



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:50 PM GMT

PDB ID : 4AMX
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

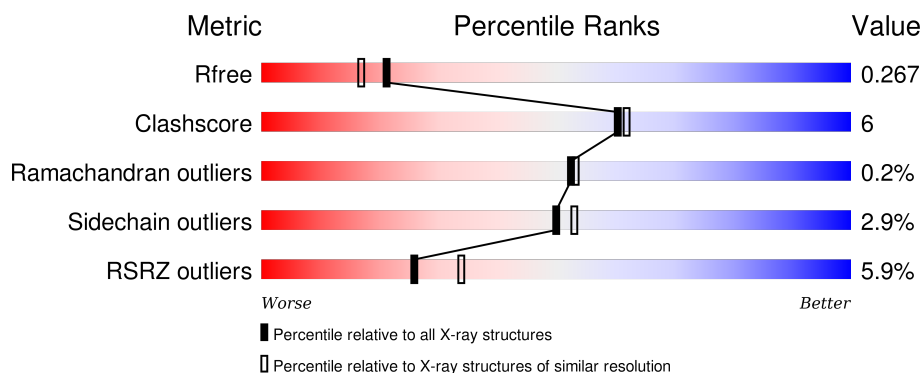
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1027	<div> <div>3%</div> <div>86%</div> <div>13%</div> </div>
1	B	1027	<div> <div>8%</div> <div>85%</div> <div>14%</div> </div>
1	C	1027	<div> <div>8%</div> <div>87%</div> <div>13%</div> </div>
1	D	1027	<div> <div>5%</div> <div>85%</div> <div>14%</div> </div>

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	-	-	-
3	GOL	A	1040	-	-	-	X
3	GOL	A	1041	-	-	-	X
3	GOL	D	1039	-	-	-	X
3	GOL	D	1040	-	-	-	X

2 Entry composition [i](#)

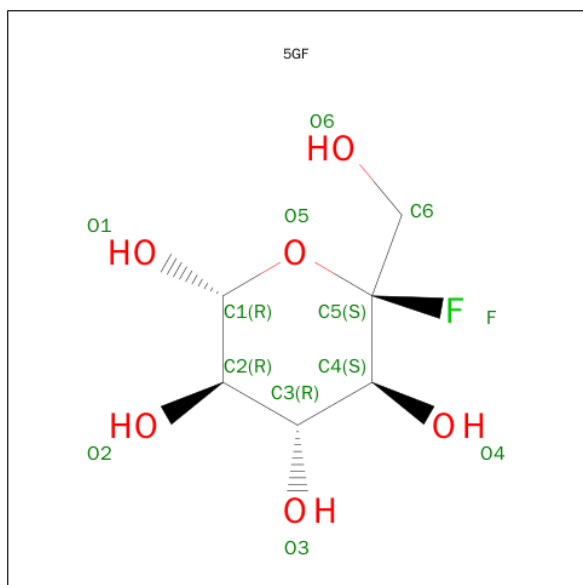
There are 5 unique types of molecules in this entry. The entry contains 33667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SUGAR (5-FLUORO-BETA-D-GLUCOPYRANOSE) (three-letter code: 5GF) (formula: C₆H₁₁FO₆).



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

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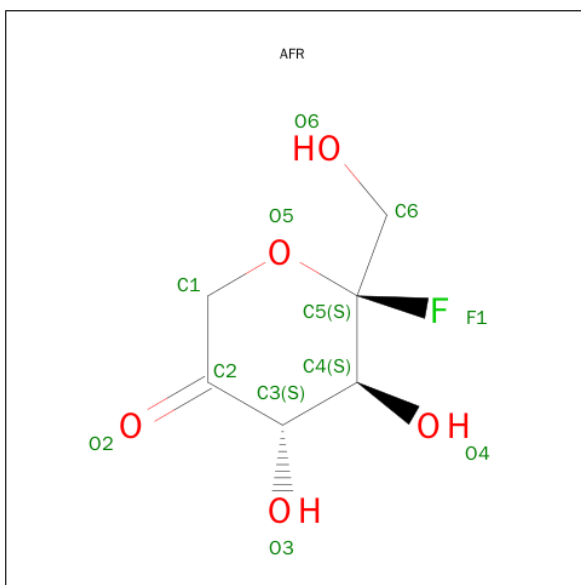
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	F	O	0	0
			12	6	1	5		

- Molecule 3 is GLYCEROL (three-letter code: 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 SUGAR (2-OXO-1,2,DIDEOXY-5F-D-GLUCOPYRANOSE) (three-letter code: 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		

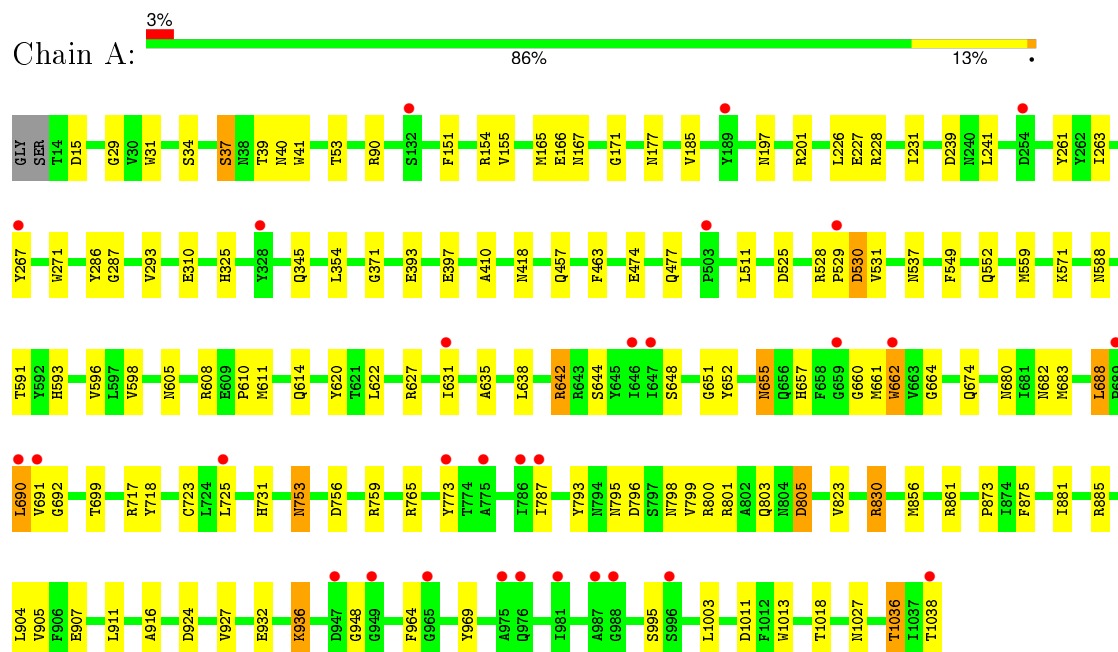
- Molecule 5 is water.

