Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 11:12 am 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

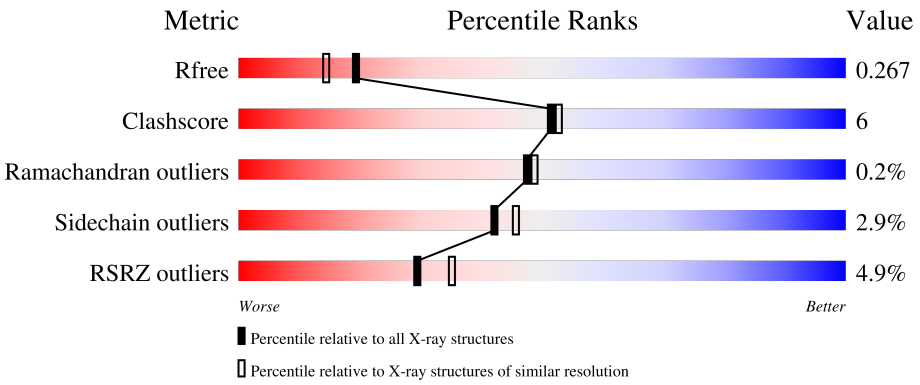
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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	3% 86% 13% •
1	B	1027	6% 85% 14% •
1	C	1027	7% 87% 13%
1	D	1027	4% 85% 14% •

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)

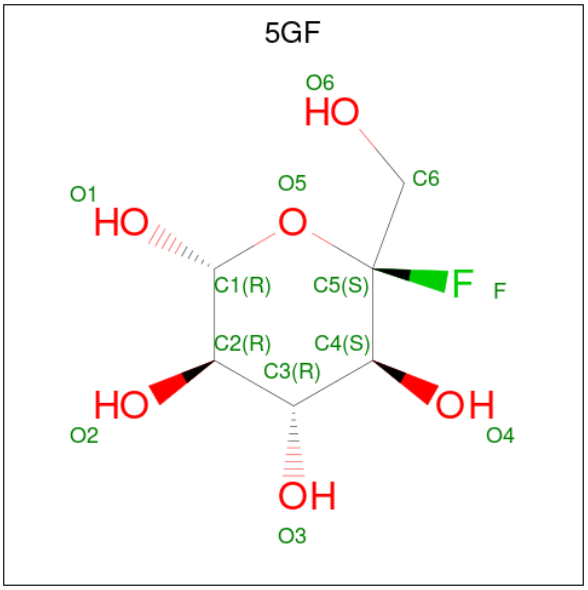
There are 5 unique types of molecules in this entry. The entry contains 33667 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	1025	8171	5143	1385	1596	47	0	1	0
1	B	1025	8162	5135	1385	1595	47	0	0	0
1	C	1025	8162	5135	1385	1595	47	0	0	0
1	D	1025	8171	5143	1385	1596	47	0	1	0

- Molecule 2 is 5-fluoro-beta-D-glucopyranose (three-letter code: 5GF) (formula: $C_6H_{11}FO_6$).



