



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:03 AM UTC

PDB ID : 4AMX / pdb_00004amx
Title : CRYSTAL STRUCTURE OF THE GRACILARIOPSIS LEMANEIFORMIS
ALPHA-1,4- GLUCAN LYASE Covalent Intermediate Complex with 5-fluoro-
glucosyl- fluoride
Authors : Rozeboom, H.J.; Yu, S.; Madrid, S.; Kalk, K.H.; Dijkstra, B.W.
Deposited on : 2012-03-14
Resolution : 2.10 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

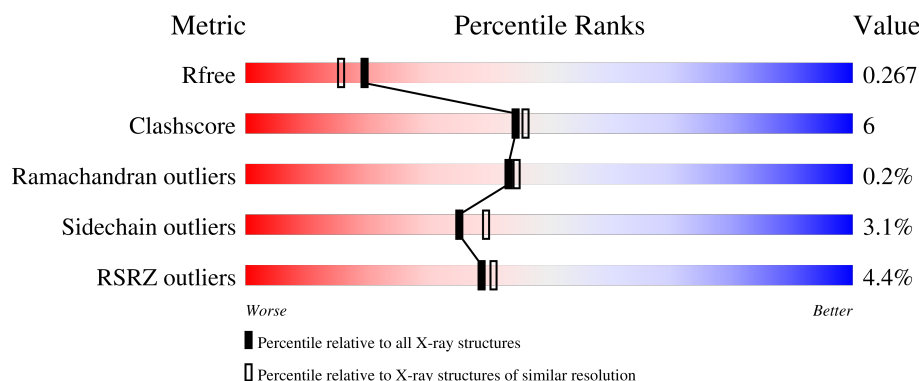
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	2% 85% 14% .
1	B	1027	7% 85% 14% .
1	C	1027	5% 86% 13% .
1	D	1027	4% 83% 16% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	5GF	B	1039	X	-	-	-

2 Entry composition [i](#)

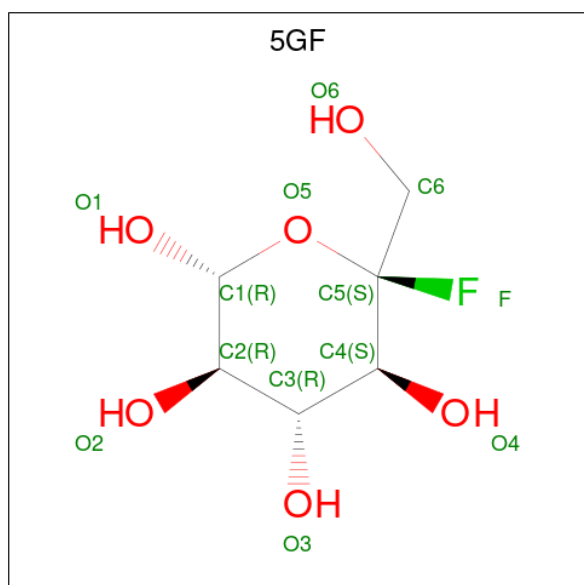
There are 5 unique types of molecules in this entry. The entry contains 33667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			8171	5143	1385	1596	47			
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	1	0
			8171	5143	1385	1596	47			

- Molecule 2 is 5-fluoro-beta-D-glucopyranose (CCD ID: 5GF) (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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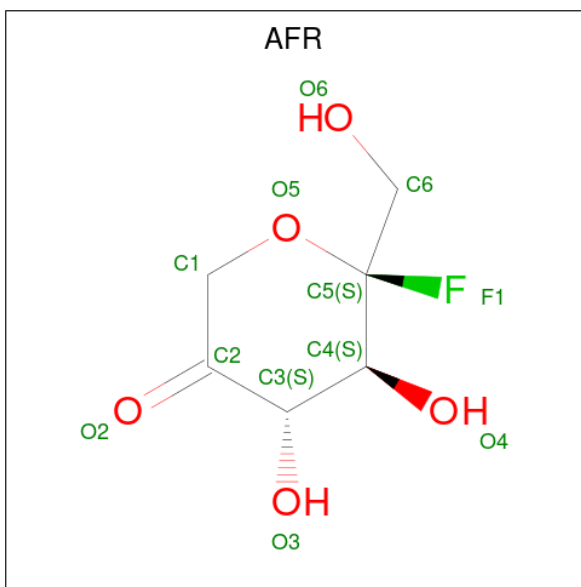
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	F	O	0	0
			12	6	1	5		

- 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	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-5,1-pyranosyl fluoride (CCD ID: AFR) (formula: $C_6H_9FO_5$).



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

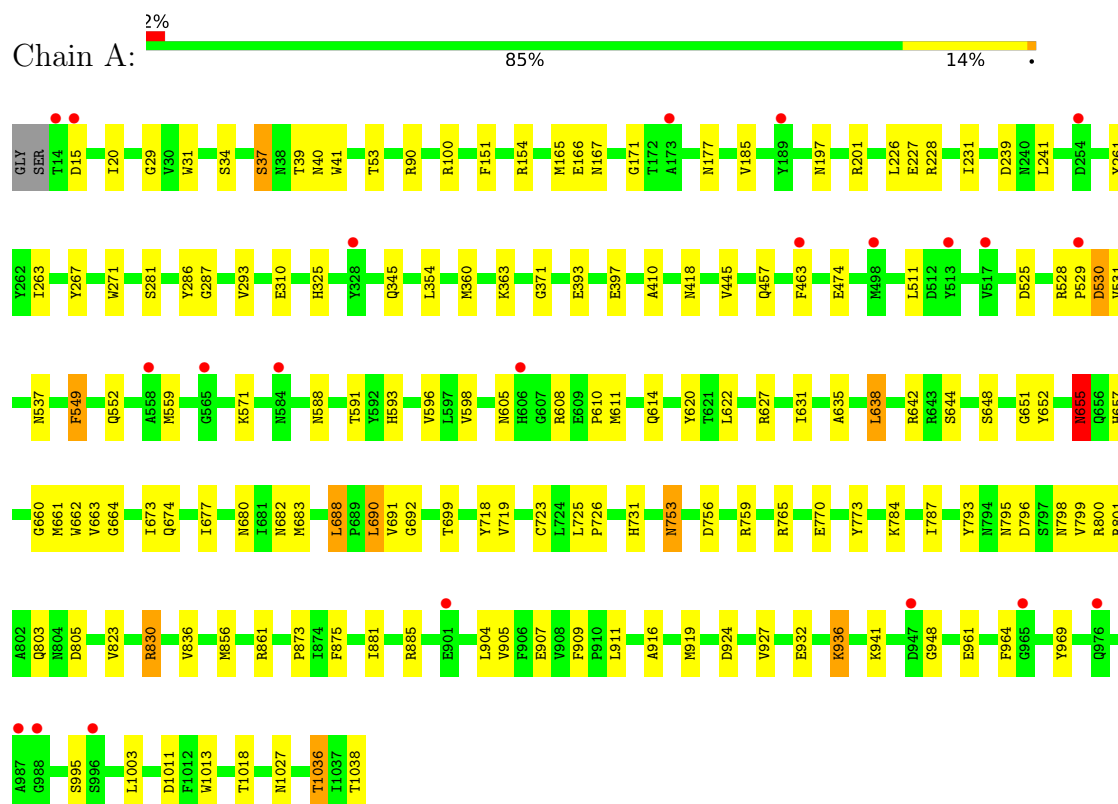
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	328	Total	O	0	0
			328	328		
5	B	147	Total	O	0	0
			147	147		
5	C	152	Total	O	0	0
			152	152		
5	D	296	Total	O	0	0
			296	296		

