D	12	0	9	4	0
5	A	901	0	0	17	0
5	B	548	0	0	14	0
5	C	581	0	0	7	0
5	D	894	0	0	28	0
All	All	35670	0	30523	334	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 5.

All (334) 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:D:37:SER:HB2	5:D:2028:HOH:O	1.27	1.34
1:B:462:CYS:HB2	5:B:2303:HOH:O	1.39	1.22
1:D:586:GLN:HG2	5:D:2529:HOH:O	1.49	1.10
1:C:776:MET:CE	1:C:786:ILE:HD11	1.81	1.09
1:C:210:PHE:H	1:C:229:THR:HG22	1.19	1.07
1:D:219:LYS:HD2	5:D:2241:HOH:O	1.55	1.06
1:D:182:LEU:HB3	5:D:2208:HOH:O	1.55	1.05
1:A:562:HIS:HD2	1:A:593:HIS:HE1	1.08	1.01
1:C:776:MET:HE2	1:C:786:ILE:HD11	1.42	1.00
1:C:598:VAL:HG11	1:C:611:MET:HE2	1.48	0.96
1:D:41:TRP:CD1	5:D:2029:HOH:O	2.27	0.88
1:C:776:MET:HE1	1:C:786:ILE:HD11	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:PHE:CE1	5:D:2208:HOH:O	2.28	0.85
1:B:38:ASN:HD21	1:B:180:ARG:HH11	1.24	0.84
1:A:562:HIS:HD2	1:A:593:HIS:CE1	1.95	0.82
1:D:165:MET:HE1	1:D:326:PHE:CD1	2.15	0.82
1:D:210:PHE:H	1:D:229:THR:HG22	1.44	0.81
1:D:463:PHE:CE2	1:D:511:LEU:HD22	2.16	0.80
1:A:1038:THR:HG22	5:A:2863:HOH:O	1.82	0.79
1:C:325:HIS:HD2	5:C:2048:HOH:O	1.66	0.79
1:D:947:ASP:HB2	5:D:2774:HOH:O	1.83	0.79
1:A:38:ASN:HD21	1:A:180:ARG:HH11	1.34	0.76
1:A:601:MET:H	1:A:614:GLN:HE22	1.32	0.75
1:B:976:GLN:HB3	5:B:2527:HOH:O	1.85	0.75
1:C:210:PHE:H	1:C:229:THR:CG2	1.95	0.75
1:A:598:VAL:HG11	1:A:611:MET:HE2	1.69	0.74
1:C:806:HIS:HE1	1:C:833:TYR:H	1.36	0.73
1:C:227:GLU:HG2	1:C:229:THR:HG23	1.71	0.72
1:B:24:THR:HG21	1:B:318:GLN:OE1	1.89	0.71
1:A:1017:GLU:OE2	5:A:2759:HOH:O	2.08	0.71
1:A:503:PRO:HG2	1:A:506:ALA:HB2	1.72	0.70
1:D:227:GLU:OE2	1:D:229:THR:CG2	2.41	0.69
1:D:227:GLU:OE2	1:D:229:THR:HG21	1.92	0.69
1:B:995:SER:HB2	1:B:1011:ASP:HB3	1.75	0.67
1:D:450:HIS:HD2	5:D:2462:HOH:O	1.76	0.67
1:B:382:HIS:CD2	1:B:432:ASN:HB2	2.29	0.67
1:B:905:VAL:HG22	1:B:969:TYR:HB2	1.75	0.67
1:D:976:GLN:HE22	1:D:1016:GLN:HA	1.59	0.67
1:A:640:LYS:HE2	5:A:2599:HOH:O	1.94	0.67
1:D:753:ASN:ND2	5:D:2616:HOH:O	2.26	0.66
1:B:383:MET:HE1	5:B:2251:HOH:O	1.95	0.66
1:A:529:PRO:O	1:A:530:ASP:HB2	1.96	0.65
1:D:562:HIS:HD2	1:D:593:HIS:NE2	1.94	0.65
1:A:562:HIS:CD2	1:A:593:HIS:HE1	2.00	0.64
1:B:856:MET:HE1	1:B:875:PHE:CE1	2.33	0.64
1:B:200:PHE:HB2	1:B:208:GLU:HG3	1.80	0.64
1:A:282:GLU:HB3	5:A:2322:HOH:O	1.97	0.63
1:B:288:TRP:NE1	1:B:324:GLN:OE1	2.30	0.63
1:C:227:GLU:OE2	1:C:229:THR:HG21	1.98	0.63
1:D:629:GLU:HG3	1:D:633:GLU:OE2	1.98	0.63
1:C:209:GLY:HA2	1:C:229:THR:HG21	1.81	0.63
1:D:995:SER:HB2	1:D:1011:ASP:HB3	1.81	0.62
1:D:513:TYR:HE1	1:D:554:MET:HE2	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:TYR:CE1	1:D:554:MET:CE	2.83	0.62
1:A:23:LYS:H	1:A:191:ASN:HD21	1.47	0.61
1:A:457:GLN:NE2	1:A:729:ARG:HH11	1.97	0.61
1:B:38:ASN:HD21	1:B:180:ARG:NH1	1.96	0.61
1:A:704:GLU:HG3	5:A:2287:HOH:O	2.00	0.61
1:D:1016:GLN:OE1	5:D:2850:HOH:O	2.16	0.61