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

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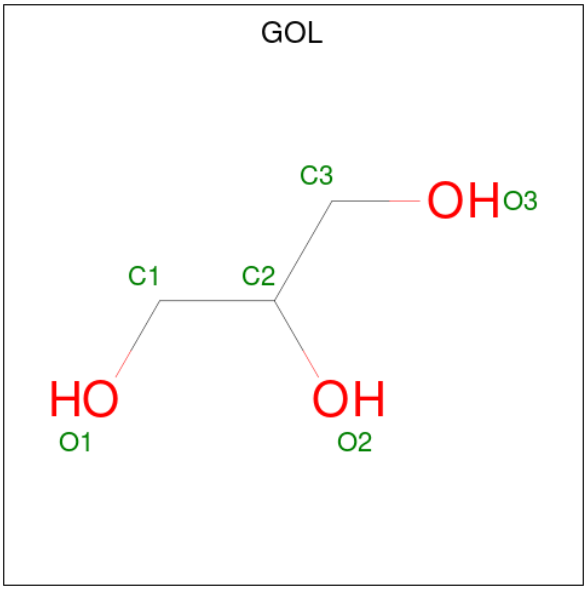
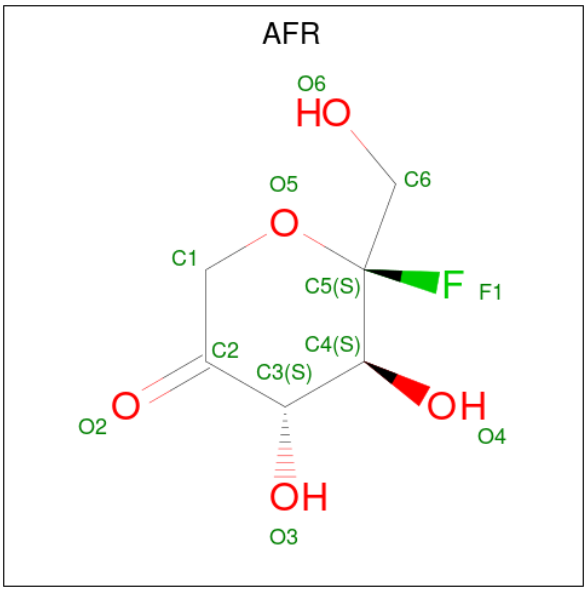
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	F	O		
2	C	1	12	6	1	5	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is alpha-D-threo-hexo-2,5-diulo-5,1-pyranosyl fluoride (three-letter code: AFR) (formula: $C_6H_9FO_5$).



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

- Molecule 5 is water.

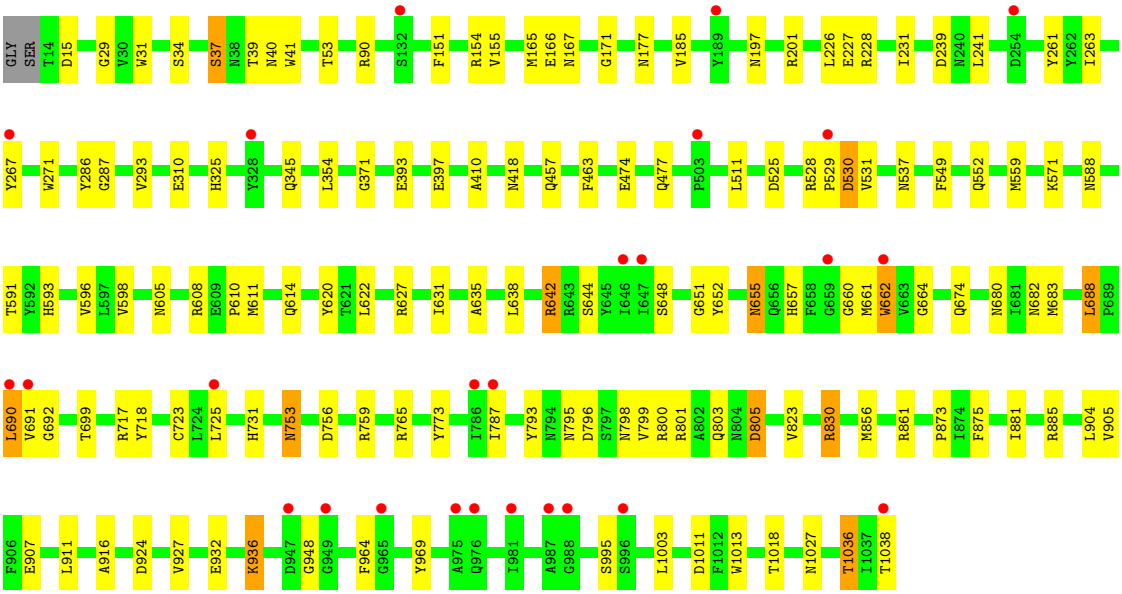
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	328	328	328	0	0
			Total	O		
5	B	147	147	147	0	0
			Total	O		
5	C	152	152	152	0	0
			Total	O		
5	D	296	296	296	0	0

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.