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		

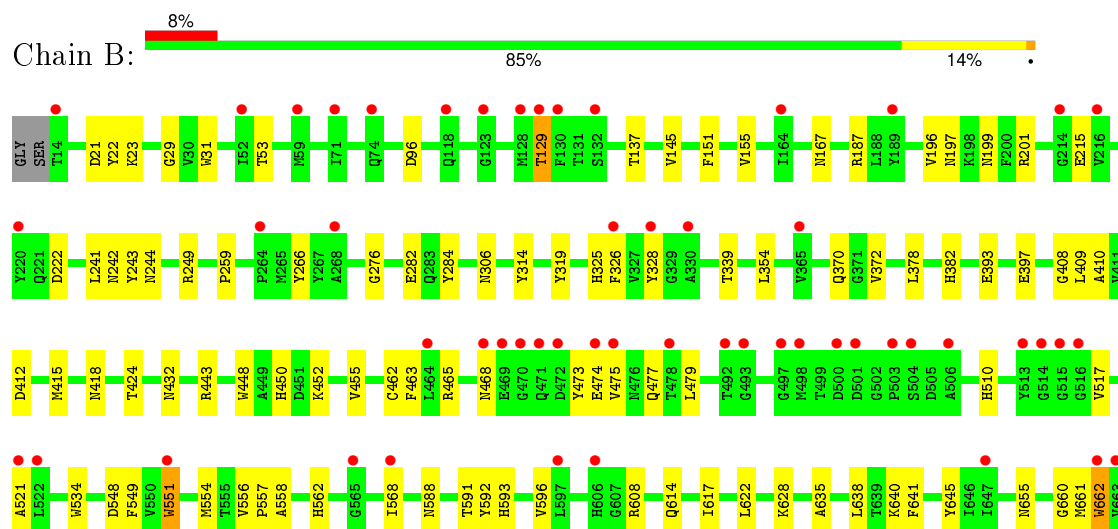
3 Residue-property plots

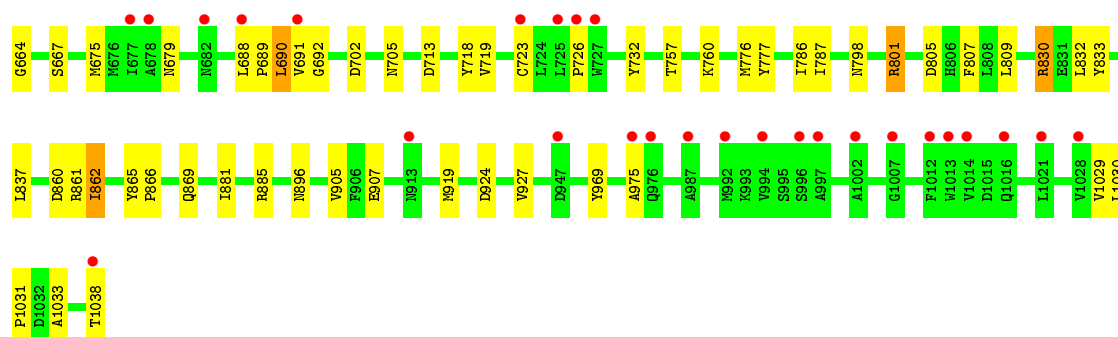
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