1:C:776:MET:CE	1:C:786:ILE:CD1	2.71	0.61
1:A:601:MET:H	1:A:614:GLN:NE2	1.97	0.61
1:A:961:GLU:HG2	5:A:2830:HOH:O	2.00	0.61
1:C:479:LEU:HD12	1:C:484:LEU:HB2	1.83	0.60
1:C:464:LEU:HD22	1:C:475:VAL:HG12	1.82	0.60
1:A:39:THR:HA	1:A:67:ASP:OD2	2.02	0.60
1:B:856:MET:HE1	1:B:875:PHE:HE1	1.67	0.60
1:A:410:ALA:HB2	1:A:457:GLN:HE21	1.67	0.60
1:C:210:PHE:N	1:C:229:THR:HG22	2.04	0.59
1:B:463:PHE:CD2	1:B:511:LEU:HD22	2.38	0.59
1:C:806:HIS:CE1	1:C:833:TYR:H	2.19	0.59
1:C:557:PRO:HD3	1:C:618:HIS:CE1	2.38	0.58
1:D:35:PRO:O	5:D:2029:HOH:O	2.17	0.58
1:D:197:ASN:ND2	5:D:2212:HOH:O	2.35	0.58
1:A:794:ASN:ND2	5:A:2325:HOH:O	2.35	0.58
1:B:657:HIS:HD2	5:B:2220:HOH:O	1.85	0.58
1:C:15:ASP:OD1	1:C:608:ARG:HD3	2.03	0.58
1:D:499:THR:HG23	1:D:568:ILE:HD12	1.86	0.58
1:C:457:GLN:HA	1:C:549:PHE:O	2.04	0.58
1:C:167:ASN:HA	1:C:197:ASN:HA	1.85	0.58
1:C:776:MET:HE1	1:C:786:ILE:CD1	2.31	0.58
1:D:137:THR:HG21	5:D:2158:HOH:O	2.03	0.58
1:B:463:PHE:CE2	1:B:511:LEU:HD22	2.38	0.57
1:C:452:LYS:HE2	5:C:2302:HOH:O	2.04	0.57
1:C:80:GLN:HE22	1:C:90:ARG:HH11	1.51	0.57
1:D:137:THR:HG23	5:D:2154:HOH:O	2.03	0.57
1:D:209:GLY:HA2	1:D:229:THR:HG21	1.86	0.57
1:B:510:HIS:C	1:B:511:LEU:HG	2.29	0.57
1:C:227:GLU:OE2	1:C:229:THR:CG2	2.53	0.56
1:C:566:ASP:HB3	1:C:570:VAL:CG2	2.35	0.56
1:C:464:LEU:HD22	1:C:475:VAL:CG1	2.35	0.56
1:D:539:TYR:OH	1:D:552:GLN:NE2	2.34	0.56
1:A:657:HIS:HE1	5:A:2370:HOH:O	1.88	0.56
1:D:165:MET:HG2	1:D:166:GLU:N	2.21	0.56
1:A:325:HIS:HE1	5:A:2112:HOH:O	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:MET:HE1	1:D:326:PHE:CE1	2.41	0.56
1:B:339:THR:HG22	5:B:2042:HOH:O	2.06	0.55
1:B:560:MET:SD	1:B:571:LYS:HG3	2.46	0.55
1:D:93:PHE:CZ	5:D:2208:HOH:O	2.52	0.55
1:B:380:ARG:HD3	5:B:2237:HOH:O	2.07	0.55
1:D:642:ARG:HD3	5:D:2555:HOH:O	2.06	0.55
1:C:588:ASN:HB3	1:C:593:HIS:CE1	2.42	0.55
1:A:794:ASN:H	3:A:1043:GOL:H31	1.71	0.55
1:D:463:PHE:CD2	1:D:511:LEU:HD13	2.42	0.55
1:A:556:VAL:N	1:A:557:PRO:HA	2.21	0.55
1:D:777:TYR:HE2	1:D:919:MET:CE	2.20	0.55
1:B:463:PHE:CD1	1:B:511:LEU:HD13	2.42	0.54
1:D:100:ARG:NH1	5:D:2115:HOH:O	2.40	0.54
1:D:371:GLY:C	1:D:731:HIS:HD2	2.15	0.54
1:C:96:ASP:OD1	1:C:187:ARG:HD2	2.08	0.54
1:A:785:PRO:O	1:A:788:LYS:HE3	2.07	0.54
1:B:594:PRO:HG3	5:B:2141:HOH:O	2.07	0.54
1:D:201:ARG:HD3	1:D:310:GLU:O	2.08	0.54
1:B:492:THR:HG23	1:B:494:THR:OG1	2.07	0.54
1:D:513:TYR:CE1	1:D:554:MET:HE2	2.43	0.54
1:A:100:ARG:HD2	5:A:2054:HOH:O	2.07	0.54
1:C:60:ASN:HB3	1:C:74:GLN:OE1	2.09	0.53
1:D:325:HIS:HE1	5:D:2101:HOH:O	1.90	0.53
1:B:479:LEU:HD12	1:B:484:LEU:HB2	1.90	0.53
1:D:154:ARG:HG2	1:D:166:GLU:HG2	1.90	0.53
1:D:165:MET:CE	1:D:326:PHE:CD1	2.89	0.53
1:D:746:GLN:CD	5:D:2579:HOH:O	2.51	0.53
1:A:737:GLU:HG3	5:A:2415:HOH:O	2.08	0.53
1:A:985:SER:O	1:A:986:GLY:C	2.51	0.53
1:A:20:ILE:HD11	1:A:96:ASP:HB3	1.90	0.53
1:A:226:LEU:H	1:A:804:ASN:ND2	2.06	0.53
1:B:136:LEU:HD23	1:B:147:ILE:HD12	1.89	0.53
