Full wwPDB X-ray Structure Validation Report ⓘ

Nov 11, 2021 – 11:09 am GMT

PDB ID	:	7P38
Title	:	4,6-alpha-glucanotransferase GtfB from Limosilactobacillus reuteri NCC 2613
Authors	:	Pijning, T.; te Poele, E.; Gangoiti, J.; Boerner, T.; Dijkhuizen, L.
Deposited on	:	2021-07-07
Resolution	:	2.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

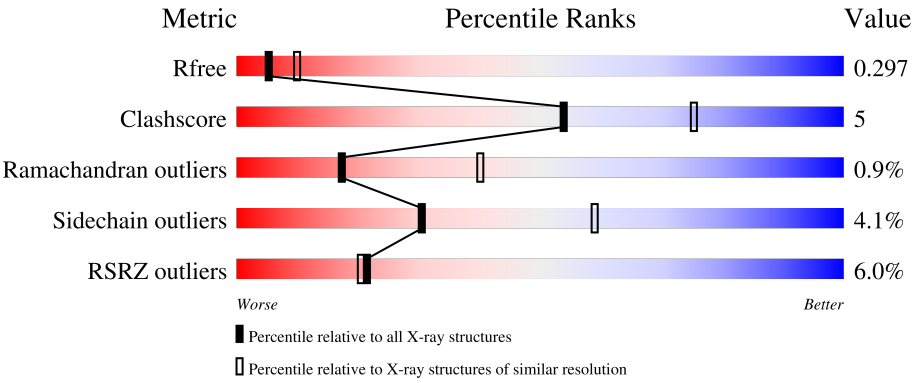
MolProbity	:	4.02b-467
Mogul	:	1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	881	6% 80% 13% • 6%
1	B	881	5% 80% 14% • 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13114 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 Dextransucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6510	4054	1101	1333	22			
1	B	830	Total	C	N	O	S	0	0	0
			6491	4040	1098	1331	22			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	MET	-	initiating methionine	UNP A0A1Z2RUH3
A	398	ALA	-	expression tag	UNP A0A1Z2RUH3
A	399	HIS	-	expression tag	UNP A0A1Z2RUH3
A	400	HIS	-	expression tag	UNP A0A1Z2RUH3
A	401	HIS	-	expression tag	UNP A0A1Z2RUH3
A	402	HIS	-	expression tag	UNP A0A1Z2RUH3
A	403	HIS	-	expression tag	UNP A0A1Z2RUH3
A	404	HIS	-	expression tag	UNP A0A1Z2RUH3
A	405	SER	-	expression tag	UNP A0A1Z2RUH3
A	406	ALA	-	expression tag	UNP A0A1Z2RUH3
A	407	ALA	-	expression tag	UNP A0A1Z2RUH3
A	408	LEU	-	expression tag	UNP A0A1Z2RUH3
A	409	GLU	-	expression tag	UNP A0A1Z2RUH3
A	410	VAL	-	expression tag	UNP A0A1Z2RUH3
A	411	LEU	-	expression tag	UNP A0A1Z2RUH3
A	412	PHE	-	expression tag	UNP A0A1Z2RUH3
A	413	GLN	-	expression tag	UNP A0A1Z2RUH3
A	414	GLY	-	expression tag	UNP A0A1Z2RUH3
A	415	PRO	-	expression tag	UNP A0A1Z2RUH3
A	416	GLY	-	expression tag	UNP A0A1Z2RUH3
B	397	MET	-	initiating methionine	UNP A0A1Z2RUH3
B	398	ALA	-	expression tag	UNP A0A1Z2RUH3
B	399	HIS	-	expression tag	UNP A0A1Z2RUH3
B	400	HIS	-	expression tag	UNP A0A1Z2RUH3
B	401	HIS	-	expression tag	UNP A0A1Z2RUH3