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

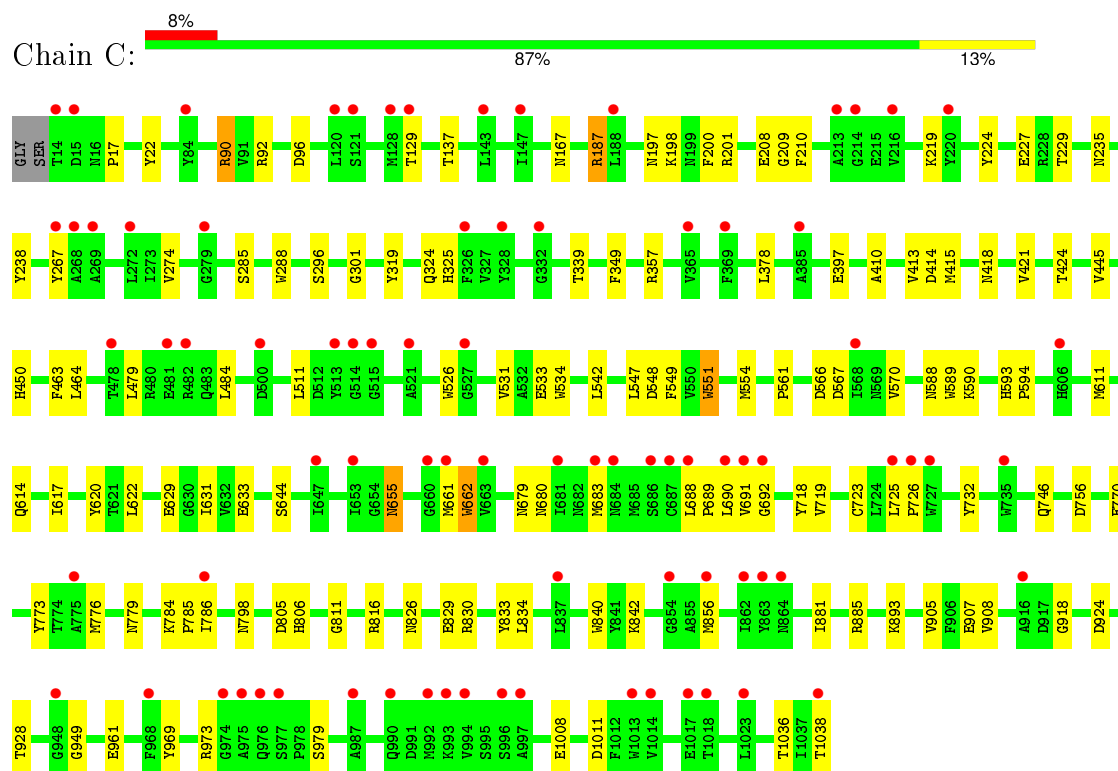


• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

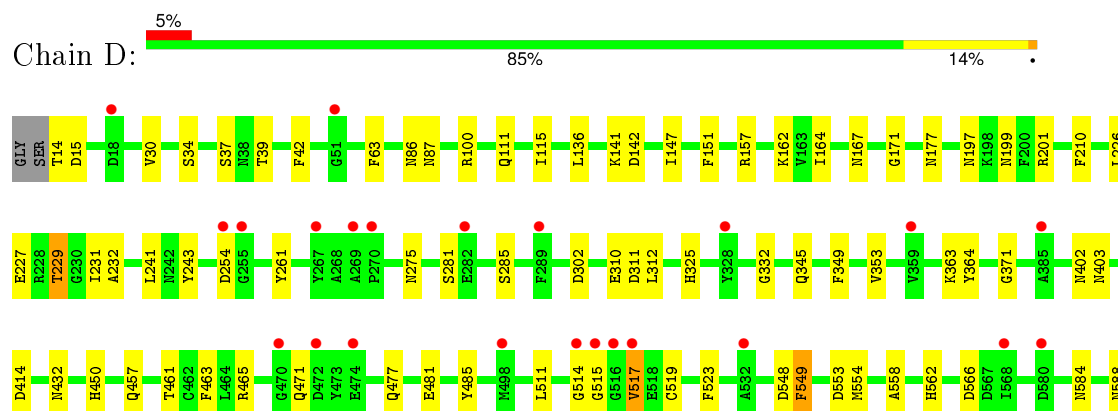


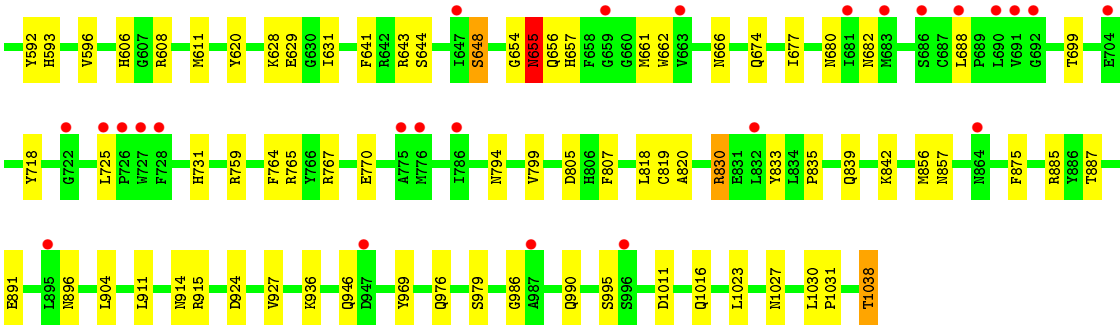


• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1



• 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) 91.3 (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 (5.32%)	DCC
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 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 255733 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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, 5GF, AFR

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	0.62	0/8387	0.70	2/11407 (0.0%)
1	B	0.49	0/8374	0.60	3/11389 (0.0%)
1	C	0.48	0/8374	0.59	0/11389
1	D	0.61	0/8387	0.67	1/11407 (0.0%)
All	All	0.56	0/33522	0.64	6/45592 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	975	ALA	O-C-N	-7.75	110.31	122.70
1	B	622	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	805	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	717	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	643	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	975	ALA	CA-C-N	5.06	128.33	117.20