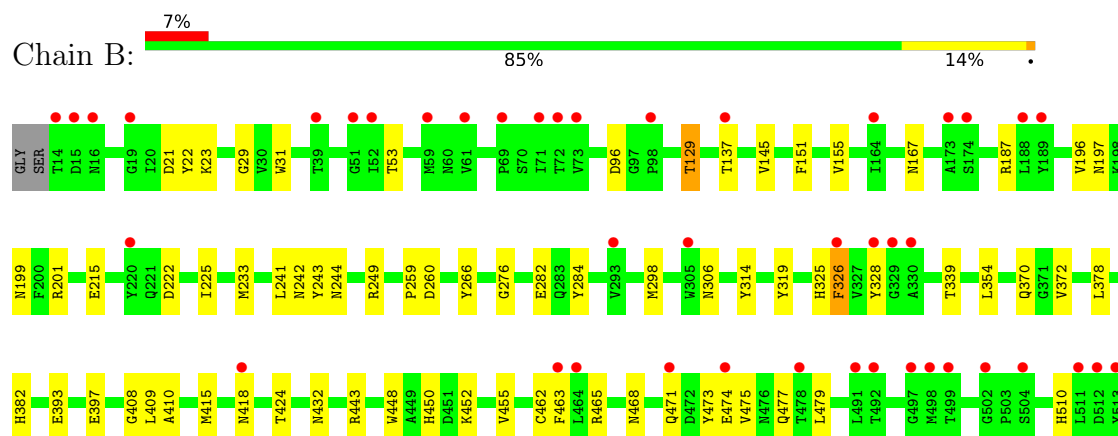
3 Residue-property plots

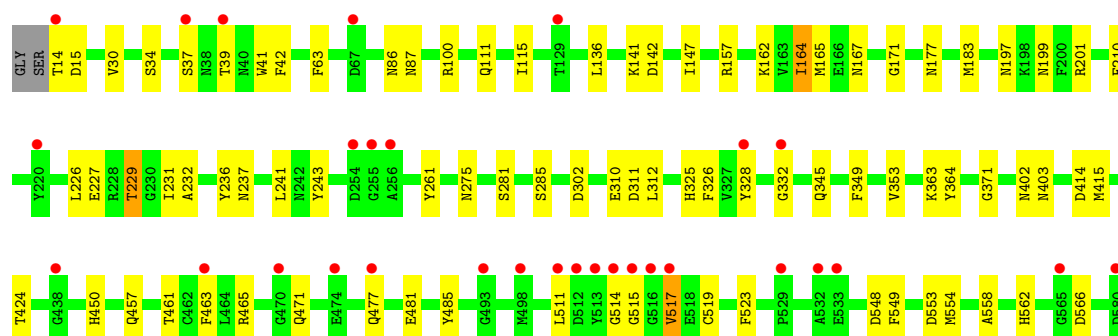
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

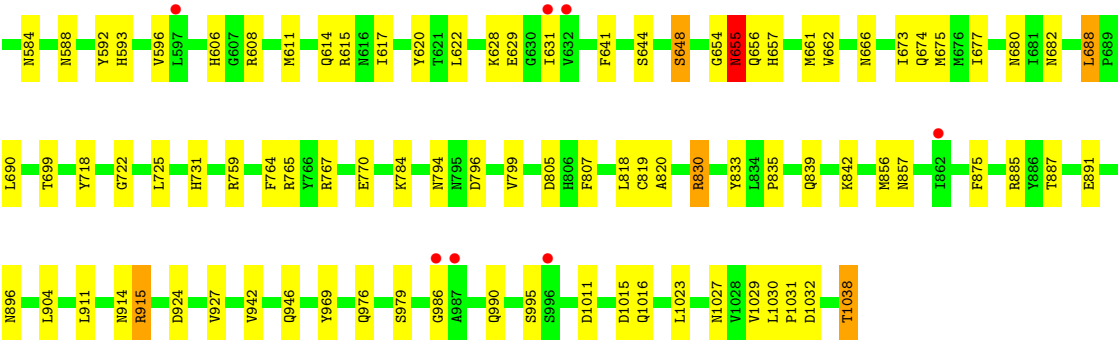
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1



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







4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	91.64Å 97.01Å 135.71Å 80.38° 83.11° 85.22°	Depositor
Resolution (Å)	46.74 – 2.10 46.74 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (46.74-2.10) 95.9 (46.74-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.267 0.222 , 0.267	Depositor DCC
R_{free} test set	12923 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.533	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.5	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	0.93	EDS
Total number of atoms	33667	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.73% 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: 5GF, CSO, AFR, 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	0.75	0/8387	0.94	9/11407 (0.1%)
1	B	0.61	2/8374 (0.0%)	0.84	6/11389 (0.1%)
1	C	0.58	0/8374	0.81	2/11389 (0.0%)
1	D	0.74	1/8387 (0.0%)	0.91	2/11407 (0.0%)
All	All	0.67	3/33522 (0.0%)	0.88	19/45592 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	975	ALA	C-N	-7.55	1.23	1.33
1	B	556	VAL	CA-CB	5.46	1.57	1.53
1	D	722	GLY	C-O	5.03	1.28	1.24

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	975	ALA	O-C-N	-11.01	110.31	122.85
1	A	673	ILE	N-CA-C	-7.74	103.15	110.42
1	B	810	GLY	N-CA-C	6.61	120.47	112.48
1	A	909	PHE	CA-C-N	-6.11	113.65	119.76
1	A	909	PHE	C-N-CA	-6.11	113.65	119.76
1	B	902	ASP	CA-C-N	6.07	126.42	119.93
1	B	902	ASP	C-N-CA	6.07	126.42	119.93
1	D	915	ARG	N-CA-C	5.47	116.59	108.60
1	B	260	ASP	N-CA-C	5.44	116.41	108.14
1	A	784	LYS	CA-C-N	-5.39	114.17	119.99
1	A	784	LYS	C-N-CA	-5.39	114.17	119.99
1	A	549	PHE	N-CA-C	5.37	116.15	108.74
1	C	803	GLN	N-CA-C	5.33	119.40	113.01
1	C	526	TRP	N-CA-C	5.20	118.41	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	225	ILE	N-CA-C	5.18	117.08	108.99
1	A	836	VAL	N-CA-C	5.16	115.68	110.05
1	D	673	ILE	N-CA-C	-5.05	105.78	110.53
1	A	655	ASN	N-CA-C	5.02	118.17	111.75
1	A	961	GLU	N-CA-C	-5.01	107.20	113.72

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	8171	0	7615	95	0
1	B	8162	0	7606	89	0
1	C	8162	0	7606	87	0
1	D	8171	0	7615	109	0
2	A	12	0	9	1	0
2	B	12	0	9	0	0
2	C	12	0	9	0	0
3	A	12	0	16	1	0
3	B	6	0	8	0	0
3	D	12	0	16	2	0
4	D	12	0	9	4	0
5	A	328	0	0	20	0
5	B	147	0	0	13	0
5	C	152	0	0	9	0
5	D	296	0	0	19	0
All	All	33667	0	30518	380	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 6.