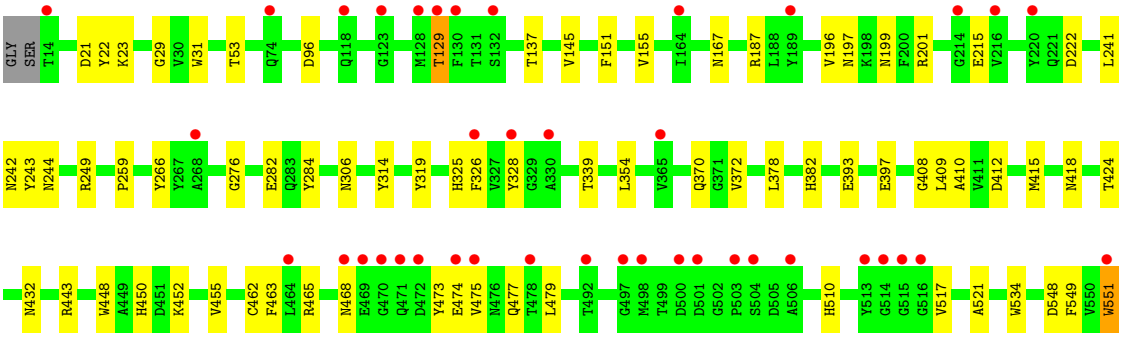
• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

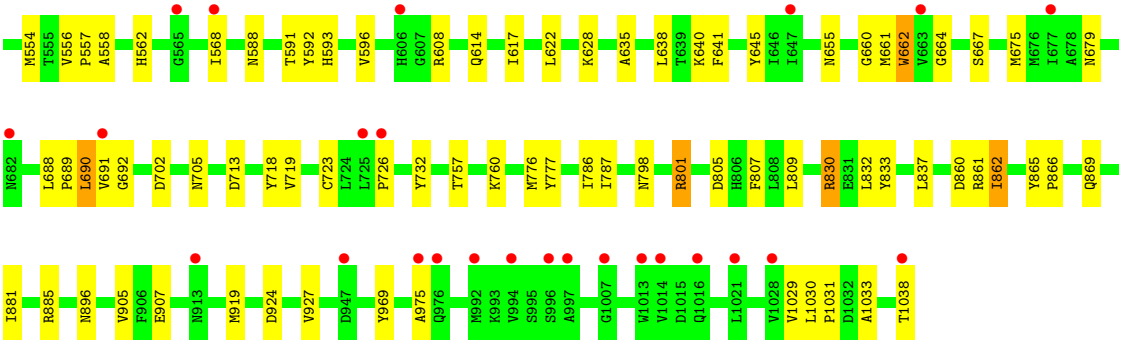
Chain A:



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

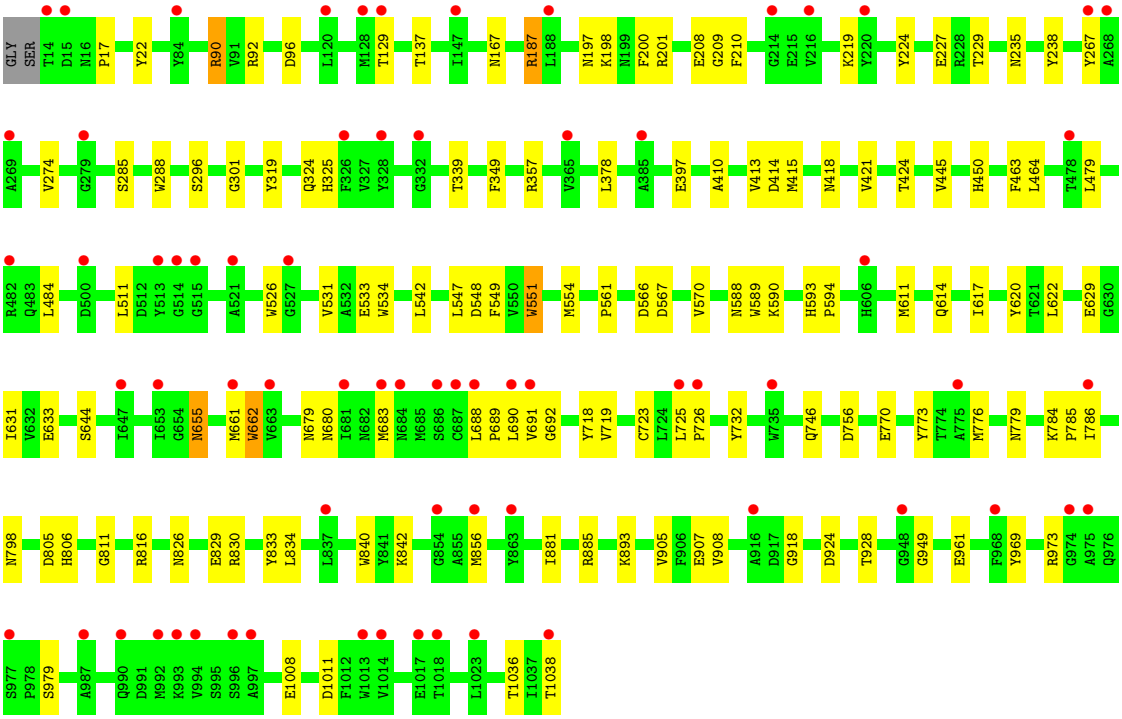
Chain B:





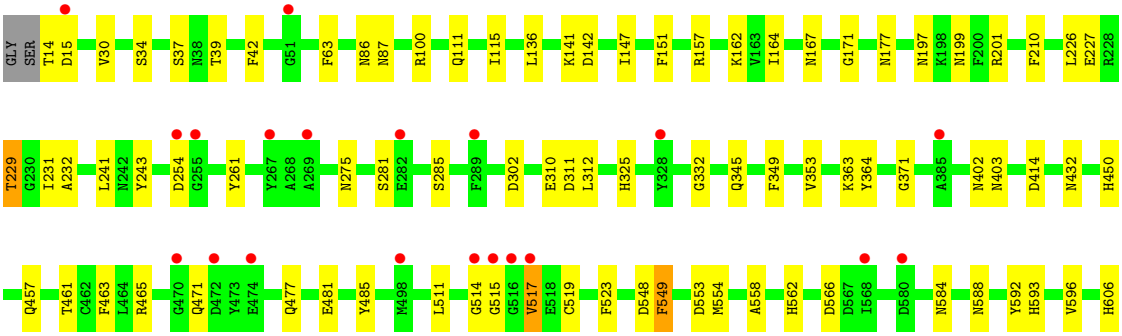
- Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

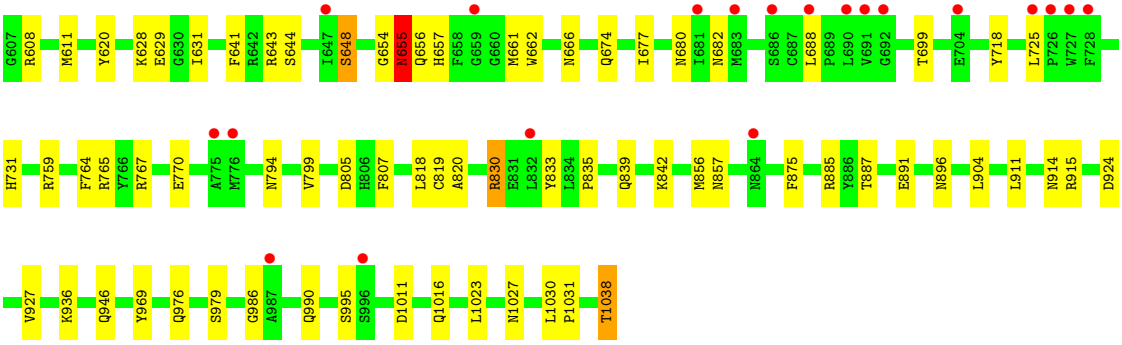
Chain C:



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

Chain D:




G607
R608
M611
Y620
K628
E629
G630
I631
F641
R642
R643
S644
I647
S648
G654
N655
Q656
H657
F658
G659
G660
M661
W662
N666
Q674
I677
N680
I681
N682
M683
S686
C687
L688
P689
L690
V691
G692
T699
E704
Y718
L725
P726
W727
F728
H731
R759
F764
R765
Y766
R767
E770
A775
M776
N794
V799
D805
H806
F807
L818
C819
A820
R830
E831
L832
Y833
L834
P835
Q839
K842
M856
N857
N864
F875
R885
Y886
T887
E891
N896
L904
L911
N914
R915
D924
V927
K936
Q946
Y969
Q976
S979
G986
A987
Q990
S995
S996
D1011
Q1016
L1023
N1027
L1030
P1031
T1038

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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	12914 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 , 36.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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, AFR, 5GF

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(^{o})	Ideal(^{o})
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: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:756:ASP:HB2	5:C:2116:HOH:O	1.92	0.68
1:C:776:MET:HE2	1:C:786:ILE:HD11	1.74	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: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: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: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: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:A:201:ARG:HD3	1:A:310:GLU:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:680:ASN:CG	5:A:2222:HOH:O	2.43	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: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

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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:A:226:LEU:HD12	1:A:682:ASN:HD21	1.75	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
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:629:GLU:HG3	1:C:633:GLU:OE1	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: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: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: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:A:856:MET:CE	1:A:875:PHE:CD2	2.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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:34:SER:C	5:A:2012:HOH:O	2.53	0.47
1:A:856:MET:HE1	1:A:875:PHE:CD2	2.50	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: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: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: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
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:B:805:ASP:CG	1:B:830:ARG:HH22	2.19	0.46
1:D:680:ASN:ND2	1:D:725:LEU:HD13	2.30	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:A:155:VAL:HG21	1:A:165:MET:HE3	1.97	0.45
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: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: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:B:776:MET:HE3	1:B:786:ILE:HD11	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:A:371:GLY:C	1:A:731:HIS:HD2	2.19	0.45
1:D:856:MET:HE1	1:D:875:PHE:HD2	1.81	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

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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:C:484:LEU:HB3	1:C:531:VAL:HG22	1.98	0.45
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:450:HIS:HE1	1:D:548:ASP:OD1	2.00	0.44
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:A:800:ARG:O	1:A:803:GLN:CD	2.55	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: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: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:D:805:ASP:CG	1:D:830:ARG:HH22	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:856:MET:HE1	1:D:875:PHE:CD2	2.53	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:B:1030:LEU:N	1:B:1031:PRO:HD2	2.34	0.42
1:C:961:GLU:HA	1:C:961:GLU:OE1	2.19	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:CG	1:D:606:HIS:O	2.71	0.42
1:A:753:ASN:HD22	1:A:753:ASN:HA	1.66	0.42
1:A:856:MET:HE3	1:A:875:PHE:CD2	2.54	0.42
1:B:241:LEU:C	1:B:243:TYR:H	2.23	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:719:VAL:O	1:C:723:CYS:HB3	2.20	0.42
1:D:86:ASN:O	1:D:87:ASN:HB2	2.19	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:415:MET:CE	1:C:424:THR:HG22	2.49	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:A:756:ASP:OD1	1:A:759:ARG:NH2	2.53	0.42
1:C:288:TRP:HE1	1:C:324:GLN:CD	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TYR:C	5:B:2034:HOH:O	2.58	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: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: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: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: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: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:415:MET:CE	1:B:424:THR:HG22	2.50	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: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:403:ASN:O	1:D:759:ARG:CD	2.68	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:A:796:ASP:CG	1:A:799:VAL:HG13	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:776:MET:CE	1:C:786:ILE:CD1	2.94	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:588:ASN:HB3	1:D:593:HIS:CE1	2.56	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%)	34	32
1	B	1022/1027 (100%)	962 (94%)	59 (6%)	1 (0%)	51	54
1	C	1022/1027 (100%)	974 (95%)	47 (5%)	1 (0%)	51	54
1	D	1023/1027 (100%)	960 (94%)	59 (6%)	4 (0%)	34	32
All	All	4090/4108 (100%)	3862 (94%)	218 (5%)	10 (0%)	47	49