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	8171	0	7615	92	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8162	0	7605	86	0
1	C	8162	0	7606	85	0
1	D	8171	0	7615	94	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	3	0
5	A	328	0	0	20	0
5	B	147	0	0	13	0
5	C	152	0	0	8	0
5	D	296	0	0	18	0
All	All	33667	0	30517	357	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 (357) 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:C:210:PHE:H	1:C:229:THR:HG22	1.26	1.00
1:A:529:PRO:O	1:A:530:ASP:HB2	1.65	0.96
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:D:677:ILE:HD13	5:D:2230:HOH:O	1.74	0.86
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: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	0.80
1:B:776:MET:HE2	1:B:786:ILE:HD11	1.64	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:B:462:CYS:HB2	5:B:2079:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:995:SER:HB2	1:A:1011:ASP:HB3	1.74	0.69
1:B:924:ASP:O	1:B:927:VAL:HG23	1.92	0.69
1:A:325:HIS:HE1	5:A:2036:HOH:O	1.76	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:776:MET:HE2	1:C:786:ILE:HD11	1.74	0.68
1:C:756:ASP:HB2	5:C:2116:HOH:O	1.92	0.68
1:A:805:ASP:CG	1:A:830:ARG:HH22	1.97	0.68
1:D:620:TYR:HA	1:D:655:ASN:HD21	1.60	0.67
1:A:598:VAL:HG11	1:A:611:MET:CE	2.25	0.67
1:B:382:HIS:CD2	1:B:432:ASN:HB2	2.31	0.66
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:677:ILE:HG21	5:D:2230:HOH:O	1.95	0.65
1:D:171:GLY:HA2	1:D:177:ASN:HD22	1.62	0.65
1:C:842:LYS:HB2	1:C:856:MET:CE	2.27	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: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: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:C:776:MET:HE3	1:C:786:ILE:HD11	1.81	0.62
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:NH1	1:B:249:ARG:HG2	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: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:598:VAL:HG11	1:A:611:MET:HE1	1.85	0.59
1:B:477:GLN:HG3	5:B:2081:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ARG:HD3	1:A:310:GLU:O	2.03	0.59
1:C:732:TYR:CD1	1:C:746:GLN:HB3	2.37	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:C:842:LYS:HB2	1:C:856:MET:HE3	1.84	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:D:136:LEU:HD23	1:D:147:ILE:HD12	1.86	0.56
1:C:811:GLY:HA3	1:C:816:ARG:CG	2.35	0.56
1:C:811:GLY:HA3	1:C:816:ARG:HG3	1.88	0.56
1:B:562:HIS:ND1	1:B:593:HIS:HE1	2.04	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:680:ASN:CG	5:A:2222:HOH:O	2.43	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: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:D:332:GLY:HA3	5:D:2114:HOH:O	2.07	0.54
1:B:554:MET:HB3	1:B:558:ALA:HB3	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:856:MET:HG2	5:D:2247:HOH:O	2.09	0.52
1:A:226:LEU:HD12	1:A:682:ASN:HD21	1.75	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
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:C:629:GLU:HG3	1:C:633:GLU:OE1	2.11	0.51
1:B:661:MET:O	1:B:691:VAL:HA	2.11	0.51
1:D:764:PHE:O	1:D:765:ARG:C	2.48	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:D:111:GLN:HE22	1:D:349:PHE:H	1.57	0.51
1:D:30:VAL:HG11	1:D:232:ALA:O	2.10	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:A:167:ASN:HA	1:A:197:ASN:HA	1.93	0.50
1:C:235:ASN:HB2	1:C:296:SER:OG	2.10	0.50
1:C:201:ARG:NH1	1:C:301:GLY:O	2.44	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: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: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:D:767:ARG:HB2	5:D:2210:HOH:O	2.12	0.48
1:D:477:GLN:O	1:D:481:GLU:HG2	2.13	0.48
1:B:719:VAL:O	1:B:723:CYS:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:MET:CE	1:A:875:PHE:CD2	2.95	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
1:D:818:LEU:HD22	1:D:835:PRO:HD2	1.95	0.48
1:B:645:TYR:CE2	1:B:690:LEU:HD13	2.48	0.48
1:C:219:LYS:HD3	1:C:224:TYR:CE1	2.48	0.48
1:D:924:ASP:OD1	1:D:924:ASP:C	2.52	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: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:553:ASP:OD2	4:D:1041:AFR:H11	2.13	0.48
1:D:241:LEU:HD21	1:D:699:THR:HG21	1.95	0.48
1:A:463:PHE:CE2	1:A:511:LEU:HD13	2.49	0.48
1:A:635:ALA:HB1	1:A:642:ARG:HG2	1.96	0.48
1:A:34:SER:O	1:A:37:SER:HB2	2.13	0.48
1:D:15:ASP:OD1	1:D:608:ARG:HD3	2.14	0.48
1:B:410:ALA:HB1	1:B:551:TRP:CZ3	2.49	0.48
1:B:832:LEU:HD23	1:B:862:ILE:HD12	1.96	0.47
1:A:598:VAL:HG11	1:A:611:MET:HE2	1.97	0.47
1:C:357:ARG:HB2	1:C:779:ASN:O	2.13	0.47
1:B:660:GLY:C	1:B:661:MET:HG2	2.35	0.47
1:C:881:ILE:HG12	1:C:908:VAL:HG22	1.95	0.47
1:C:614:GLN:O	1:C:617:ILE:HG22	2.15	0.47
1:A:34:SER:C	5:A:2012:HOH:O	2.53	0.47
1:A:1003:LEU:HD22	1:A:1013:TRP:CB	2.44	0.47
1:A:856:MET:HE1	1:A:875:PHE:CD2	2.50	0.47
1:D:227:GLU:OE2	1:D:229:THR:CG2	2.62	0.47
1:A:801:ARG:HH21	1:A:861:ARG:HD3	1.79	0.47
1:D:1030:LEU:N	1:D:1031:PRO:CD	2.78	0.47
1:B:556:VAL:N	1:B:557:PRO:HA	2.29	0.47
1:D:281:SER:HA	5:D:2105:HOH:O	2.13	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:D:805:ASP:HA	5:D:2230:HOH:O	2.15	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:A:41:TRP:CE2	1:A:185:VAL:HG22	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ILE:CA	1:D:302:ASP:HB2	2.45	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:656:GLN:HG2	1:D:657:HIS:N	2.31	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:680:ASN:ND2	1:D:725:LEU:HD13	2.30	0.46
1:B:805:ASP:CG	1:B:830:ARG:HH22	2.19	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:C:227:GLU:OE2	1:C:229:THR:CG2	2.64	0.45
1:B:266:TYR:CE2	1:B:664:GLY:HA3	2.51	0.45
1:B:22:TYR:HD1	1:B:319:TYR:CE2	2.34	0.45
1:A:155:VAL:HG21	1:A:165:MET:HE3	1.97	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:C:905:VAL:HG22	1:C:969:TYR:HB2	1.97	0.45