All (380) 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:598:VAL:HG11	1:A:611:MET:HE2	1.35	1.07
1:C:210:PHE:H	1:C:229:THR:HG22	1.26	1.00
1:C:776:MET:HE2	1:C:786:ILE:HD11	1.47	0.96
1:A:529:PRO:O	1:A:530:ASP:HB2	1.65	0.96
1:B:776:MET:HE2	1:B:786:ILE:HD11	1.49	0.94
1:D:584:ASN:HB3	5:D:2168:HOH:O	1.68	0.94
1:A:642:ARG:HD2	5:A:2210:HOH:O	1.69	0.92
1:C:210:PHE:H	1:C:229:THR:CG2	1.85	0.88
1:C:806:HIS:HE1	1:C:833:TYR:H	1.19	0.87
1:A:856:MET:HE1	1:A:875:PHE:CD2	2.10	0.86
1:D:677:ILE:HD13	5:D:2230:HOH:O	1.74	0.86
1:C:842:LYS:HB2	1:C:856:MET:HE1	1.58	0.85
1:A:795:ASN:HB3	5:A:2267:HOH:O	1.76	0.85
1:A:725:LEU:HD22	5:A:2222:HOH:O	1.76	0.85
1:A:856:MET:HE1	1:A:875:PHE:CE2	2.14	0.82
1:B:259:PRO:HG3	5:B:2034:HOH:O	1.79	0.82
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.46	0.81
1:C:776:MET:CE	1:C:786:ILE:HD11	2.12	0.79
1:C:210:PHE:N	1:C:229:THR:HG22	2.00	0.76
1:B:776:MET:CE	1:B:786:ILE:HD11	2.15	0.75
1:D:210:PHE:HD1	1:D:229:THR:HB	1.51	0.75
1:C:806:HIS:CE1	1:C:833:TYR:H	2.03	0.75
1:B:635:ALA:HA	1:B:638:LEU:HD12	1.68	0.74
1:A:805:ASP:CG	1:A:830:ARG:HH22	1.97	0.73
1:B:462:CYS:HB2	5:B:2079:HOH:O	1.88	0.72
1:A:635:ALA:HA	1:A:638:LEU:HD12	1.71	0.72
1:B:905:VAL:HG22	1:B:969:TYR:HB2	1.72	0.72
1:D:794:ASN:H	3:D:1040:GOL:H31	1.54	0.71
1:B:243:TYR:HB2	5:B:2034:HOH:O	1.91	0.71
1:D:856:MET:HE1	1:D:875:PHE:HD2	1.56	0.70
1:B:415:MET:HE3	1:B:424:THR:HG22	1.74	0.69
1:A:995:SER:HB2	1:A:1011:ASP:HB3	1.74	0.69
1:D:856:MET:HE1	1:D:875:PHE:CD2	2.27	0.69
1:A:325:HIS:HE1	5:A:2036:HOH:O	1.76	0.69
1:B:924:ASP:O	1:B:927:VAL:HG23	1.92	0.69
1:A:525:ASP:HB3	1:A:528:ARG:HD2	1.74	0.68
1:D:450:HIS:HD2	5:D:2154:HOH:O	1.76	0.68
1:C:415:MET:HE3	1:C:424:THR:HG22	1.75	0.68
1:C:756:ASP:HB2	5:C:2116:HOH:O	1.92	0.68
1:A:919:MET:HE3	1:A:941:LYS:HE2	1.75	0.68
1:D:620:TYR:HA	1:D:655:ASN:HD21	1.60	0.67
1:B:382:HIS:CD2	1:B:432:ASN:HB2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:GLN:HA	5:D:2190:HOH:O	1.94	0.66
1:A:529:PRO:O	1:A:530:ASP:CB	2.43	0.65
1:D:171:GLY:HA2	1:D:177:ASN:HD22	1.62	0.65
1:D:677:ILE:HG21	5:D:2230:HOH:O	1.95	0.65
1:D:162:LYS:NZ	5:D:2057:HOH:O	2.30	0.65
1:C:325:HIS:HE1	5:C:2048:HOH:O	1.80	0.64
1:A:363:LYS:NZ	1:A:770:GLU:OE2	2.29	0.64
1:A:631:ILE:HG23	1:A:644:SER:HB3	1.79	0.64
1:C:661:MET:HB2	1:C:691:VAL:HG23	1.80	0.64
1:C:842:LYS:HB2	1:C:856:MET:CE	2.27	0.64
1:A:263:ILE:O	5:A:2086:HOH:O	2.15	0.64
1:A:34:SER:HA	5:A:2012:HOH:O	1.98	0.63
1:B:1029:VAL:O	1:B:1033:ALA:HB2	1.99	0.63
1:C:526:TRP:CZ2	1:C:622:LEU:HD13	2.32	0.63
1:B:339:THR:HG22	5:B:2007:HOH:O	1.99	0.62
1:C:805:ASP:OD1	1:C:806:HIS:HD2	1.83	0.62
1:B:249:ARG:HG2	1:B:249:ARG:NH1	2.13	0.61
1:D:167:ASN:HA	1:D:197:ASN:HA	1.83	0.61
1:C:464:LEU:HD11	1:C:534:TRP:HH2	1.67	0.60
1:A:680:ASN:CG	5:A:2222:HOH:O	2.43	0.60
1:A:588:ASN:HB3	1:A:593:HIS:CE1	2.36	0.59
1:D:363:LYS:NZ	1:D:770:GLU:OE2	2.31	0.59
1:D:1016:GLN:HG2	5:D:2295:HOH:O	2.02	0.59
1:D:311:ASP:O	1:D:312:LEU:HD23	2.02	0.59
1:C:209:GLY:HA2	1:C:229:THR:HG21	1.85	0.59
1:A:201:ARG:HD3	1:A:310:GLU:O	2.03	0.59
1:B:477:GLN:HG3	5:B:2081:HOH:O	2.02	0.59
1:C:732:TYR:CD1	1:C:746:GLN:HB3	2.37	0.58
1:D:611:MET:HE3	5:D:2163:HOH:O	2.02	0.58
1:D:210:PHE:CD1	1:D:229:THR:HB	2.36	0.58
1:A:723:CYS:O	1:A:765:ARG:NH1	2.34	0.58
1:C:566:ASP:HB3	1:C:570:VAL:HG13	1.86	0.58
1:A:873:PRO:HA	5:A:2295:HOH:O	2.03	0.58
1:B:801:ARG:HG2	1:B:861:ARG:NH2	2.19	0.58
1:C:92:ARG:HD2	5:C:2015:HOH:O	2.03	0.58
1:C:631:ILE:HD13	1:C:644:SER:HB3	1.86	0.57
1:D:231:ILE:HD12	1:D:261:TYR:HB2	1.85	0.57
1:A:798:ASN:HB3	1:A:861:ARG:HH21	1.70	0.57
1:C:811:GLY:HA3	1:C:816:ARG:CG	2.35	0.56
1:D:136:LEU:HD23	1:D:147:ILE:HD12	1.86	0.56
1:B:562:HIS:ND1	1:B:593:HIS:HE1	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:811:GLY:HA3	1:C:816:ARG:HG3	1.88	0.56
1:D:969:TYR:HA	1:D:1023:LEU:O	2.06	0.56
1:A:661:MET:O	1:A:691:VAL:HA	2.06	0.56
1:A:37:SER:HB3	5:A:2010:HOH:O	2.06	0.56
1:A:267:TYR:CD2	1:A:683:MET:SD	2.99	0.56
1:D:514:GLY:H	1:D:517:VAL:HG13	1.71	0.56
1:D:157:ARG:HB2	1:D:164:ILE:HD13	1.86	0.56
1:D:764:PHE:O	1:D:765:ARG:C	2.48	0.56
1:A:1003:LEU:HD22	1:A:1013:TRP:HB3	1.87	0.55
1:D:201:ARG:HD3	1:D:310:GLU:O	2.06	0.55
1:C:464:LEU:HD12	1:C:479:LEU:HD22	1.89	0.55
1:A:905:VAL:HG22	1:A:969:TYR:HB2	1.89	0.55
1:D:463:PHE:CE2	1:D:511:LEU:HD22	2.41	0.55