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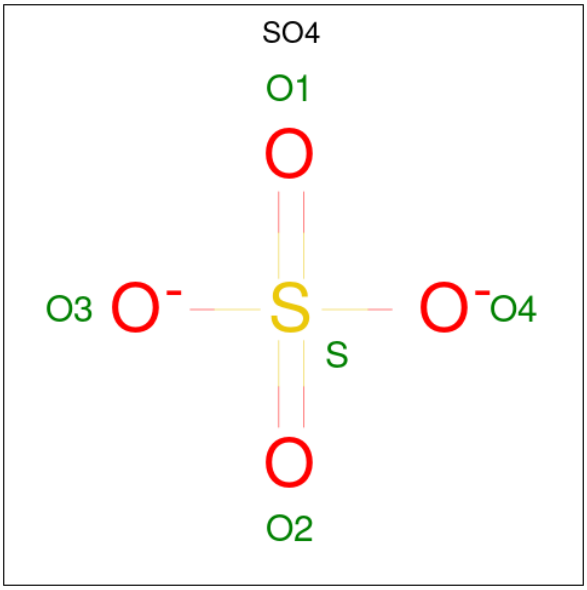
Chain	Residue	Modelled	Actual	Comment	Reference
B	402	HIS	-	expression tag	UNP A0A1Z2RUH3
B	403	HIS	-	expression tag	UNP A0A1Z2RUH3
B	404	HIS	-	expression tag	UNP A0A1Z2RUH3
B	405	SER	-	expression tag	UNP A0A1Z2RUH3
B	406	ALA	-	expression tag	UNP A0A1Z2RUH3
B	407	ALA	-	expression tag	UNP A0A1Z2RUH3
B	408	LEU	-	expression tag	UNP A0A1Z2RUH3
B	409	GLU	-	expression tag	UNP A0A1Z2RUH3
B	410	VAL	-	expression tag	UNP A0A1Z2RUH3
B	411	LEU	-	expression tag	UNP A0A1Z2RUH3
B	412	PHE	-	expression tag	UNP A0A1Z2RUH3
B	413	GLN	-	expression tag	UNP A0A1Z2RUH3
B	414	GLY	-	expression tag	UNP A0A1Z2RUH3
B	415	PRO	-	expression tag	UNP A0A1Z2RUH3
B	416	GLY	-	expression tag	UNP A0A1Z2RUH3

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

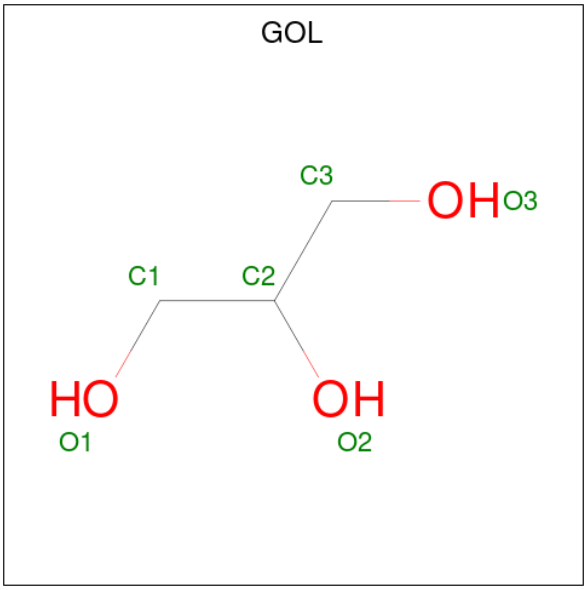
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

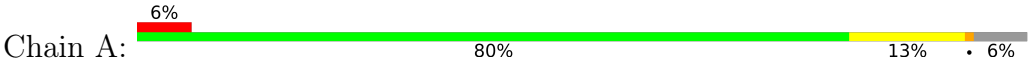
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	45	Total O 45 45	0	0