1:D:371:GLY:C	1:D:731:HIS:HD2	2.18	0.45
1:B:776:MET:HE3	1:B:786:ILE:HD11	1.98	0.45
1:A:525:ASP:O	1:A:531:VAL:HG21	2.16	0.45
1:D:111:GLN:O	1:D:115:ILE:HG13	2.17	0.45
1:C:238:TYR:HE1	1:C:589:TRP:HB3	1.80	0.45
1:B:450:HIS:HE1	1:B:548:ASP:OD1	1.98	0.45
1:C:594:PRO:HG3	5:C:2037:HOH:O	2.16	0.45
1:B:463:PHE:HB2	1:B:521:ALA:CB	2.46	0.45
1:A:773:TYR:HB3	5:A:2256:HOH:O	2.15	0.45
1:D:856:MET:HE1	1:D:875:PHE:HD2	1.81	0.45
1:A:371:GLY:C	1:A:731:HIS:HD2	2.19	0.45
1:B:881:ILE:HA	1:B:907:GLU:O	2.16	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:D:15:ASP:HA	1:D:608:ARG:H	1.82	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:A:90:ARG:HB2	1:A:325:HIS:CD2	2.52	0.45
1:C:484:LEU:HB3	1:C:531:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:VAL:HG23	1:A:614:GLN:HA	1.99	0.45
1:A:154:ARG:NH1	1:A:166:GLU:OE2	2.50	0.45
1:D:450:HIS:HE1	1:D:548:ASP:OD1	2.00	0.44
1:C:842:LYS:HB2	1:C:856:MET:HE1	1.99	0.44
1:D:42:PHE:HB3	1:D:63:PHE:HB3	1.98	0.44
1:D:799:VAL:HG13	1:D:833:TYR:HE2	1.82	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:A:620:TYR:HA	1:A:655:ASN:HD21	1.83	0.44
1:D:631:ILE:HG23	1:D:644:SER:HB3	2.00	0.44
1:B:325:HIS:HD2	5:B:2006:HOH:O	2.00	0.44
1:A:393:GLU:HG2	1:A:397:GLU:OE2	2.17	0.44
1:D:226:LEU:HD12	1:D:682:ASN:ND2	2.33	0.44
1:A:165:MET:HG3	1:A:286:TYR:CZ	2.53	0.44
1:A:800:ARG:O	1:A:803:GLN:CD	2.55	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: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:D:592:TYR:CD1	1:D:596:VAL:HG11	2.53	0.43
1:D:141:LYS:HE3	1:D:142:ASP:OD2	2.18	0.43
1:B:689:PRO:O	1:B:726:PRO:HG2	2.18	0.43
1:D:275:ASN:OD1	1:D:285:SER:OG	2.35	0.43
1:D:805:ASP:CG	1:D:830:ARG:HH22	2.22	0.43
1:A:787:ILE:HG13	5:A:2222:HOH:O	2.18	0.43
1:B:713:ASP:OD1	1:B:869:GLN:HG3	2.18	0.43
1:B:588:ASN:HB2	1:B:591:THR:O	2.18	0.43
1:B:326:PHE:CE1	1:B:328:TYR:HB2	2.54	0.43
1:D:924:ASP:O	1:D:927:VAL:HG23	2.18	0.43
1:D:842:LYS:O	5:D:2241:HOH:O	2.21	0.43
1:D:231:ILE:N	1:D:302:ASP:HB2	2.32	0.43
1:B:242:ASN:ND2	1:B:667:SER:HB2	2.34	0.43
1:A:354:LEU:HD23	1:A:932:GLU:HB3	1.99	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:856:MET:HE1	1:D:875:PHE:CD2	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:641:PHE:CZ	1:B:896:ASN:HB2	2.54	0.43
1:A:793:TYR:HA	3:A:1041:GOL:H12	2.01	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
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:C:961:GLU:HA	1:C:961:GLU:OE1	2.19	0.42
1:B:1030:LEU:N	1:B:1031:PRO:HD2	2.34	0.42
1:D:794:ASN:N	3:D:1040:GOL:H31	2.29	0.42
1:D:554:MET:HB3	1:D:558:ALA:HB3	2.01	0.42
1:A:525:ASP:HB3	1:A:528:ARG:CD	2.48	0.42
1:A:29:GLY:HA3	1:A:31:TRP:CE2	2.53	0.42
1:A:964:PHE:O	1:A:1027:ASN:HB2	2.20	0.42
1:D:606:HIS:O	1:D:606:HIS:CG	2.71	0.42
1:B:222:ASP:HB2	5:B:2023:HOH:O	2.18	0.42
1:C:227:GLU:HB2	5:C:2033:HOH:O	2.19	0.42
1:B:241:LEU:C	1:B:243:TYR:H	2.23	0.42
1:A:856:MET:HE3	1:A:875:PHE:CD2	2.54	0.42
4:D:1041:AFR:H12	5:D:2186:HOH:O	2.18	0.42
1:D:86:ASN:O	1:D:87:ASN:HB2	2.19	0.42
1:C:719:VAL:O	1:C:723:CYS:HB3	2.20	0.42
1:B:370:GLN:O	1:B:409:LEU:HA	2.19	0.42
1:A:753:ASN:HD22	1:A:753:ASN:HA	1.66	0.42
1:B:591:THR:OG1	1:B:592:TYR:N	2.53	0.42
1:A:15:ASP:OD1	1:A:608:ARG:HD3	2.20	0.42
1:C:421:VAL:HG12	5:C:2075:HOH:O	2.20	0.42
1:C:415:MET:CE	1:C:424:THR:HG22	2.49	0.42
1:D:628:LYS:HD3	1:D:629:GLU:OE2	2.19	0.42
1:C:784:LYS:HA	1:C:785:PRO:HD2	1.91	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:A:756:ASP:OD1	1:A:759:ARG:NH2	2.53	0.42
1:D:648:SER:O	1:D:661:MET:HA	2.20	0.42
1:C:288:TRP:HE1	1:C:324:GLN:CD	2.23	0.42
1:C:885:ARG:HA	1:C:885:ARG:HD2	1.87	0.42
1:C:826:ASN:ND2	5:C:2133:HOH:O	2.53	0.42
1:A:34:SER:CA	5:A:2012:HOH:O	2.63	0.42
1:C:567:ASP:O	1:C:570:VAL:HG12	2.20	0.42
1:C:90:ARG:NH2	1:C:92:ARG:HD3	2.35	0.42
1:B:196:VAL:HG22	1:B:314:TYR:HB3	2.02	0.42
1:B:243:TYR:C	5:B:2034:HOH:O	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:267:TYR:CE1	1:A:651:GLY:C	2.94	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
1:D:517:VAL:HG22	1:D:517:VAL:O	2.20	0.41
1:B:276:GLY:HA3	1:B:284:TYR:CE1	2.55	0.41
1:D:485:TYR:HA	1:D:523:PHE:O	2.19	0.41
1:C:200:PHE:HB2	1:C:208:GLU:HG3	2.02	0.41
1:D:654:GLY:C	1:D:656:GLN:OE1	2.59	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:C:463:PHE:CD1	1:C:511:LEU:HD13	2.56	0.41
1:D:887:THR:HG21	1:D:891:GLU:O	2.21	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:770:GLU:HG2	1:C:885:ARG:HG2	2.03	0.41
1:B:675:MET:O	1:B:679:ASN:ND2	2.53	0.41
1:A:241:LEU:HD21	1:A:699:THR:HG21	2.02	0.41
1:B:415:MET:CE	1:B:424:THR:HG22	2.50	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:662:TRP:HA	1:A:692:GLY:O	2.21	0.41
1:B:259:PRO:CG	5:B:2034:HOH:O	2.52	0.41
1:D:403:ASN:O	1:D:759:ARG:CD	2.68	0.41
1:B:242:ASN:HA	1:B:242:ASN:HD22	1.71	0.41
1:A:231:ILE:HD12	1:A:261:TYR:HB2	2.03	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:A:271:TRP:CH2	1:A:287:GLY:HA3	2.56	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:796:ASP:CG	1:A:799:VAL:HG13	2.42	0.41
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:A:559:MET:HG3	1:A:591:THR:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:776:MET:CE	1:C:786:ILE:CD1	2.94	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
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:D:199:ASN:OD1	1:D:201:ARG:HB3	2.22	0.40
1:D:588:ASN:HB3	1:D:593:HIS:CE1	2.56	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1023/1027 (100%)	966 (94%)	53 (5%)	4 (0%)	39	37
1	B	1022/1027 (100%)	962 (94%)	59 (6%)	1 (0%)	56	58
1	C	1022/1027 (100%)	974 (95%)	47 (5%)	1 (0%)	56	58
1	D	1023/1027 (100%)	960 (94%)	59 (6%)	4 (0%)	39	37
All	All	4090/4108 (100%)	3862 (94%)	218 (5%)	10 (0%)	52	53