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 (i)

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%)	46	50
1	B	877/878 (100%)	852 (97%)	25 (3%)	42	46
1	C	877/878 (100%)	852 (97%)	25 (3%)	42	46
1	D	878/878 (100%)	850 (97%)	28 (3%)	39	41
All	All	3510/3512 (100%)	3409 (97%)	101 (3%)	42	46

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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	C	336	1	3,6,7	0.56	0	0,6,8	-	-
1	CSO	D	336	1	3,6,7	0.47	0	0,6,8	-	-
1	CSO	B	336	1	3,6,7	0.69	0	0,6,8	-	-
1	CSO	A	336	1	3,6,7	0.54	0	0,6,8	-	-

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	C	336	1	-	0/1/5/7	-
1	CSO	D	336	1	-	0/1/5/7	-
1	CSO	B	336	1	-	1/1/5/7	-
1	CSO	A	336	1	-	0/1/5/7	-

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 monosaccharides 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	C	1039	1	9,12,13	1.28	1 (11%)	14,18,20	0.80	1 (7%)
3	GOL	A	1041	-	5,5,5	0.30	0	5,5,5	0.44	0
3	GOL	D	1040	-	5,5,5	0.40	0	5,5,5	0.63	0
4	AFR	D	1041	-	9,12,12	5.24	3 (33%)	10,18,18	0.95	0
3	GOL	D	1039	-	5,5,5	0.34	0	5,5,5	0.65	0
2	5GF	A	1039	1	9,12,13	1.44	1 (11%)	14,18,20	1.07	1 (7%)
3	GOL	B	1040	-	5,5,5	0.41	0	5,5,5	0.27	0
2	5GF	B	1039	1	9,12,13	1.17	1 (11%)	14,18,20	0.86	0
3	GOL	A	1040	-	5,5,5	0.34	0	5,5,5	0.14	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	C	1039	1	-	2/2/23/26	0/1/1/1
3	GOL	A	1041	-	-	4/4/4/4	-
3	GOL	D	1040	-	-	0/4/4/4	-
4	AFR	D	1041	-	-	0/2/23/23	0/1/1/1
3	GOL	D	1039	-	-	4/4/4/4	-
2	5GF	A	1039	1	-	0/2/23/26	0/1/1/1
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
3	GOL	A	1040	-	-	2/4/4/4	-

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	2.99	1.46	1.43
4	D	1041	AFR	O5-C5	2.83	1.43	1.37

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1039	5GF	O2-C2-C1	2.11	113.48	109.15
2	C	1039	5GF	C1-C2-C3	2.04	112.17	109.67

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	O5-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	D	1039	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	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
3	A	1041	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1041	GOL	1	0
3	D	1040	GOL	2	0
4	D	1041	AFR	3	0
2	A	1039	5GF	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.26	26 (2%)	57	62	16, 30, 44, 68	0
1	B	1024/1027 (99%)	0.51	65 (6%)	20	24	24, 40, 58, 79	0
1	C	1024/1027 (99%)	0.56	69 (6%)	17	22	24, 40, 57, 78	0
1	D	1024/1027 (99%)	0.35	40 (3%)	39	45	17, 30, 48, 81	0
All	All	4096/4108 (99%)	0.42	200 (4%)	29	35	16, 35, 55, 81	0