1:B:490:SER:HB2	1:B:492:THR:HG22	1.91	0.53
1:C:905:VAL:HG22	1:C:969:TYR:HB2	1.90	0.53
1:A:345:GLN:NE2	1:A:656:GLN:HE22	2.07	0.53
1:A:834:LEU:O	1:A:859:GLY:N	2.30	0.53
1:C:69:PRO:HB2	1:C:175:SER:OG	2.08	0.53
1:A:22:TYR:OH	1:A:609:GLU:OE1	2.25	0.52
1:B:463:PHE:HB2	1:B:521:ALA:HB1	1.92	0.52
1:B:744:ASP:OD2	3:B:1040:GOL:H31	2.09	0.52
1:A:74:GLN:NE2	5:A:2086:HOH:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:696:GLY:HA3	5:D:2579:HOH:O	2.10	0.52
1:C:464:LEU:HD13	1:C:479:LEU:HD22	1.90	0.52
1:D:450:HIS:HE1	1:D:548:ASP:OD1	1.92	0.52
1:B:978:PRO:HG3	1:B:981:ILE:HD11	1.92	0.52
1:B:562:HIS:ND1	1:B:593:HIS:HE1	2.08	0.51
1:D:286:TYR:HB3	1:D:328:TYR:CD2	2.46	0.51
1:C:641:PHE:CZ	1:C:896:ASN:HB2	2.44	0.51
1:D:1026:PRO:O	1:D:1029:VAL:HG22	2.10	0.51
1:A:554[A]:MET:HE3	2:A:1039:B9D:C5	2.41	0.51
1:C:484:LEU:HB3	1:C:531:VAL:HG22	1.92	0.51
1:B:165:MET:HG2	1:B:166:GLU:N	2.26	0.51
1:B:325:HIS:HD2	5:B:2041:HOH:O	1.93	0.51
1:D:661:MET:O	1:D:691:VAL:HA	2.11	0.51
1:A:441:ASN:ND2	1:C:403:ASN:HD22	2.08	0.51
1:C:378:LEU:HD13	1:C:445:VAL:HG23	1.93	0.51
1:B:805:ASP:CG	1:B:830:ARG:HH22	2.19	0.50
1:C:452:LYS:CE	5:C:2302:HOH:O	2.59	0.50
1:B:770:GLU:HG2	1:B:885:ARG:HG2	1.93	0.50
1:C:100:ARG:HG3	1:C:603:TYR:CE1	2.46	0.50
1:C:850:LYS:HB2	1:C:851:PRO:HD2	1.92	0.50
1:D:533:GLU:HA	1:D:629:GLU:HG2	1.93	0.50
1:D:986:GLY:O	1:D:987:ALA:HB3	2.12	0.50
1:D:513:TYR:CE1	1:D:554:MET:HE3	2.46	0.50
1:D:111:GLN:HE21	1:D:111:GLN:HA	1.78	0.49
1:A:252:HIS:HE1	1:A:580:ASP:OD1	1.95	0.49
1:A:657:HIS:HD2	5:A:2388:HOH:O	1.96	0.49
1:C:982:HIS:HB3	1:C:1036:THR:CG2	2.42	0.49
1:D:111:GLN:HE22	1:D:349:PHE:H	1.60	0.49
1:A:363:LYS:NZ	1:A:769:GLN:HE21	2.10	0.49
1:A:961:GLU:CG	5:A:2830:HOH:O	2.59	0.49
1:C:915:ARG:NH1	1:C:945:GLU:OE2	2.45	0.49
1:D:114:TRP:O	1:D:118:GLN:HG2	2.12	0.49
1:C:412:ASP:HB3	1:C:414:ASP:OD1	2.12	0.49
1:B:511:LEU:O	1:B:518:GLU:HB2	2.13	0.48
1:C:881:ILE:HB	1:C:918:GLY:HA3	1.95	0.48
1:D:1032:ASP:CG	1:D:1032:ASP:O	2.55	0.48
1:A:777:TYR:HE2	1:A:919:MET:CE	2.26	0.48
1:A:885:ARG:HD2	1:A:904:LEU:HA	1.96	0.48
1:C:361:PRO:CD	1:C:776:MET:HG2	2.42	0.48
1:C:661:MET:HB2	1:C:691:VAL:HG23	1.95	0.48
1:C:1008:GLU:O	1:C:1011:ASP:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:GLU:OE1	1:A:864:ASN:HA	2.14	0.48
1:B:777:TYR:CE2	1:B:919:MET:CE	2.97	0.48
1:A:457:GLN:HE22	1:A:729:ARG:HH11	1.60	0.48
1:A:529:PRO:O	1:A:530:ASP:CB	2.61	0.48
1:B:593:HIS:HD2	5:B:2348:HOH:O	1.95	0.48
1:D:133:GLU:CD	1:D:133:GLU:H	2.21	0.48
1:A:216:VAL:O	1:A:228:ARG:NH2	2.40	0.48
1:A:556:VAL:N	1:A:557:PRO:CA	2.77	0.48
1:C:325:HIS:HE1	5:C:2053:HOH:O	1.96	0.48
1:B:474:GLU:HA	1:B:477:GLN:HB2	1.95	0.48
1:D:553:ASP:OD2	4:D:1041:5DI:H12C	2.12	0.48
1:A:976:GLN:HE22	1:A:1016:GLN:HG2	1.77	0.47
1:C:539:TYR:OH	1:C:552:GLN:NE2	2.46	0.47
1:C:812:HIS:CE1	5:C:2470:HOH:O	2.67	0.47
1:D:200:PHE:HB2	1:D:208:GLU:HG3	1.96	0.47