1:D:403:ASN:O	1:D:759:ARG:HD2	2.06	0.55
1:D:562:HIS:HD2	1:D:593:HIS:NE2	2.04	0.55
1:C:798:ASN:HB2	1:C:833:TYR:CZ	2.42	0.54
1:A:627:ARG:NH1	5:A:2205:HOH:O	2.40	0.54
1:B:554:MET:HB3	1:B:558:ALA:HB3	1.89	0.54
1:D:332:GLY:HA3	5:D:2114:HOH:O	2.07	0.54
1:D:807:PHE:CE1	1:D:819:CYS:HB2	2.42	0.54
1:D:641:PHE:CZ	1:D:896:ASN:HB2	2.43	0.54
1:D:976:GLN:HE22	1:D:1016:GLN:HA	1.72	0.54
1:A:657:HIS:HE1	5:A:2137:HOH:O	1.91	0.53
1:A:397:GLU:OE2	1:C:397:GLU:OE2	2.26	0.53
1:C:227:GLU:OE2	1:C:229:THR:HG21	2.07	0.53
1:B:757:THR:HA	1:B:760:LYS:HE2	1.91	0.53
1:D:457:GLN:HA	1:D:549:PHE:O	2.08	0.53
1:B:777:TYR:HE2	1:B:919:MET:CE	2.21	0.53
1:D:165:MET:HE3	1:D:328[A]:TYR:OH	2.09	0.53
1:D:924:ASP:OD1	1:D:924:ASP:C	2.52	0.53
1:B:393:GLU:O	1:B:397:GLU:HG3	2.09	0.52
1:C:96:ASP:OD1	1:C:187:ARG:HD2	2.09	0.52
1:B:660:GLY:C	1:B:661:MET:HG2	2.35	0.52
1:B:465:ARG:HG2	1:B:468:ASN:OD1	2.10	0.52
1:B:479:LEU:HD13	1:B:534:TRP:CH2	2.45	0.52
1:A:34:SER:C	5:A:2012:HOH:O	2.53	0.52
1:A:226:LEU:HD12	1:A:682:ASN:HD21	1.75	0.52
1:B:233:MET:HE3	1:B:298:MET:HB2	1.91	0.52
1:D:856:MET:HG2	5:D:2247:HOH:O	2.09	0.52
1:D:1038:THR:HB	5:D:2283:HOH:O	2.09	0.52
1:A:795:ASN:CB	5:A:2267:HOH:O	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:HIS:HB2	1:B:568:ILE:HG22	1.91	0.51
1:A:657:HIS:CE1	5:A:2137:HOH:O	2.63	0.51
1:C:588:ASN:HB3	1:C:593:HIS:CE1	2.45	0.51
1:B:661:MET:O	1:B:691:VAL:HA	2.11	0.51
1:C:298:MET:HG2	1:C:315:MET:HE2	1.93	0.51
1:C:629:GLU:HG3	1:C:633:GLU:OE1	2.11	0.51
1:A:39:THR:O	1:A:40:ASN:HB2	2.10	0.51
1:A:674:GLN:HG3	1:A:823:VAL:HB	1.93	0.51
1:B:452:LYS:HE2	5:B:2077:HOH:O	2.10	0.51
1:A:226:LEU:HD12	1:A:682:ASN:ND2	2.26	0.51
1:A:731:HIS:HE1	2:A:1039:5GF:O4	1.94	0.51
1:B:805:ASP:CG	1:B:830:ARG:HH22	2.19	0.51
1:D:111:GLN:HE22	1:D:349:PHE:H	1.57	0.51
1:B:129:THR:HG23	1:B:137:THR:HG22	1.93	0.51
1:B:662:TRP:HA	1:B:692:GLY:O	2.11	0.51
1:D:30:VAL:HG11	1:D:232:ALA:O	2.10	0.51
1:A:167:ASN:HA	1:A:197:ASN:HA	1.93	0.50
1:C:201:ARG:NH1	1:C:301:GLY:O	2.44	0.50
1:C:235:ASN:HB2	1:C:296:SER:OG	2.10	0.50
1:A:598:VAL:HG11	1:A:611:MET:CE	2.25	0.50
1:A:856:MET:HE1	1:A:875:PHE:HD2	1.71	0.50
1:B:777:TYR:CE2	1:B:919:MET:CE	2.94	0.50
1:C:533:GLU:HA	1:C:629:GLU:HG2	1.94	0.50
1:D:995:SER:HB2	1:D:1011:ASP:HB3	1.93	0.50
1:B:372:VAL:HG22	1:B:732:TYR:CE1	2.46	0.50
1:C:167:ASN:HA	1:C:197:ASN:HA	1.94	0.50
1:D:371:GLY:C	1:D:731:HIS:HD2	2.18	0.50
1:A:371:GLY:C	1:A:731:HIS:HD2	2.19	0.49
1:D:165:MET:HE2	1:D:326:PHE:CD1	2.47	0.49
1:A:345:GLN:HA	5:A:2048:HOH:O	2.11	0.49
1:C:661:MET:O	1:C:691:VAL:HA	2.12	0.49
1:A:171:GLY:HA2	1:A:177:ASN:HD22	1.78	0.49
1:B:777:TYR:HE2	1:B:919:MET:HE1	1.78	0.49
1:C:267:TYR:CD2	1:C:683:MET:SD	3.06	0.49
1:C:1008:GLU:O	1:C:1011:ASP:HB2	2.13	0.49
1:A:800:ARG:O	1:A:803:GLN:CD	2.55	0.49
1:D:477:GLN:O	1:D:481:GLU:HG2	2.13	0.48
1:D:767:ARG:HB2	5:D:2210:HOH:O	2.12	0.48
1:B:719:VAL:O	1:B:723:CYS:HB3	2.13	0.48
1:A:537:ASN:HB3	5:A:2185:HOH:O	2.13	0.48
1:D:226:LEU:HD12	1:D:682:ASN:HD21	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:TYR:CE2	1:B:690:LEU:HD13	2.48	0.48
1:D:818:LEU:HD22	1:D:835:PRO:HD2	1.95	0.48
1:C:219:LYS:HD3	1:C:224:TYR:CE1	2.48	0.48
1:D:805:ASP:CG	1:D:830:ARG:HH22	2.22	0.48
1:A:661:MET:HG2	1:A:688:LEU:HD11	1.96	0.48
1:B:443:ARG:NE	5:B:2073:HOH:O	2.25	0.48
1:A:463:PHE:CE2	1:A:511:LEU:HD13	2.49	0.48
1:C:227:GLU:HG2	1:C:229:THR:HG23	1.95	0.48
1:C:479:LEU:HD12	1:C:484:LEU:HB2	1.95	0.48
1:D:241:LEU:HD21	1:D:699:THR:HG21	1.95	0.48
1:D:553:ASP:OD2	4:D:1041:AFR:H11	2.13	0.48
1:A:34:SER:O	1:A:37:SER:HB2	2.13	0.48
1:A:635:ALA:HB1	1:A:642:ARG:HG2	1.96	0.48
1:B:410:ALA:HB1	1:B:551:TRP:CZ3	2.49	0.48
1:D:15:ASP:OD1	1:D:608:ARG:HD3	2.14	0.48
1:B:832:LEU:HD23	1:B:862:ILE:HD12	1.96	0.47
1:C:357:ARG:HB2	1:C:779:ASN:O	2.13	0.47
1:C:614:GLN:O	1:C:617:ILE:HG22	2.15	0.47
1:C:881:ILE:HG12	1:C:908:VAL:HG22	1.95	0.47
1:A:1003:LEU:HD22	1:A:1013:TRP:CB	2.44	0.47
1:A:801:ARG:HH21	1:A:861:ARG:HD3	1.79	0.47
1:B:241:LEU:C	1:B:243:TYR:H	2.23	0.47
1:B:556:VAL:N	1:B:557:PRO:HA	2.29	0.47
1:D:227:GLU:OE2	1:D:229:THR:CG2	2.62	0.47
1:D:281:SER:HA	5:D:2105:HOH:O	2.13	0.47
1:D:1030:LEU:N	1:D:1031:PRO:CD	2.78	0.47
1:A:267:TYR:CE1	1:A:652:TYR:N	2.83	0.47
1:B:96:ASP:OD1	1:B:187:ARG:HD2	2.14	0.47