All (200) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	ALA	6.2
1	C	837	LEU	4.9
1	B	514	GLY	4.6
1	A	988	GLY	4.5
1	C	514	GLY	4.4
1	D	516	GLY	4.4
1	B	976	GLN	4.3
1	D	515	GLY	4.2
1	A	976	GLN	4.2
1	D	517	VAL	4.1
1	C	1013	TRP	4.0
1	B	129	THR	3.7
1	B	504	SER	3.7
1	B	123	GLY	3.6
1	B	1028	VAL	3.6
1	B	565	GLY	3.6
1	C	948	GLY	3.6
1	B	470	GLY	3.5
1	D	254	ASP	3.5
1	C	688	LEU	3.5
1	C	1014	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	515	GLY	3.4
1	C	691	VAL	3.4
1	D	470	GLY	3.4
1	C	996	SER	3.3
1	D	725	LEU	3.3
1	C	269	ALA	3.3
1	B	503	PRO	3.3
1	B	994	VAL	3.2
1	C	515	GLY	3.2
1	D	996	SER	3.2
1	C	220	TYR	3.2
1	C	326	PHE	3.1
1	C	690	LEU	3.1
1	C	992	MET	3.1
1	D	255	GLY	3.1
1	D	472	ASP	3.1
1	B	474	GLU	3.1
1	C	653	ILE	3.1
1	D	692	GLY	3.1
1	C	686	SER	3.1
1	C	14	THR	3.0
1	C	1017	GLU	3.0
1	B	326	PHE	3.0
1	B	691	VAL	3.0
1	B	471	GLN	3.0
1	A	947	ASP	2.9
1	C	1038	THR	2.9
1	D	498	MET	2.9
1	B	500	ASP	2.9
1	D	987	ALA	2.9
1	A	996	SER	2.9
1	B	189	TYR	2.8
1	B	975	ALA	2.8
1	B	130	PHE	2.8
1	C	15	ASP	2.8
1	C	975	ALA	2.8
1	C	994	VAL	2.7
1	B	220	TYR	2.7
1	C	478	THR	2.7
1	A	725	LEU	2.7
1	C	84	TYR	2.7
1	C	863	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	568	ILE	2.7
1	C	385	ALA	2.7
1	C	267	TYR	2.7
1	B	663	VAL	2.7
1	A	787	ILE	2.7
1	D	647	ILE	2.7
1	C	268	ALA	2.6
1	D	727	TRP	2.6
1	C	977	SER	2.6
1	C	725	LEU	2.6
1	B	996	SER	2.6
1	A	254	ASP	2.6
1	C	681	ILE	2.6
1	C	527	GLY	2.6
1	C	216	VAL	2.6
1	D	691	VAL	2.6
1	B	1014	VAL	2.5
1	C	147	ILE	2.5
1	A	503	PRO	2.5
1	A	690	LEU	2.5
1	B	725	LEU	2.5
1	C	214	GLY	2.5
1	D	688	LEU	2.5
1	B	516	GLY	2.5
1	B	330	ALA	2.5
1	B	365	VAL	2.5
1	B	647	ILE	2.5
1	C	854	GLY	2.5
1	B	128	MET	2.4
1	B	472	ASP	2.4
1	C	683	MET	2.4
1	B	677	ILE	2.4
1	C	856	MET	2.4
1	D	289	PHE	2.4
1	D	690	LEU	2.4
1	B	164	ILE	2.4
1	D	681	ILE	2.4
1	C	328	TYR	2.4
1	C	500	ASP	2.4
1	D	728	PHE	2.3
1	B	913	ASN	2.3
1	D	726	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	659	GLY	2.3
1	B	492	THR	2.3
1	A	662	TRP	2.3
1	C	974	GLY	2.3
1	C	987	ALA	2.3
1	B	606	HIS	2.3
1	B	132	SER	2.3
1	B	214	GLY	2.3
1	B	464	LEU	2.3
1	B	497	GLY	2.3
1	C	129	THR	2.3
1	C	188	LEU	2.3
1	D	328[A]	TYR	2.3
1	B	1013	TRP	2.3
1	C	990	GLN	2.3