1:C:526:TRP:CZ2	1:C:622:LEU:HD13	2.48	0.47
1:B:463:PHE:HB2	1:B:521:ALA:CB	2.43	0.47
1:C:410:ALA:HB2	1:C:457:GLN:HE21	1.78	0.47
1:D:553:ASP:CG	4:D:1041:5DI:H12C	2.39	0.47
1:A:325:HIS:HD2	5:A:2099:HOH:O	1.98	0.47
1:A:554[A]:MET:HE2	1:A:649:ARG:CZ	2.44	0.47
1:A:976:GLN:HE22	1:A:1016:GLN:HA	1.78	0.47
1:B:422:PHE:HA	1:B:542:LEU:HD11	1.95	0.47
1:B:380:ARG:NH2	1:B:397:GLU:OE1	2.32	0.47
1:D:915:ARG:NH1	1:D:945:GLU:OE2	2.47	0.47
1:A:661:MET:HG2	1:A:688:LEU:HD11	1.96	0.47
1:C:612:VAL:O	5:C:2195:HOH:O	2.21	0.47
1:C:463:PHE:CD1	1:C:511:LEU:HD13	2.50	0.47
1:D:185:VAL:HG12	1:D:186:ASP:O	2.14	0.47
1:D:553:ASP:OD1	4:D:1041:5DI:H12C	2.15	0.47
1:A:976:GLN:NE2	1:A:1016:GLN:HG2	2.30	0.46
1:B:139:GLU:HB2	1:B:143:LEU:O	2.15	0.46
1:A:661:MET:HG3	1:A:688:LEU:HG	1.97	0.46
1:A:245:GLN:HE21	1:A:590:LYS:NZ	2.12	0.46
1:A:661:MET:O	1:A:691:VAL:HA	2.16	0.46
1:C:288:TRP:HE1	1:C:324:GLN:CD	2.24	0.46
1:D:942:VAL:HA	1:D:954:THR:O	2.15	0.46
1:B:450:HIS:HE1	1:B:548:ASP:OD1	1.98	0.46
1:B:484:LEU:HB3	1:B:531:VAL:HG22	1.97	0.46
1:B:661:MET:O	1:B:691:VAL:HA	2.15	0.46
1:A:226:LEU:H	1:A:804:ASN:HD22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:SER:HA	5:D:2647:HOH:O	2.16	0.46
1:B:474:GLU:O	1:B:474:GLU:HG2	2.16	0.46
1:D:60:ASN:HB3	1:D:74:GLN:HE21	1.80	0.46
1:D:696:GLY:CA	5:D:2579:HOH:O	2.63	0.46
1:A:201:ARG:HD3	1:A:310:GLU:O	2.16	0.46
1:B:23:LYS:H	1:B:191:ASN:HD21	1.64	0.46
1:B:777:TYR:CE2	1:B:919:MET:HE1	2.50	0.46
1:C:80:GLN:NE2	1:C:90:ARG:HH11	2.14	0.46
1:D:865:TYR:HA	1:D:866:PRO:HD3	1.85	0.46
1:A:777:TYR:CE2	1:A:919:MET:CE	2.99	0.46
1:B:661:MET:HG3	1:B:688:LEU:HG	1.96	0.46
1:B:243:TYR:CD1	1:B:265:MET:HE1	2.50	0.45
1:A:684:ASN:C	5:A:2620:HOH:O	2.58	0.45
1:B:513:TYR:CE1	1:B:554:MET:HE3	2.51	0.45
1:D:201:ARG:NH1	1:D:301:GLY:O	2.49	0.45
1:D:227:GLU:OE2	1:D:229:THR:HG23	2.14	0.45
1:D:363:LYS:NZ	1:D:770:GLU:OE2	2.44	0.45
1:D:793:TYR:HA	3:D:1040:GOL:H31	1.98	0.45
1:A:200:PHE:HB2	1:A:208:GLU:HG3	1.97	0.45
1:D:777:TYR:CE2	1:D:919:MET:HE2	2.51	0.45
1:B:777:TYR:HE2	1:B:919:MET:HE1	1.81	0.45
1:A:942:VAL:HA	1:A:954:THR:O	2.16	0.45
1:B:550:VAL:HG21	1:B:552:GLN:HE21	1.82	0.45
1:B:533:GLU:HA	1:B:629:GLU:HG2	1.99	0.45
1:A:1032:ASP:O	1:A:1032:ASP:CG	2.60	0.45
1:B:689:PRO:O	1:B:726:PRO:HG2	2.17	0.45
1:C:657:HIS:HD2	5:C:2237:HOH:O	1.99	0.45
1:C:732:TYR:CD1	1:C:746:GLN:HB3	2.52	0.44
1:B:554:MET:HE2	2:B:1039:B9D:O5	2.17	0.44
1:C:811:GLY:HA3	1:C:816:ARG:HG3	2.00	0.44
1:C:1038:THR:HG22	1:C:1038:THR:OXT	2.18	0.44
1:D:243:TYR:OH	1:D:666:ASN:HB3	2.17	0.44
1:A:286:TYR:HB3	1:A:328:TYR:CD2	2.52	0.44
1:B:383:MET:CE	5:B:2251:HOH:O	2.61	0.44
1:C:964:PHE:O	1:C:1027:ASN:HB2	2.17	0.44
1:A:20:ILE:CD1	1:A:96:ASP:HB3	2.48	0.44
1:C:408:GLY:HA3	1:C:455:VAL:O	2.17	0.44
1:C:34:SER:HA	1:C:35:PRO:HD2	1.92	0.44
1:D:360:MET:HE3	1:D:360:MET:HB3	1.90	0.44
1:A:29:GLY:HA3	1:A:31:TRP:CE2	2.53	0.44