1:D:661:MET:HG2	1:D:688:LEU:HD11	1.96	0.47
1:B:473:TYR:CZ	1:B:475:VAL:HB	2.49	0.47
1:C:463:PHE:CG	1:C:511:LEU:HD13	2.50	0.47
1:D:805:ASP:HA	5:D:2230:HOH:O	2.15	0.47
1:A:41:TRP:CE2	1:A:185:VAL:HG22	2.50	0.46
1:C:288:TRP:HE1	1:C:324:GLN:CD	2.23	0.46
1:B:661:MET:HB2	1:B:691:VAL:HG23	1.96	0.46
1:C:410:ALA:HB1	1:C:551:TRP:CZ3	2.50	0.46
1:B:378:LEU:HD11	1:B:448:TRP:CE3	2.51	0.46
1:B:798:ASN:HB2	1:B:833:TYR:CZ	2.50	0.46
1:C:561:PRO:HD3	1:C:590:LYS:HG2	1.97	0.46
1:D:231:ILE:CA	1:D:302:ASP:HB2	2.45	0.46
1:D:656:GLN:HG2	1:D:657:HIS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TYR:CE1	1:A:651:GLY:C	2.94	0.46
1:B:244:ASN:HB3	5:B:2034:HOH:O	2.14	0.46
1:B:463:PHE:HB2	1:B:521:ALA:HB1	1.97	0.46
1:D:465:ARG:HG3	1:D:519:CYS:HB2	1.97	0.46
1:D:654:GLY:C	1:D:656:GLN:OE1	2.59	0.46
1:D:680:ASN:ND2	1:D:725:LEU:HD13	2.30	0.46
1:B:243:TYR:C	5:B:2034:HOH:O	2.58	0.46
1:D:562:HIS:HE1	1:D:566:ASP:O	1.99	0.46
1:C:679:ASN:O	1:C:683:MET:HB2	2.16	0.46
1:D:325:HIS:HE1	5:D:2033:HOH:O	1.98	0.46
1:C:620:TYR:HA	1:C:655:ASN:HD21	1.81	0.46
1:B:22:TYR:HD1	1:B:319:TYR:CE2	2.34	0.45
1:B:266:TYR:CE2	1:B:664:GLY:HA3	2.51	0.45
1:C:227:GLU:OE2	1:C:229:THR:CG2	2.64	0.45
1:B:372:VAL:HG22	1:B:732:TYR:HE1	1.81	0.45
1:C:378:LEU:HD13	1:C:445:VAL:HA	1.97	0.45
1:A:796:ASP:CG	1:A:799:VAL:HG13	2.42	0.45
1:C:905:VAL:HG22	1:C:969:TYR:HB2	1.97	0.45
1:B:233:MET:HB2	1:B:298:MET:HE3	1.98	0.45
1:A:525:ASP:O	1:A:531:VAL:HG21	2.16	0.45
1:B:450:HIS:HE1	1:B:548:ASP:OD1	1.98	0.45
1:C:238:TYR:HE1	1:C:589:TRP:HB3	1.80	0.45
1:C:594:PRO:HG3	5:C:2037:HOH:O	2.16	0.45
1:D:111:GLN:O	1:D:115:ILE:HG13	2.17	0.45
1:A:773:TYR:HB3	5:A:2256:HOH:O	2.15	0.45
1:B:463:PHE:HB2	1:B:521:ALA:CB	2.46	0.45
1:B:167:ASN:HA	1:B:197:ASN:HA	1.99	0.45
1:B:199:ASN:OD1	1:B:201:ARG:HG2	2.16	0.45
1:B:787:ILE:HG23	1:B:807:PHE:CD1	2.51	0.45
1:B:881:ILE:HA	1:B:907:GLU:O	2.16	0.45
1:A:911:LEU:HD22	1:A:916:ALA:HB2	1.98	0.45
1:C:689:PRO:O	1:C:726:PRO:HG2	2.17	0.45
1:D:15:ASP:HA	1:D:608:ARG:H	1.82	0.45
1:A:90:ARG:HB2	1:A:325:HIS:CD2	2.52	0.45
1:A:154:ARG:NH1	1:A:166:GLU:OE2	2.50	0.45
1:A:293:VAL:HG23	1:A:614:GLN:HA	1.99	0.45
1:C:484:LEU:HB3	1:C:531:VAL:HG22	1.98	0.45
1:C:611:MET:HE3	5:C:2091:HOH:O	2.16	0.44
1:D:796:ASP:CG	1:D:799:VAL:HG13	2.42	0.44
1:D:42:PHE:HB3	1:D:63:PHE:HB3	1.98	0.44
1:D:450:HIS:HE1	1:D:548:ASP:OD1	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:VAL:HG13	1:D:833:TYR:HE2	1.82	0.44
1:A:620:TYR:HA	1:A:655:ASN:HD21	1.83	0.44
1:B:325:HIS:HD2	5:B:2006:HOH:O	2.00	0.44
1:B:354:LEU:HD11	1:B:777:TYR:HD1	1.83	0.44
1:C:907:GLU:OE2	1:C:973:ARG:NE	2.47	0.44
1:D:631:ILE:HG23	1:D:644:SER:HB3	2.00	0.44
1:A:165:MET:HG3	1:A:286:TYR:CZ	2.53	0.44
1:A:393:GLU:HG2	1:A:397:GLU:OE2	2.17	0.44
1:B:661:MET:HE3	1:B:661:MET:HB3	1.75	0.44
1:D:226:LEU:HD12	1:D:682:ASN:ND2	2.33	0.44
1:A:660:GLY:HA3	1:A:690:LEU:O	2.18	0.44
1:D:111:GLN:NE2	1:D:349:PHE:H	2.16	0.44
1:A:856:MET:HE1	1:A:875:PHE:HE2	1.79	0.44
1:C:450:HIS:HE1	1:C:548:ASP:OD1	2.00	0.44
1:D:553:ASP:OD1	4:D:1041:AFR:H11	2.17	0.44
1:A:1036:THR:CG2	5:A:2319:HOH:O	2.66	0.43
1:C:662:TRP:HA	1:C:692:GLY:O	2.18	0.43
1:D:805:ASP:O	1:D:820:ALA:HA	2.18	0.43
1:B:689:PRO:O	1:B:726:PRO:HG2	2.18	0.43
1:D:141:LYS:HE3	1:D:142:ASP:OD2	2.18	0.43
1:D:275:ASN:OD1	1:D:285:SER:OG	2.35	0.43
1:D:553:ASP:CG	4:D:1041:AFR:H11	2.44	0.43
1:D:592:TYR:CD1	1:D:596:VAL:HG11	2.53	0.43
1:A:787:ILE:HG13	5:A:2222:HOH:O	2.18	0.43
1:B:326:PHE:CE1	1:B:328:TYR:HB2	2.54	0.43
1:B:588:ASN:HB2	1:B:591:THR:O	2.18	0.43
1:B:713:ASP:OD1	1:B:869:GLN:HG3	2.18	0.43
1:A:725:LEU:O	1:A:726:PRO:C	2.61	0.43
1:D:842:LYS:O	5:D:2241:HOH:O	2.21	0.43
1:D:924:ASP:O	1:D:927:VAL:HG23	2.18	0.43
1:A:354:LEU:HD23	1:A:932:GLU:HB3	1.99	0.43
1:B:242:ASN:ND2	1:B:667:SER:HB2	2.34	0.43
1:D:231:ILE:N	1:D:302:ASP:HB2	2.32	0.43
1:A:793:TYR:HA	3:A:1041:GOL:H12	2.01	0.43
1:B:129:THR:HG23	1:B:137:THR:CG2	2.48	0.43
1:B:640:LYS:HB3	1:B:641:PHE:CD1	2.54	0.43
1:B:641:PHE:CZ	1:B:896:ASN:HB2	2.54	0.43
1:C:566:ASP:HB3	1:C:570:VAL:CG1	2.49	0.43
1:D:231:ILE:HA	1:D:302:ASP:HB2	2.00	0.43
1:D:243:TYR:OH	1:D:666:ASN:HB3	2.19	0.43
1:B:592:TYR:CD1	1:B:596:VAL:HG11	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:TRP:CE3	1:D:183:MET:HE2	2.53	0.43
1:D:885:ARG:HD2	1:D:904:LEU:HA	2.00	0.43