1	D	51	GLY	2.3
1	B	469	GLU	2.3
1	B	328	TYR	2.2
1	C	120	LEU	2.2
1	A	975	ALA	2.2
1	A	949	GLY	2.2
1	B	551	TRP	2.2
1	A	647	ILE	2.2
1	C	661	MET	2.2
1	D	385	ALA	2.2
1	C	1018	THR	2.2
1	B	468	ASN	2.2
1	A	267	TYR	2.2
1	B	216	VAL	2.2
1	D	580	ASP	2.2
1	D	683	MET	2.2
1	A	646	ILE	2.2
1	B	14	THR	2.2
1	A	132	SER	2.2
1	A	529	PRO	2.2
1	C	997	ALA	2.2
1	C	687	CYS	2.2
1	C	993	LYS	2.2
1	C	968	PHE	2.2
1	D	267	TYR	2.2
1	B	992	MET	2.2
1	C	128	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1038	THR	2.2
1	B	268	ALA	2.2
1	B	506	ALA	2.2
1	B	947	ASP	2.2
1	C	775	ALA	2.2
1	A	786	ILE	2.1
1	D	568	ILE	2.1
1	D	832	LEU	2.1
1	C	365	VAL	2.1
1	D	864	ASN	2.1
1	B	501	ASP	2.1
1	A	659	GLY	2.1
1	D	775	ALA	2.1
1	A	328[A]	TYR	2.1
1	B	1016	GLN	2.1
1	D	514	GLY	2.1
1	C	916	ALA	2.1
1	D	269	ALA	2.1
1	A	981	ILE	2.1
1	C	647	ILE	2.1
1	C	1023	LEU	2.1
1	B	1007	GLY	2.1
1	B	498	MET	2.1
1	C	482	ARG	2.1
1	D	474	GLU	2.1
1	B	1021	LEU	2.1
1	A	691	VAL	2.1
1	B	475	VAL	2.1
1	C	521	ALA	2.1
1	C	735	TRP	2.1
1	D	282	GLU	2.1
1	C	279	GLY	2.1
1	B	997	ALA	2.1
1	A	189	TYR	2.1
1	C	684	ASN	2.0
1	C	786	ILE	2.0
1	B	74	GLN	2.0
1	B	118	GLN	2.0
1	C	726	PRO	2.0
1	B	1038	THR	2.0
1	C	663	VAL	2.0
1	A	965	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	726	PRO	2.0
1	C	606	HIS	2.0
1	B	478	THR	2.0
1	C	332	GLY	2.0
1	B	682	ASN	2.0
1	D	15	ASP	2.0
1	B	513	TYR	2.0
1	C	513	TYR	2.0
1	D	686	SER	2.0
1	D	776	MET	2.0
1	D	704	GLU	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(Å^2)	Q<0.9
1	CSO	B	336	7/8	0.90	0.14	36,37,42,44	0
1	CSO	A	336	7/8	0.94	0.12	26,27,35,37	0
1	CSO	D	336	7/8	0.94	0.14	27,27,29,31	0
1	CSO	C	336	7/8	0.95	0.11	36,37,41,43	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1040	6/6	0.73	0.23	47,49,50,52	0
3	GOL	A	1041	6/6	0.83	0.19	45,46,46,47	0
3	GOL	D	1040	6/6	0.86	0.18	43,46,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	5GF	B	1039	12/13	0.88	0.15	42,44,46,47	0
4	AFR	D	1041	12/12	0.88	0.17	45,47,48,49	0
2	5GF	A	1039	12/13	0.89	0.16	35,36,38,39	0
3	GOL	B	1040	6/6	0.89	0.13	41,44,44,46	0
3	GOL	D	1039	6/6	0.90	0.17	34,35,37,37	0
2	5GF	C	1039	12/13	0.91	0.12	42,44,44,46	0

6.5 Other polymers (i)

There are no such residues in this entry.