1:D:182:LEU:CB	5:D:2208:HOH:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:886:TYR:O	1:D:902:ASP:HB3	2.17	0.44
1:D:98:PRO:HD2	5:D:2115:HOH:O	2.17	0.44
1:D:286:TYR:OH	5:D:2213:HOH:O	2.20	0.44
1:D:969:TYR:HA	1:D:1023:LEU:O	2.18	0.44
1:B:702:ASP:HB3	1:B:705:ASN:O	2.18	0.44
1:B:415:MET:HE3	1:B:424:THR:HG22	2.00	0.43
1:C:811:GLY:HA3	1:C:816:ARG:CG	2.48	0.43
1:A:98:PRO:HG2	1:A:100:ARG:NH1	2.34	0.43
1:C:601:MET:HE1	1:C:611:MET:HE1	1.99	0.43
1:C:766:TYR:CE2	1:C:895:LEU:HG	2.54	0.43
1:D:93:PHE:HE1	5:D:2208:HOH:O	1.86	0.43
1:D:162:LYS:HE2	1:D:282:GLU:OE1	2.19	0.43
1:A:554[A]:MET:CE	1:A:649:ARG:NH1	2.81	0.43
1:C:450:HIS:HE1	1:C:548:ASP:OD1	2.01	0.43
1:C:36:LEU:HD12	1:C:308:GLY:HA2	2.01	0.43
1:D:903:PRO:HG2	1:D:1004:PHE:CD2	2.54	0.43
1:A:808:LEU:HA	1:A:817:ILE:O	2.18	0.43
1:C:836:VAL:HG22	1:C:837:LEU:N	2.34	0.43
1:B:662:TRP:HZ2	2:B:1039:B9D:H4	1.84	0.43
1:D:241:LEU:O	1:D:242:ASN:HB2	2.19	0.43
1:B:433:ARG:HD3	5:B:2278:HOH:O	2.19	0.42
1:D:559:MET:HG3	1:D:591:THR:HA	2.01	0.42
1:B:130:PHE:HA	1:B:135:PHE:O	2.19	0.42
1:C:463:PHE:HB2	1:C:521:ALA:HB1	2.02	0.42
1:D:1027:ASN:N	1:D:1027:ASN:HD22	2.17	0.42
1:D:210:PHE:H	1:D:229:THR:CG2	2.23	0.42
1:D:231:ILE:HB	1:D:261:TYR:CD1	2.54	0.42
1:D:361:PRO:CD	1:D:776:MET:HG2	2.50	0.42
1:A:17:PRO:HG3	1:A:606:HIS:O	2.20	0.42
1:C:474:GLU:OE2	1:C:478:THR:HG21	2.19	0.42
1:C:649:ARG:HB2	1:C:662:TRP:CH2	2.55	0.42
1:D:661:MET:HB3	1:D:661:MET:HE3	1.78	0.42
1:C:463:PHE:CG	1:C:511:LEU:HD13	2.54	0.42
1:D:273:ILE:HG21	1:D:334:MET:HG2	2.01	0.42
1:A:785:PRO:O	1:A:788:LYS:CE	2.67	0.42
1:B:380:ARG:NH1	5:B:2237:HOH:O	2.08	0.42
1:D:39:THR:HG21	5:D:2018:HOH:O	2.18	0.42
1:B:582:PRO:HG3	5:B:2345:HOH:O	2.20	0.42
1:D:483:GLN:HE21	1:D:483:GLN:HB2	1.52	0.42
1:A:372:VAL:HG22	1:A:732:TYR:CE1	2.55	0.41
1:B:415:MET:SD	1:B:424:THR:HG22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:PRO:HD3	1:C:776:MET:HG2	2.01	0.41
1:D:167:ASN:HA	1:D:197:ASN:HA	2.01	0.41
1:D:484:LEU:HB3	1:D:531:VAL:HG22	2.02	0.41
1:B:593:HIS:CD2	5:B:2348:HOH:O	2.72	0.41
1:D:372:VAL:HG22	1:D:732:TYR:CE1	2.55	0.41
1:A:60:ASN:HB3	1:A:74:GLN:HE21	1.85	0.41
1:A:955:PHE:O	1:A:1032:ASP:HA	2.20	0.41
1:A:990:GLN:HB3	5:A:2870:HOH:O	2.20	0.41
1:A:688:LEU:HD12	1:A:691:VAL:HB	2.02	0.41
1:C:834:LEU:HB3	1:C:840:TRP:CD1	2.55	0.41
1:A:140:THR:OG1	1:A:143:LEU:HB2	2.21	0.41
1:C:629:GLU:HG3	1:C:633:GLU:OE2	2.20	0.41
1:D:171:GLY:HA2	1:D:177:ASN:HD22	1.86	0.41
1:D:807:PHE:CE1	1:D:819:CYS:HB2	2.56	0.41
1:B:777:TYR:HE2	1:B:919:MET:CE	2.33	0.41
1:C:228:ARG:HB3	1:C:231:ILE:HD11	2.02	0.41
1:D:165:MET:HG2	1:D:166:GLU:H	1.85	0.41
1:D:674:GLN:HG3	1:D:823:VAL:HB	2.01	0.41
1:A:364:TYR:CD1	1:A:364:TYR:C	2.99	0.41
1:A:911:LEU:HD12	1:A:946:GLN:HB2	2.02	0.41
1:B:881:ILE:HA	1:B:907:GLU:O	2.21	0.41
1:A:36:LEU:HD12	1:A:308:GLY:HA2	2.03	0.41
1:A:235:ASN:ND2	1:A:269:ALA:H	2.19	0.41