1:C:198:LYS:HD3	1:C:198:LYS:HA	1.85	0.43
1:B:1030:LEU:N	1:B:1031:PRO:HD2	2.34	0.42
1:C:805:ASP:CG	1:C:830:ARG:HH22	2.27	0.42
1:C:961:GLU:HA	1:C:961:GLU:OE1	2.19	0.42
1:D:236:TYR:O	1:D:237:ASN:C	2.62	0.42
1:D:554:MET:HB3	1:D:558:ALA:HB3	2.01	0.42
1:D:794:ASN:N	3:D:1040:GOL:H31	2.29	0.42
1:A:29:GLY:HA3	1:A:31:TRP:CE2	2.53	0.42
1:A:525:ASP:HB3	1:A:528:ARG:CD	2.48	0.42
1:A:964:PHE:O	1:A:1027:ASN:HB2	2.20	0.42
1:B:222:ASP:HB2	5:B:2023:HOH:O	2.18	0.42
1:D:606:HIS:O	1:D:606:HIS:CG	2.71	0.42
1:A:753:ASN:HD22	1:A:753:ASN:HA	1.66	0.42
1:B:370:GLN:O	1:B:409:LEU:HA	2.19	0.42
1:C:227:GLU:HB2	5:C:2033:HOH:O	2.19	0.42
1:C:363:LYS:NZ	1:C:770:GLU:OE2	2.45	0.42
1:C:719:VAL:O	1:C:723:CYS:HB3	2.20	0.42
4:D:1041:AFR:H12	5:D:2186:HOH:O	2.18	0.42
1:A:15:ASP:OD1	1:A:608:ARG:HD3	2.20	0.42
1:B:591:THR:OG1	1:B:592:TYR:N	2.53	0.42
1:C:421:VAL:HG12	5:C:2075:HOH:O	2.20	0.42
1:D:628:LYS:HD3	1:D:629:GLU:OE2	2.19	0.42
1:A:881:ILE:HA	1:A:907:GLU:O	2.19	0.42
1:B:408:GLY:HA3	1:B:455:VAL:O	2.20	0.42
1:C:784:LYS:HA	1:C:785:PRO:HD2	1.91	0.42
1:D:1015:ASP:OD1	1:D:1015:ASP:C	2.63	0.42
1:A:756:ASP:OD1	1:A:759:ARG:NH2	2.53	0.42
1:C:826:ASN:ND2	5:C:2133:HOH:O	2.53	0.42
1:C:885:ARG:HD2	1:C:885:ARG:HA	1.87	0.42
1:D:648:SER:O	1:D:661:MET:HA	2.20	0.42
1:A:34:SER:CA	5:A:2012:HOH:O	2.63	0.42
1:B:196:VAL:HG22	1:B:314:TYR:HB3	2.02	0.42
1:C:90:ARG:NH2	1:C:92:ARG:HD3	2.35	0.42
1:C:567:ASP:O	1:C:570:VAL:HG12	2.20	0.42
1:B:29:GLY:HA3	1:B:31:TRP:CE2	2.55	0.41
1:D:34:SER:O	1:D:37:SER:HB2	2.19	0.41
1:B:702:ASP:HB3	1:B:705:ASN:O	2.20	0.41
1:C:542:LEU:HB3	1:C:547:LEU:HD22	2.01	0.41
1:C:924:ASP:OD2	1:C:928:THR:OG1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ASN:O	1:D:87:ASN:HB2	2.19	0.41
1:B:276:GLY:HA3	1:B:284:TYR:CE1	2.55	0.41
1:C:200:PHE:HB2	1:C:208:GLU:HG3	2.02	0.41
1:D:415:MET:HE3	1:D:424:THR:HG22	2.01	0.41
1:D:485:TYR:HA	1:D:523:PHE:O	2.19	0.41
1:D:517:VAL:HG22	1:D:517:VAL:O	2.20	0.41
1:C:881:ILE:HA	1:C:907:GLU:O	2.19	0.41
1:D:402:ASN:HA	5:D:2143:HOH:O	2.20	0.41
1:A:227:GLU:O	1:A:228:ARG:NH1	2.52	0.41
1:A:596:VAL:O	1:A:610:PRO:HA	2.21	0.41
1:C:463:PHE:CD1	1:C:511:LEU:HD13	2.56	0.41
1:D:614:GLN:O	1:D:615:ARG:C	2.63	0.41
1:D:887:THR:HG21	1:D:891:GLU:O	2.21	0.41
1:A:241:LEU:HD21	1:A:699:THR:HG21	2.02	0.41
1:B:675:MET:O	1:B:679:ASN:ND2	2.53	0.41
1:C:770:GLU:HG2	1:C:885:ARG:HG2	2.03	0.41
1:D:30:VAL:HG11	1:D:232:ALA:C	2.46	0.41
1:A:662:TRP:HA	1:A:692:GLY:O	2.21	0.41
1:A:885:ARG:HD2	1:A:904:LEU:HA	2.02	0.41
1:C:17:PRO:HB3	5:C:2095:HOH:O	2.20	0.41
1:A:231:ILE:HD12	1:A:261:TYR:HB2	2.03	0.41
1:B:242:ASN:HD22	1:B:242:ASN:HA	1.71	0.41
1:B:259:PRO:CG	5:B:2034:HOH:O	2.52	0.41
1:D:364:TYR:CD1	1:D:364:TYR:C	2.98	0.41
1:D:403:ASN:O	1:D:759:ARG:CD	2.68	0.41
1:D:674:GLN:O	1:D:675:MET:C	2.61	0.41
1:A:271:TRP:CH2	1:A:287:GLY:HA3	2.56	0.41
1:A:648:SER:O	1:A:661:MET:HA	2.20	0.41
1:B:21:ASP:OD2	1:B:23:LYS:HE2	2.21	0.41
1:B:885:ARG:HA	1:B:885:ARG:HD2	1.95	0.41
1:C:834:LEU:HB3	1:C:840:TRP:CD1	2.56	0.41
1:D:911:LEU:CD1	1:D:946:GLN:HB2	2.51	0.41
1:A:559:MET:HG3	1:A:591:THR:HA	2.03	0.40
1:B:259:PRO:CB	5:B:2034:HOH:O	2.69	0.40
1:C:881:ILE:HB	1:C:918:GLY:HA3	2.03	0.40
1:D:345:GLN:HA	5:D:2045:HOH:O	2.21	0.40
1:A:410:ALA:HA	1:A:457:GLN:HG3	2.02	0.40
1:C:274:VAL:O	1:C:285:SER:HA	2.21	0.40
1:D:1032:ASP:O	1:D:1032:ASP:CG	2.64	0.40
1:A:924:ASP:O	1:A:927:VAL:HG23	2.22	0.40
1:A:936:LYS:HD3	1:A:936:LYS:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:TYR:HA	1:B:866:PRO:HD3	1.91	0.40
1:C:680:ASN:ND2	1:C:725:LEU:HD13	2.37	0.40
1:C:776:MET:CE	1:C:786:ILE:CD1	2.94	0.40
1:A:360:MET:HE3	1:A:360:MET:HB3	1.83	0.40
1:B:145:VAL:HG22	1:B:155:VAL:HG13	2.04	0.40
1:B:614:GLN:O	1:B:617:ILE:HG22	2.21	0.40
1:C:22:TYR:HD1	1:C:319:TYR:CE2	2.39	0.40
1:D:199:ASN:OD1	1:D:201:ARG:HB3	2.22	0.40
1:D:261:TYR:CD1	1:D:261:TYR:C	2.99	0.40
1:D:588:ASN:HB3	1:D:593:HIS:CE1	2.56	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%)	966 (94%)	53 (5%)	4 (0%)	30	28
1	B	1022/1027 (100%)	962 (94%)	59 (6%)	1 (0%)	48	50
1	C	1022/1027 (100%)	974 (95%)	47 (5%)	1 (0%)	48	50
1	D	1023/1027 (100%)	960 (94%)	59 (6%)	4 (0%)	30	28
All	All	4090/4108 (100%)	3862 (94%)	218 (5%)	10 (0%)	43	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	ASP
1	A	530	ASP
1	A	664	GLY
1	D	655	ASN
1	C	949	GLY