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%)	855 (97%)	23 (3%)	54	58
1	B	877/878 (100%)	852 (97%)	25 (3%)	50	53
1	C	877/878 (100%)	852 (97%)	25 (3%)	50	53
1	D	878/878 (100%)	850 (97%)	28 (3%)	46	48
All	All	3510/3512 (100%)	3409 (97%)	101 (3%)	50	53

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	SER
1	A	53	THR
1	A	151	PHE
1	A	418	ASN
1	A	474	GLU
1	A	477	GLN
1	A	549	PHE
1	A	552	GLN
1	A	571	LYS
1	A	605	ASN
1	A	622	LEU
1	A	642	ARG
1	A	655	ASN
1	A	662	TRP
1	A	688	LEU
1	A	690	LEU

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Mol	Chain	Res	Type
1	A	718	TYR
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	412	ASP
1	B	418	ASN
1	B	474	GLU
1	B	517	VAL
1	B	549	PHE
1	B	551	TRP
1	B	608	ARG
1	B	628	LYS
1	B	655	ASN
1	B	662	TRP
1	B	688	LEU
1	B	690	LEU
1	B	718	TYR
1	B	801	ARG
1	B	809	LEU
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
1	C	339	THR
1	C	349	PHE
1	C	413	VAL
1	C	414	ASP
1	C	418	ASN
1	C	549	PHE

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Mol	Chain	Res	Type
1	C	551	TRP
1	C	554	MET
1	C	611	MET
1	C	655	ASN
1	C	662	TRP
1	C	688	LEU
1	C	690	LEU
1	C	718	TYR
1	C	773	TYR
1	C	829	GLU
1	C	830	ARG
1	C	893	LYS
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	151	PHE
1	D	229	THR
1	D	254	ASP
1	D	353	VAL
1	D	364	TYR
1	D	414	ASP
1	D	432	ASN
1	D	461	THR
1	D	471	GLN
1	D	517	VAL
1	D	549	PHE
1	D	611	MET
1	D	648	SER
1	D	655	ASN
1	D	662	TRP
1	D	718	TYR
1	D	830	ARG
1	D	839	GLN
1	D	857	ASN
1	D	915	ARG
1	D	936	LYS
1	D	979	SER
1	D	990	GLN
1	D	1027	ASN

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Mol	Chain	Res	Type
1	D	1038	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
1	A	242	ASN
1	A	325	HIS
1	A	552	GLN
1	A	586	GLN
1	A	655	ASN
1	A	657	HIS
1	A	671	ASN
1	A	731	HIS
1	A	753	ASN
1	A	812	HIS
1	A	930	ASN
1	A	934	ASN
1	B	16	ASN
1	B	197	ASN
1	B	221	GLN
1	B	242	ASN
1	B	325	HIS
1	B	418	ASN
1	B	450	HIS
1	B	593	HIS
1	B	671	ASN
1	B	839	GLN
1	B	930	ASN
1	B	934	ASN
1	C	80	GLN
1	C	207	GLN
1	C	242	ASN
1	C	325	HIS
1	C	450	HIS
1	C	457	GLN
1	C	655	ASN
1	C	657	HIS
1	C	671	ASN
1	C	806	HIS
1	C	812	HIS
1	C	826	ASN

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Mol	Chain	Res	Type
1	C	930	ASN
1	C	934	ASN
1	C	990	GLN
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	432	ASN
1	D	450	HIS
1	D	562	HIS
1	D	655	ASN
1	D	671	ASN
1	D	731	HIS
1	D	753	ASN
1	D	826	ASN
1	D	839	GLN
1	D	896	ASN
1	D	930	ASN
1	D	934	ASN
1	D	957	ASN
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	A	336	1	3,6,7	0.47	0	1,6,8	2.23	1 (100%)
1	CSO	B	336	1	3,6,7	0.61	0	1,6,8	1.81	0
1	CSO	C	336	1	3,6,7	0.49	0	1,6,8	1.94	0
1	CSO	D	336	1	3,6,7	0.41	0	1,6,8	1.96	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	A	336	1	-	0/1/5/7	0/0/0/0
1	CSO	B	336	1	-	0/1/5/7	0/0/0/0
1	CSO	C	336	1	-	0/1/5/7	0/0/0/0
1	CSO	D	336	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	CSO	O-C-CA	-2.23	119.69	125.49

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 [i](#)