1:B:872:SER:HA	1:B:873:PRO:HD3	1.96	0.40
1:C:907:GLU:OE2	1:C:973:ARG:NE	2.45	0.40
1:A:562:HIS:CD2	1:A:593:HIS:CE1	2.88	0.40
1:B:474:GLU:O	1:B:478:THR:HG23	2.21	0.40
1:D:553:ASP:OD2	4:D:1041:5DI:C1	2.69	0.40
1:D:588:ASN:HB3	1:D:593:HIS:CE1	2.56	0.40
1:B:216:VAL:O	1:B:228:ARG:NH2	2.53	0.40
1:B:354:LEU:HD21	1:B:360:MET:HG3	2.03	0.40
1:C:125:ASP:HA	1:C:126:PRO:HD2	1.98	0.40
1:C:663:VAL:HG11	1:C:679:ASN:ND2	2.36	0.40
1:D:182:LEU:CA	5:D:2208:HOH:O	2.67	0.40
1:B:661:MET:HB3	1:B:661:MET:HE3	1.80	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	1023/1027 (100%)	981 (96%)	38 (4%)	4 (0%)	30	22
1	B	1022/1027 (100%)	980 (96%)	39 (4%)	3 (0%)	36	29
1	C	1022/1027 (100%)	988 (97%)	34 (3%)	0	100	100
1	D	1022/1027 (100%)	977 (96%)	44 (4%)	1 (0%)	48	40
All	All	4089/4108 (100%)	3926 (96%)	155 (4%)	8 (0%)	43	36

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	530	ASP
1	B	948	GLY
1	D	986	GLY
1	A	530	ASP
1	A	986	GLY
1	B	746	GLN
1	A	239	ASP
1	A	987	ALA

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	878/878 (100%)	864 (98%)	14 (2%)	55	54
1	B	877/878 (100%)	854 (97%)	23 (3%)	40	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	877/878 (100%)	857 (98%)	20 (2%)	44	40
1	D	877/878 (100%)	850 (97%)	27 (3%)	35	29
All	All	3509/3512 (100%)	3425 (98%)	84 (2%)	43	38

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	A	144	SER
1	A	324	GLN
1	A	445	VAL
1	A	571	LYS
1	A	662	TRP
1	A	688	LEU
1	A	718	TYR
1	A	753	ASN
1	A	830	ARG
1	A	838	THR
1	A	936	LYS
1	A	945	GLU
1	A	1038	THR
1	B	18	ASP
1	B	39	THR
1	B	53	THR
1	B	164	ILE
1	B	165	MET
1	B	282	GLU
1	B	306	ASN
1	B	418	ASN
1	B	462	CYS
1	B	474	GLU
1	B	487	LYS
1	B	494	THR
1	B	511	LEU
1	B	549	PHE
1	B	550	VAL
1	B	611	MET
1	B	655	ASN
1	B	688	LEU
1	B	690	LEU
1	B	718	TYR

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Mol	Chain	Res	Type
1	B	830	ARG
1	B	979	SER
1	B	984	SER
1	C	175	SER
1	C	282	GLU
1	C	413	VAL
1	C	414	ASP
1	C	462	CYS
1	C	483	GLN
1	C	551	TRP
1	C	571	LYS
1	C	655	ASN
1	C	688	LEU
1	C	690	LEU
1	C	704	GLU
1	C	718	TYR
1	C	829	GLU
1	C	830	ARG
1	C	837	LEU
1	C	860	ASP
1	C	893	LYS
1	C	942	VAL
1	C	990	GLN
1	D	14	THR
1	D	92	ARG
1	D	100	ARG
1	D	107	ILE
1	D	164	ILE
1	D	165	MET
1	D	198	LYS
1	D	229	THR
1	D	254	ASP
1	D	359	VAL
1	D	432	ASN
1	D	474	GLU
1	D	483	GLN
1	D	511	LEU
1	D	550	VAL
1	D	605	ASN
1	D	608	ARG
1	D	655	ASN
1	D	688	LEU

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Mol	Chain	Res	Type
1	D	690	LEU
1	D	718	TYR
1	D	830	ARG
1	D	915	ARG
1	D	942	VAL
1	D	990	GLN
1	D	1027	ASN
1	D	1038	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	74	GLN
1	A	86	ASN
1	A	118	GLN
1	A	202	ASN
1	A	217	ASN
1	A	221	GLN
1	A	235	ASN
1	A	245	GLN
1	A	252	HIS
1	A	318	GLN
1	A	325	HIS
1	A	345	GLN
1	A	432	ASN
1	A	457	GLN
1	A	471	GLN
1	A	483	GLN
1	A	510	HIS
1	A	538	ASN
1	A	552	GLN
1	A	562	HIS
1	A	593	HIS
1	A	614	GLN