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Mol	Chain	Res	Type
1	D	986	GLY
1	B	151	PHE
1	D	914	ASN
1	A	948	GLY
1	D	515	GLY

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%)	850 (97%)	28 (3%)	34	38
1	B	877/878 (100%)	851 (97%)	26 (3%)	36	41
1	C	877/878 (100%)	852 (97%)	25 (3%)	37	42
1	D	878/878 (100%)	849 (97%)	29 (3%)	33	37
All	All	3510/3512 (100%)	3402 (97%)	108 (3%)	35	39

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ILE
1	A	37	SER
1	A	53	THR
1	A	100	ARG
1	A	151	PHE
1	A	281	SER
1	A	418	ASN
1	A	445	VAL
1	A	474	GLU
1	A	549	PHE
1	A	552	GLN
1	A	571	LYS
1	A	605	ASN
1	A	622	LEU
1	A	638	LEU
1	A	655	ASN

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Mol	Chain	Res	Type
1	A	663	VAL
1	A	677	ILE
1	A	688	LEU
1	A	690	LEU
1	A	718	TYR
1	A	719	VAL
1	A	753	ASN
1	A	830	ARG
1	A	936	LYS
1	A	1018	THR
1	A	1036	THR
1	A	1038	THR
1	B	53	THR
1	B	129	THR
1	B	215	GLU
1	B	282	GLU
1	B	306	ASN
1	B	326	PHE
1	B	418	ASN
1	B	471	GLN
1	B	474	GLU
1	B	517	VAL
1	B	551	TRP
1	B	571	LYS
1	B	622	LEU
1	B	628	LYS
1	B	640	LYS
1	B	655	ASN
1	B	661	MET
1	B	688	LEU
1	B	690	LEU
1	B	718	TYR
1	B	801	ARG
1	B	830	ARG
1	B	837	LEU
1	B	860	ASP
1	B	862	ILE
1	B	1038	THR
1	C	90	ARG
1	C	129	THR
1	C	137	THR
1	C	187	ARG

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Mol	Chain	Res	Type
1	C	339	THR
1	C	413	VAL
1	C	414	ASP
1	C	418	ASN
1	C	549	PHE
1	C	551	TRP
1	C	554	MET
1	C	655	ASN
1	C	662	TRP
1	C	688	LEU
1	C	690	LEU
1	C	718	TYR
1	C	829	GLU
1	C	830	ARG
1	C	849	THR
1	C	891	GLU
1	C	893	LYS
1	C	942	VAL
1	C	979	SER
1	C	1036	THR
1	C	1038	THR
1	D	14	THR
1	D	39	THR
1	D	100	ARG
1	D	164	ILE
1	D	229	THR
1	D	353	VAL
1	D	414	ASP
1	D	461	THR
1	D	471	GLN
1	D	517	VAL
1	D	617	ILE
1	D	622	LEU
1	D	648	SER
1	D	655	ASN
1	D	662	TRP
1	D	688	LEU
1	D	690	LEU
1	D	718	TYR
1	D	784	LYS
1	D	830	ARG
1	D	839	GLN

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Mol	Chain	Res	Type
1	D	857	ASN
1	D	915	ARG
1	D	942	VAL
1	D	979	SER
1	D	990	GLN
1	D	1027	ASN
1	D	1029	VAL
1	D	1038	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	177	ASN
1	A	242	ASN
1	A	253	HIS
1	A	325	HIS
1	A	468	ASN
1	A	616	ASN
1	A	655	ASN
1	A	657	HIS
1	A	671	ASN
1	A	679	ASN
1	A	684	ASN
1	A	731	HIS
1	A	753	ASN
1	A	803	GLN
1	A	812	HIS
1	A	864	ASN
1	A	930	ASN
1	A	957	ASN
1	A	980	ASN
1	B	16	ASN
1	B	62	ASN
1	B	191	ASN
1	B	217	ASN
1	B	221	GLN
1	B	242	ASN
1	B	325	HIS
1	B	416	GLN
1	B	418	ASN
1	B	450	HIS

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Mol	Chain	Res	Type
1	B	471	GLN
1	B	593	HIS
1	B	679	ASN
1	B	839	GLN
1	B	869	GLN
1	B	930	ASN
1	B	980	ASN
1	C	40	ASN
1	C	80	GLN
1	C	207	GLN
1	C	217	ASN
1	C	242	ASN
1	C	325	HIS
1	C	432	ASN
1	C	450	HIS
1	C	457	GLN
1	C	468	ASN
1	C	606	HIS
1	C	655	ASN
1	C	657	HIS
1	C	671	ASN
1	C	803	GLN
1	C	806	HIS
1	C	812	HIS
1	C	826	ASN
1	C	839	GLN
1	C	857	ASN
1	C	914	ASN
1	C	930	ASN
1	C	934	ASN
1	C	980	ASN
1	C	990	GLN
1	C	1009	ASN
1	D	62	ASN
1	D	111	GLN
1	D	177	ASN
1	D	197	ASN
1	D	242	ASN
1	D	258	ASN
1	D	309	GLN
1	D	325	HIS
1	D	382	HIS

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Mol	Chain	Res	Type
1	D	402	ASN
1	D	432	ASN
1	D	450	HIS
1	D	468	ASN
1	D	562	HIS
1	D	655	ASN
1	D	731	HIS
1	D	753	ASN
1	D	803	GLN
1	D	826	ASN
1	D	839	GLN
1	D	896	ASN
1	D	930	ASN
1	D	976	GLN
1	D	980	ASN
1	D	990	GLN

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	0.48	0	1,6,8	0.72	0
1	CSO	A	336	1	3,6,7	0.55	0	1,6,8	0.20	0
1	CSO	C	336	1	3,6,7	0.57	0	1,6,8	0.44	0
1	CSO	B	336	1	3,6,7	0.70	0	1,6,8	1.02	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	C	336	1	-	0/1/5/7	-
1	CSO	B	336	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	336	CSO	N-CA-CB-SG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	5GF	A	1039	1	9,12,13	1.43	1 (11%)	14,18,20	1.27	1 (7%)
3	GOL	A	1041	-	5,5,5	0.31	0	5,5,5	0.46	0
3	GOL	A	1040	-	5,5,5	0.35	0	5,5,5	0.16	0
2	5GF	C	1039	1	9,12,13	1.28	1 (11%)	14,18,20	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	AFR	D	1041	-	9,12,12	5.24	3 (33%)	9,18,18	0.79	0
3	GOL	D	1039	-	5,5,5	0.34	0	5,5,5	0.72	0
3	GOL	D	1040	-	5,5,5	0.40	0	5,5,5	0.70	0
3	GOL	B	1040	-	5,5,5	0.42	0	5,5,5	0.26	0
2	5GF	B	1039	1	9,12,13	1.17	1 (11%)	14,18,20	0.87	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	5GF	A	1039	1	-	0/2/23/26	0/1/1/1
3	GOL	A	1041	-	-	4/4/4/4	-
3	GOL	A	1040	-	-	2/4/4/4	-
2	5GF	C	1039	1	-	2/2/23/26	0/1/1/1
4	AFR	D	1041	-	-	0/2/23/23	0/1/1/1
3	GOL	D	1039	-	-	4/4/4/4	-
3	GOL	D	1040	-	-	0/4/4/4	-
3	GOL	B	1040	-	-	2/4/4/4	-
2	5GF	B	1039	1	1/1/4/5	2/2/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1041	AFR	C1-C2	-15.10	1.35	1.51
2	A	1039	5GF	O5-C5	3.69	1.45	1.37
2	C	1039	5GF	O5-C5	3.55	1.44	1.37
2	B	1039	5GF	O5-C5	3.08	1.43	1.37
4	D	1041	AFR	O5-C1	3.04	1.46	1.43
4	D	1041	AFR	O5-C5	2.83	1.43	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1039	5GF	C5-C4-C3	-2.56	107.89	110.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1039	5GF	C1