There are no carbohydrates 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	12,12,13	1.46	2 (16%)	14,18,20	1.33	2 (14%)
3	GOL	A	1040	-	5,5,5	0.30	0	5,5,5	0.18	0
3	GOL	A	1041	-	5,5,5	0.27	0	5,5,5	0.46	0
2	5GF	B	1039	1	12,12,13	1.21	1 (8%)	14,18,20	1.04	1 (7%)
3	GOL	B	1040	-	5,5,5	0.38	0	5,5,5	0.31	0
2	5GF	C	1039	1	12,12,13	1.25	1 (8%)	14,18,20	1.05	2 (14%)
3	GOL	D	1039	-	5,5,5	0.33	0	5,5,5	0.59	0
3	GOL	D	1040	-	5,5,5	0.41	0	5,5,5	0.60	0
4	AFR	D	1041	-	11,12,12	5.37	3 (27%)	7,18,18	0.94	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	1040	-	-	0/4/4/4	0/0/0/0
3	GOL	A	1041	-	-	0/4/4/4	0/0/0/0
2	5GF	B	1039	1	1/1/4/5	0/2/23/26	0/1/1/1
3	GOL	B	1040	-	-	0/4/4/4	0/0/0/0
2	5GF	C	1039	1	-	0/2/23/26	0/1/1/1
3	GOL	D	1039	-	-	0/4/4/4	0/0/0/0
3	GOL	D	1040	-	-	0/4/4/4	0/0/0/0
4	AFR	D	1041	-	-	0/2/23/23	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	AFR	C1-C2	-17.21	1.35	1.51
2	A	1039	5GF	C5-C4	-2.28	1.52	1.54
4	D	1041	AFR	O5-C1	2.67	1.46	1.43
4	D	1041	AFR	O5-C5	2.83	1.43	1.37
2	B	1039	5GF	O5-C5	3.07	1.43	1.37
2	C	1039	5GF	O5-C5	3.54	1.44	1.37
2	A	1039	5GF	O5-C5	3.68	1.45	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1039	5GF	O2-C2-C1	2.13	113.48	109.21
2	C	1039	5GF	C1-C2-C3	2.22	112.17	109.54
2	B	1039	5GF	O5-C5-C6	2.37	109.67	105.85
2	C	1039	5GF	O5-C5-C6	2.60	110.04	105.85
2	A	1039	5GF	O5-C5-C6	3.05	110.76	105.85