1	A	657	HIS
1	A	679	ASN
1	A	769	GLN
1	A	795	ASN
1	A	804	ASN
1	A	864	ASN
1	A	913	ASN

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Mol	Chain	Res	Type
1	A	914	ASN
1	A	930	ASN
1	A	934	ASN
1	A	976	GLN
1	A	1009	ASN
1	A	1016	GLN
1	B	38	ASN
1	B	60	ASN
1	B	74	GLN
1	B	78	GLN
1	B	191	ASN
1	B	197	ASN
1	B	221	GLN
1	B	242	ASN
1	B	252	HIS
1	B	325	HIS
1	B	416	GLN
1	B	418	ASN
1	B	450	HIS
1	B	552	GLN
1	B	584	ASN
1	B	586	GLN
1	B	593	HIS
1	B	657	HIS
1	B	779	ASN
1	B	864	ASN
1	B	930	ASN
1	B	934	ASN
1	B	1016	GLN
1	C	62	ASN
1	C	80	GLN
1	C	197	ASN
1	C	207	GLN
1	C	217	ASN
1	C	242	ASN
1	C	325	HIS
1	C	382	HIS
1	C	402	ASN
1	C	403	ASN
1	C	450	HIS
1	C	457	GLN
1	C	483	GLN

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Mol	Chain	Res	Type
1	C	552	GLN
1	C	586	GLN
1	C	605	ASN
1	C	606	HIS
1	C	655	ASN
1	C	657	HIS
1	C	671	ASN
1	C	679	ASN
1	C	806	HIS
1	C	812	HIS
1	C	826	ASN
1	C	864	ASN
1	C	930	ASN
1	C	934	ASN
1	C	946	GLN
1	D	62	ASN
1	D	74	GLN
1	D	75	HIS
1	D	78	GLN
1	D	111	GLN
1	D	177	ASN
1	D	197	ASN
1	D	242	ASN
1	D	325	HIS
1	D	432	ASN
1	D	450	HIS
1	D	483	GLN
1	D	562	HIS
1	D	655	ASN
1	D	731	HIS
1	D	795	ASN
1	D	930	ASN
1	D	934	ASN
1	D	946	GLN
1	D	976	GLN
1	D	990	GLN
1	D	1027	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	D	336	1	3,6,7	0.69	0	1,6,8	0.24	0
1	CSO	A	336	1	3,6,7	0.50	0	1,6,8	0.16	0
1	CSO	B	336	1	3,6,7	0.66	0	1,6,8	0.19	0
1	CSO	C	336	1	3,6,7	0.66	0	1,6,8	0.26	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
1	CSO	D	336	1	-	0/1/5/7	-
1	CSO	A	336	1	-	0/1/5/7	-
1	CSO	B	336	1	-	0/1/5/7	-
1	CSO	C	336	1	-	0/1/5/7	-

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.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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
3	GOL	A	1042	-	5,5,5	0.38	0	5,5,5	0.32	0
2	B9D	B	1039	1	9,12,13	1.24	1 (11%)	14,18,20	0.96	0
3	GOL	A	1040	-	5,5,5	0.44	0	5,5,5	0.60	0
3	GOL	A	1041	-	5,5,5	0.24	0	5,5,5	0.72	0
3	GOL	D	1039	-	5,5,5	0.52	0	5,5,5	0.55	0
4	5DI	D	1041	-	9,12,12	6.07	4 (44%)	9,18,18	1.01	0
3	GOL	D	1040	-	5,5,5	0.33	0	5,5,5	0.33	0
3	GOL	A	1043	-	5,5,5	0.29	0	5,5,5	0.56	0
2	B9D	A	1039	1	9,12,13	1.20	1 (11%)	14,18,20	1.19	1 (7%)
3	GOL	B	1040	-	5,5,5	0.49	0	5,5,5	0.48	0
2	B9D	C	1039	1	9,12,13	1.33	1 (11%)	14,18,20	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1042	-	-	2/4/4/4	-
2	B9D	B	1039	1	-	0/2/23/26	0/1/1/1
3	GOL	A	1040	-	-	0/4/4/4	-
3	GOL	A	1041	-	-	3/4/4/4	-
3	GOL	D	1039	-	-	2/4/4/4	-
4	5DI	D	1041	-	-	0/2/23/23	0/1/1/1
3	GOL	D	1040	-	-	0/4/4/4	-
3	GOL	A	1043	-	-	0/4/4/4	-
2	B9D	A	1039	1	-	0/2/23/26	0/1/1/1
3	GOL	B	1040	-	-	4/4/4/4	-
2	B9D	C	1039	1	-	0/2/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1041	5DI	C1-C2	-16.07	1.34	1.51
4	D	1041	5DI	O2-C2	7.44	1.33	1.21
2	C	1039	B9D	O5-C1	3.73	1.45	1.37
2	A	1039	B9D	O5-C1	3.19	1.44	1.37
2	B	1039	B9D	O5-C1	3.04	1.43	1.37