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1039	5GF	O5-C5-C6-O6
2	B	1039	5GF	C4-C5-C6-O6
2	C	1039	5GF	C4-C5-C6-O6
3	A	1041	GOL	O1-C1-C2-C3
3	B	1040	GOL	C1-C2-C3-O3
3	A	1041	GOL	O1-C1-C2-O2
3	A	1040	GOL	O1-C1-C2-C3
3	A	1041	GOL	C1-C2-C3-O3
3	D	1039	GOL	O1-C1-C2-C3
3	D	1039	GOL	C1-C2-C3-O3
3	A	1040	GOL	O1-C1-C2-O2
3	B	1040	GOL	O2-C2-C3-O3
3	D	1039	GOL	O2-C2-C3-O3
3	D	1039	GOL	O1-C1-C2-O2
2	C	1039	5GF	O5-C5-C6-O6
3	A	1041	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1039	5GF	1	0
3	A	1041	GOL	1	0
4	D	1041	AFR	4	0
3	D	1040	GOL	2	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%)	0.39	22 (2%)	63	66	14, 30, 44, 68	1 (0%)
1	B	1024/1027 (99%)	0.84	74 (7%)	21	23	24, 40, 58, 79	0
1	C	1024/1027 (99%)	0.80	49 (4%)	35	38	24, 40, 57, 78	0
1	D	1024/1027 (99%)	0.49	37 (3%)	46	48	15, 30, 48, 81	1 (0%)
All	All	4096/4108 (99%)	0.63	182 (4%)	39	41	14, 35, 55, 81	2 (0%)

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	517	VAL	5.3
1	B	514	GLY	4.6
1	A	987	ALA	4.5
1	C	514	GLY	4.5
1	D	515	GLY	4.3
1	B	326	PHE	4.1
1	C	326	PHE	4.0
1	B	530	ASP	3.9
1	B	516	GLY	3.8
1	B	515	GLY	3.8
1	A	14	THR	3.7
1	C	279	GLY	3.7
1	D	470	GLY	3.7
1	B	14	THR	3.7
1	C	948	GLY	3.6
1	D	514	GLY	3.6
1	C	328	TYR	3.5
1	D	516	GLY	3.4
1	B	606	HIS	3.4
1	B	529	PRO	3.4
1	A	976	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	994	VAL	3.2
1	B	976	GLN	3.2
1	C	14	THR	3.2
1	A	965	GLY	3.2
1	C	606	HIS	3.2
1	B	517	VAL	3.2
1	C	515	GLY	3.2
1	B	19	GLY	3.1
1	B	492	THR	3.1
1	B	220	TYR	3.1
1	B	328	TYR	3.1
1	A	947	ASP	3.1
1	A	529	PRO	3.0
1	B	558	ALA	3.0
1	D	987	ALA	3.0
1	C	527	GLY	3.0
1	D	513	TYR	3.0
1	B	551	TRP	3.0
1	C	517	VAL	2.9
1	D	254	ASP	2.9
1	B	996	SER	2.9
1	D	511	LEU	2.9
1	B	164	ILE	2.9
1	C	220	TYR	2.9
1	C	513	TYR	2.9
1	C	500	ASP	2.9
1	B	635	ALA	2.9
1	C	516	GLY	2.8
1	D	986	GLY	2.8
1	B	52	ILE	2.8
1	A	498	MET	2.7
1	B	527	GLY	2.7
1	B	330	ALA	2.7
1	D	498	MET	2.7
1	B	39	THR	2.7
1	B	73	VAL	2.7
1	A	988	GLY	2.7
1	C	478	THR	2.7
1	C	837	LEU	2.7
1	D	474	GLU	2.6
1	A	463	PHE	2.6
1	B	1038	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	14	THR	2.6
1	C	73	VAL	2.6
1	C	568	ILE	2.6
1	C	255	GLY	2.6
1	B	464	LEU	2.6
1	B	513	TYR	2.6
1	B	61	VAL	2.6
1	C	521	ALA	2.6
1	D	529	PRO	2.6
1	D	996	SER	2.6
1	C	164	ILE	2.6
1	B	565	GLY	2.6
1	A	254	ASP	2.6
1	D	512	ASP	2.6
1	A	996	SER	2.6
1	B	188	LEU	2.6
1	C	551	TRP	2.6
1	D	632	VAL	2.5
1	C	863	TYR	2.5
1	B	98	PRO	2.5
1	B	189	TYR	2.5
1	B	491	LEU	2.5
1	B	305	TRP	2.5
1	B	948	GLY	2.5
1	A	517	VAL	2.5
1	C	188	LEU	2.5
1	C	332	GLY	2.5
1	B	173	ALA	2.4
1	B	463	PHE	2.4
1	C	866	PRO	2.4
1	B	568	ILE	2.4
1	C	205	VAL	2.4
1	A	513	TYR	2.3
1	C	975	ALA	2.3
1	D	533	GLU	2.3
1	B	913	ASN	2.3
1	A	565	GLY	2.3
1	C	173	ALA	2.3
1	D	256	ALA	2.3
1	B	522	LEU	2.3
1	D	255	GLY	2.3
1	D	332	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	15	ASP	2.3
1	D	565	GLY	2.3
1	C	996	SER	2.3
1	A	558	ALA	2.3
1	C	916	ALA	2.3
1	C	997	ALA	2.3
1	D	67	ASP	2.3
1	B	71	ILE	2.2
1	B	571	LYS	2.2
1	C	493	GLY	2.2
1	D	597	LEU	2.2
1	B	474	GLU	2.2
1	B	704	GLU	2.2
1	B	72	THR	2.2
1	B	498	MET	2.2
1	B	975	ALA	2.2
1	A	606	HIS	2.2
1	D	220	TYR	2.2
1	D	37	SER	2.2
1	C	20	ILE	2.2
1	B	983	VAL	2.2
1	B	1007	GLY	2.2
1	A	173	ALA	2.2
1	D	328[A]	TYR	2.2
1	A	584	ASN	2.2
1	C	114	TRP	2.2
1	B	15	ASP	2.2
1	B	499	THR	2.2
1	B	512	ASP	2.2
1	D	580	ASP	2.2
1	C	641	PHE	2.1
1	B	329	GLY	2.1
1	B	511	LEU	2.1
1	A	189	TYR	2.1
1	A	328[A]	TYR	2.1
1	B	629	GLU	2.1
1	B	582	PRO	2.1
1	C	990	GLN	2.1
1	D	463	PHE	2.1
1	D	862	ILE	2.1
1	B	497	GLY	2.1
1	B	174	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	15	ASP	2.1
1	B	502	GLY	2.1
1	C	66	ILE	2.1
1	C	99	ILE	2.1
1	C	862	ILE	2.1
1	D	438	GLY	2.1
1	C	836	VAL	2.1
1	C	984	SER	2.1
1	B	59	MET	2.1
1	B	16	ASN	2.1
1	D	39	THR	2.1
1	B	51	GLY	2.1
1	B	949	GLY	2.1
1	B	293	VAL	2.1
1	A	901	GLU	2.0
1	D	532	ALA	2.1
1	C	498	MET	2.0
1	B	634	ASN	2.0
1	B	471	GLN	2.0
1	B	756	ASP	2.0
1	D	477	GLN	2.0
1	D	129	THR	2.0
1	C	22	TYR	2.0
1	C	1007	GLY	2.0
1	D	631	ILE	2.0
1	B	905	VAL	2.0
1	B	504	SER	2.0
1	B	418	ASN	2.0
1	C	471	GLN	2.0
1	B	69	PRO	2.0
1	B	137	THR	2.0
1	B	478	THR	2.0
1	C	1018	THR	2.0
1	B	974	GLY	2.0
1	D	493	GLY	2.0

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

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	B	336	7/8	0.86	0.12	36,37,42,44	0
1	CSO	C	336	7/8	0.94	0.09	36,37,41,43	0
1	CSO	D	336	7/8	0.94	0.09	27,27,29,31	0
1	CSO	A	336	7/8	0.95	0.08	26,27,35,37	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	A	1040	6/6	0.83	0.18	47,49,50,52	0
3	GOL	D	1040	6/6	0.84	0.18	43,46,48,48	0
3	GOL	A	1041	6/6	0.88	0.15	45,46,46,47	0
3	GOL	D	1039	6/6	0.88	0.14	34,35,37,37	0
2	5GF	B	1039	12/13	0.88	0.12	42,44,46,47	0
2	5GF	A	1039	12/13	0.89	0.11	35,36,38,39	0
3	GOL	B	1040	6/6	0.89	0.12	41,44,44,46	0
4	AFR	D	1041	12/12	0.89	0.12	45,47,48,49	0
2	5GF	C	1039	12/13	0.90	0.10	42,44,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.