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1039	5GF	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1039	5GF	1	0
3	A	1041	GOL	1	0
3	D	1040	GOL	2	0
4	D	1041	AFR	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	1024/1027 (99%)	0.34	30 (2%) 55 63	16, 30, 44, 68	0
1	B	1024/1027 (99%)	0.59	81 (7%) 15 21	24, 40, 58, 79	0
1	C	1024/1027 (99%)	0.64	82 (8%) 15 21	24, 40, 57, 78	0
1	D	1024/1027 (99%)	0.43	48 (4%) 35 44	17, 30, 48, 81	0
All	All	4096/4108 (99%)	0.50	241 (5%) 26 34	16, 35, 55, 81	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	ALA	6.1
1	C	837	LEU	4.9
1	D	516	GLY	4.7
1	A	988	GLY	4.7
1	C	514	GLY	4.5
1	D	517	VAL	4.4
1	B	976	GLN	4.3
1	B	514	GLY	4.3
1	A	976	GLN	4.3
1	C	1013	TRP	4.1
1	D	515	GLY	4.0
1	B	129	THR	4.0
1	C	1014	VAL	3.9
1	B	504	SER	3.9
1	C	688	LEU	3.9
1	B	123	GLY	3.9
1	C	691	VAL	3.8
1	B	565	GLY	3.8
1	D	470	GLY	3.8
1	B	1028	VAL	3.7
1	C	269	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	254	ASP	3.6
1	B	470	GLY	3.6
1	C	515	GLY	3.6
1	D	725	LEU	3.6
1	C	948	GLY	3.6
1	C	653	ILE	3.5
1	B	515	GLY	3.5
1	C	996	SER	3.5
1	C	14	THR	3.4
1	C	690	LEU	3.4
1	B	503	PRO	3.4
1	C	326	PHE	3.4
1	C	220	TYR	3.4
1	D	692	GLY	3.2
1	B	691	VAL	3.2
1	D	255	GLY	3.2
1	C	686	SER	3.2
1	D	996	SER	3.2
1	C	992	MET	3.2
1	D	472	ASP	3.2
1	C	1038	THR	3.2
1	B	474	GLU	3.1
1	B	994	VAL	3.1
1	B	130	PHE	3.1
1	B	663	VAL	3.1
1	A	725	LEU	3.1
1	D	987	ALA	3.1
1	C	975	ALA	3.1
1	B	326	PHE	3.1
1	C	268	ALA	3.0
1	C	994	VAL	3.0
1	B	500	ASP	3.0
1	B	471	GLN	3.0
1	C	725	LEU	3.0
1	C	863	TYR	3.0
1	A	947	ASP	3.0
1	C	15	ASP	3.0
1	C	1017	GLU	3.0
1	B	975	ALA	3.0
1	D	647	ILE	3.0
1	D	498	MET	3.0
1	C	214	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	691	VAL	2.9
1	B	220	TYR	2.9
1	C	478	THR	2.9
1	B	1014	VAL	2.9
1	A	996	SER	2.9
1	A	690	LEU	2.9
1	B	568	ILE	2.9
1	C	681	ILE	2.9
1	C	267	TYR	2.9
1	B	189	TYR	2.8
1	C	527	GLY	2.8
1	A	787	ILE	2.8
1	C	216	VAL	2.8
1	D	727	TRP	2.8
1	D	690	LEU	2.8
1	A	254	ASP	2.8
1	B	725	LEU	2.8
1	C	84	TYR	2.8
1	C	977	SER	2.8
1	B	128	MET	2.7
1	C	385	ALA	2.7
1	C	147	ILE	2.7
1	B	365	VAL	2.7
1	B	330	ALA	2.7
1	B	647	ILE	2.7
1	D	289	PHE	2.7
1	D	688	LEU	2.7
1	D	728	PHE	2.7
1	B	996	SER	2.7
1	B	677	ILE	2.6
1	D	681	ILE	2.6
1	A	662	TRP	2.6
1	B	472	ASP	2.6
1	C	854	GLY	2.6
1	C	856	MET	2.6
1	B	469	GLU	2.6
1	C	1023	LEU	2.6
1	B	14	THR	2.6
1	D	659	GLY	2.6
1	C	974	GLY	2.5
1	D	51	GLY	2.5
1	C	683	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	214	GLY	2.5
1	A	691	VAL	2.5
1	B	516	GLY	2.5
1	A	786	ILE	2.5
1	B	497	GLY	2.5
1	A	503	PRO	2.5
1	C	328	TYR	2.5
1	A	529	PRO	2.5
1	B	606	HIS	2.5
1	C	521	ALA	2.5
1	D	580	ASP	2.5
1	D	726	PRO	2.5
1	A	975	ALA	2.4
1	B	268	ALA	2.4
1	A	132	SER	2.4
1	B	132	SER	2.4
1	B	947	ASP	2.4
1	D	328[A]	TYR	2.4
1	C	120	LEU	2.4
1	A	1038	THR	2.4
1	B	216	VAL	2.4
1	B	164	ILE	2.4
1	D	775	ALA	2.4
1	A	267	TYR	2.4
1	C	188	LEU	2.4
1	D	683	MET	2.4
1	A	949	GLY	2.4
1	C	365	VAL	2.4
1	B	997	ALA	2.4
1	D	269	ALA	2.4
1	B	328	TYR	2.4
1	B	1013	TRP	2.4
1	B	1038	THR	2.4
1	C	661	MET	2.4
1	C	987	ALA	2.3
1	C	997	ALA	2.3
1	B	475	VAL	2.3
1	C	663	VAL	2.3
1	C	990	GLN	2.3
1	A	659	GLY	2.3
1	C	993	LYS	2.3
1	D	532	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	647	ILE	2.3
1	A	981	ILE	2.3
1	C	786	ILE	2.3
1	B	464	LEU	2.3
1	B	506	ALA	2.3
1	C	687	CYS	2.3
1	D	385	ALA	2.3
1	A	646	ILE	2.3
1	B	913	ASN	2.3
1	C	647	ILE	2.3
1	C	775	ALA	2.3
1	C	500	ASP	2.3
1	D	864	ASN	2.3
1	B	71	ILE	2.3
1	D	568	ILE	2.3
1	B	492	THR	2.3
1	C	129	THR	2.3
1	A	328[A]	TYR	2.3
1	D	267	TYR	2.3
1	A	965	GLY	2.2
1	C	692	GLY	2.2
1	C	968	PHE	2.2
1	D	663	VAL	2.2
1	A	775	ALA	2.2
1	C	279	GLY	2.2
1	A	189	TYR	2.2
1	B	498	MET	2.2
1	C	1018	THR	2.2
1	B	551	TRP	2.2
1	B	1021	LEU	2.2
1	B	468	ASN	2.2
1	B	682	ASN	2.2
1	C	568	ILE	2.2
1	B	74	GLN	2.2
1	B	678	ALA	2.2
1	C	976	GLN	2.2
1	D	832	LEU	2.2
1	B	513	TYR	2.2
1	C	332	GLY	2.2
1	B	501	ASP	2.2
1	C	862	ILE	2.2
1	D	474	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	514	GLY	2.2
1	C	369	PHE	2.2
1	C	513	TYR	2.2
1	D	282	GLU	2.2
1	D	704	GLU	2.2
1	B	521	ALA	2.2
1	B	1002	ALA	2.2
1	C	916	ALA	2.2
1	A	631	ILE	2.2
1	C	726	PRO	2.2
1	B	118	GLN	2.1
1	C	660	GLY	2.1
1	C	727	TRP	2.1
1	B	1012	PHE	2.1
1	D	270	PRO	2.1
1	D	776	MET	2.1
1	B	522	LEU	2.1
1	C	735	TRP	2.1
1	B	264	PRO	2.1
1	D	947	ASP	2.1
1	B	1007	GLY	2.1
1	B	688	LEU	2.1
1	C	272	LEU	2.1
1	C	213	ALA	2.1
1	C	128	MET	2.1
1	D	359	VAL	2.1
1	D	686	SER	2.1
1	B	52	ILE	2.1
1	B	478	THR	2.1
1	B	1016	GLN	2.1
1	D	786	ILE	2.1
1	C	143	LEU	2.1
1	D	18	ASP	2.1
1	A	689	PRO	2.1
1	B	726	PRO	2.1
1	B	59	MET	2.1
1	B	723	CYS	2.1
1	B	992	MET	2.1
1	C	684	ASN	2.1
1	B	727	TRP	2.1
1	C	482	ARG	2.1
1	B	493	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	864	ASN	2.1
1	A	773	TYR	2.1
1	B	597	LEU	2.0
1	D	895	LEU	2.0
1	C	606	HIS	2.0
1	B	662	TRP	2.0
1	B	987	ALA	2.0
1	C	481	GLU	2.0
1	D	722	GLY	2.0
1	C	121	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	CSO	A	336	7/8	0.95	0.12	-	26,27,35,37	0
1	CSO	D	336	7/8	0.93	0.14	-	27,27,29,31	0
1	CSO	B	336	7/8	0.89	0.14	-	36,37,42,44	0
1	CSO	C	336	7/8	0.95	0.11	-	36,37,41,43	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	D	1040	6/6	0.87	0.18	4.37	43,46,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	A	1040	6/6	0.68	0.23	3.95	47,49,50,52	0
3	GOL	A	1041	6/6	0.84	0.18	3.50	45,46,46,47	0
3	GOL	D	1039	6/6	0.90	0.16	2.27	34,35,37,37	0
3	GOL	B	1040	6/6	0.90	0.13	0.90	41,44,44,46	0
2	5GF	A	1039	12/13	0.89	0.17	0.46	35,36,38,39	0
4	AFR	D	1041	12/12	0.89	0.17	0.32	45,47,48,49	0
2	5GF	B	1039	12/13	0.88	0.15	-0.20	42,44,46,47	0
2	5GF	C	1039	12/13	0.90	0.12	-1.07	42,44,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.