4	D	1041	5DI	O5-C1	2.77	1.46	1.43
4	D	1041	5DI	O5-C5	2.53	1.42	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1039	B9D	O2-C2-C1	3.14	116.12	110.05

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1042	GOL	C1-C2-C3-O3
3	B	1040	GOL	C1-C2-C3-O3
3	B	1040	GOL	O2-C2-C3-O3
3	D	1039	GOL	C1-C2-C3-O3
3	D	1039	GOL	O2-C2-C3-O3
3	A	1041	GOL	C1-C2-C3-O3
3	B	1040	GOL	O1-C1-C2-C3
3	A	1042	GOL	O2-C2-C3-O3
3	B	1040	GOL	O1-C1-C2-O2
3	A	1041	GOL	O2-C2-C3-O3
3	A	1041	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1039	B9D	2	0
4	D	1041	5DI	4	0
3	D	1040	GOL	1	0
3	A	1043	GOL	1	0
2	A	1039	B9D	1	0
3	B	1040	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1024/1027 (99%)	-0.15	7 (0%) 84 86	8, 16, 31, 46	1 (0%)
1	B	1024/1027 (99%)	0.30	22 (2%) 63 67	13, 29, 49, 69	0
1	C	1024/1027 (99%)	0.30	19 (1%) 66 70	13, 29, 45, 72	0
1	D	1024/1027 (99%)	-0.08	14 (1%) 73 76	8, 17, 36, 59	0
All	All	4096/4108 (99%)	0.09	62 (1%) 72 75	8, 22, 44, 72	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	THR	5.3
1	C	514	GLY	4.8
1	A	987	ALA	4.3
1	A	988	GLY	3.8
1	C	515	GLY	3.8
1	B	976	GLN	3.6
1	D	511	LEU	3.5
1	D	529	PRO	3.4
1	D	515	GLY	3.4
1	B	463	PHE	3.2
1	D	516	GLY	3.1
1	D	14	THR	3.1
1	C	987	ALA	3.1
1	B	511	LEU	3.0
1	D	514	GLY	3.0
1	A	328	TYR	3.0
1	C	513	TYR	2.9
1	B	529	PRO	2.9
1	C	463	PHE	2.9
1	D	18	ASP	2.9
1	B	1038	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	987	ALA	2.8
1	C	14	THR	2.8
1	B	514	GLY	2.6
1	B	551	TRP	2.6
1	C	517	VAL	2.6
1	D	328	TYR	2.6
1	B	492	THR	2.6
1	B	530	ASP	2.5
1	D	513	TYR	2.5
1	B	639	THR	2.5
1	C	529	PRO	2.5
1	A	331	GLY	2.5
1	D	132	SER	2.4
1	D	463	PHE	2.4
1	C	947	ASP	2.4
1	C	551	TRP	2.4
1	B	994	VAL	2.3
1	B	72	THR	2.3
1	C	1007	GLY	2.3
1	D	568	ILE	2.3
1	A	529	PRO	2.2
1	C	1017	GLU	2.2
1	C	568	ILE	2.2
1	C	606	HIS	2.2
1	C	913	ASN	2.2
1	B	73	VAL	2.2
1	D	986	GLY	2.2
1	A	254	ASP	2.1
1	B	53	THR	2.1
1	B	515	GLY	2.1
1	B	188	LEU	2.1
1	C	120	LEU	2.1
1	C	837	LEU	2.1
1	C	173	ALA	2.1
1	B	565	GLY	2.1
1	D	987	ALA	2.1
1	B	860	ASP	2.1
1	A	605	ASN	2.1
1	C	994	VAL	2.1
1	B	1001	ALA	2.0
1	B	482	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	A	336	7/8	0.90	0.11	18,20,28,32	0
1	CSO	B	336	7/8	0.91	0.10	23,24,31,32	0
1	CSO	C	336	7/8	0.92	0.10	25,26,33,34	0
1	CSO	D	336	7/8	0.93	0.09	13,15,25,28	0

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
3	GOL	D	1039	6/6	0.79	0.22	37,37,38,41	0
3	GOL	B	1040	6/6	0.81	0.16	56,57,57,57	0
3	GOL	A	1040	6/6	0.87	0.15	35,36,37,39	0
4	5DI	D	1041	12/12	0.87	0.12	38,41,43,43	0
3	GOL	A	1043	6/6	0.88	0.13	35,38,38,40	0
2	B9D	C	1039	12/13	0.89	0.11	36,38,40,40	0
2	B9D	B	1039	12/13	0.89	0.11	40,42,42,45	0
3	GOL	D	1040	6/6	0.90	0.16	37,41,44,44	0
3	GOL	A	1042	6/6	0.93	0.11	28,34,35,37	0
3	GOL	A	1041	6/6	0.93	0.09	31,36,37,37	0
2	B9D	A	1039	12/13	0.94	0.08	25,28,29,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.