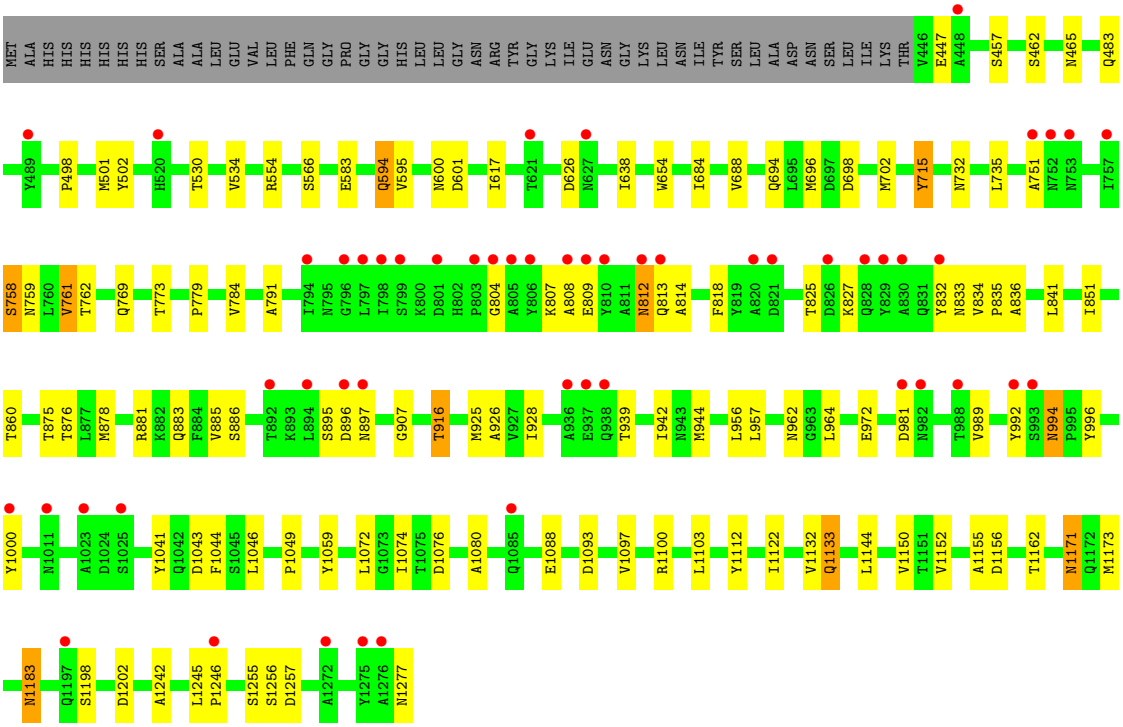
3 Residue-property plots (i)

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: Dextransucrase

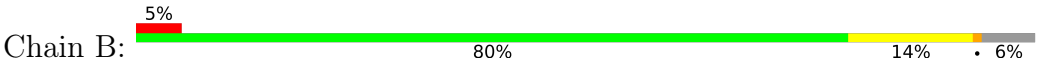
Chain A:

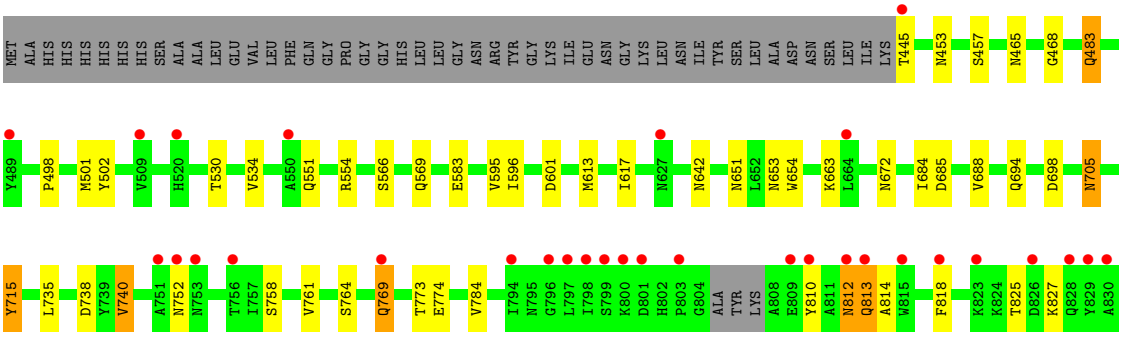


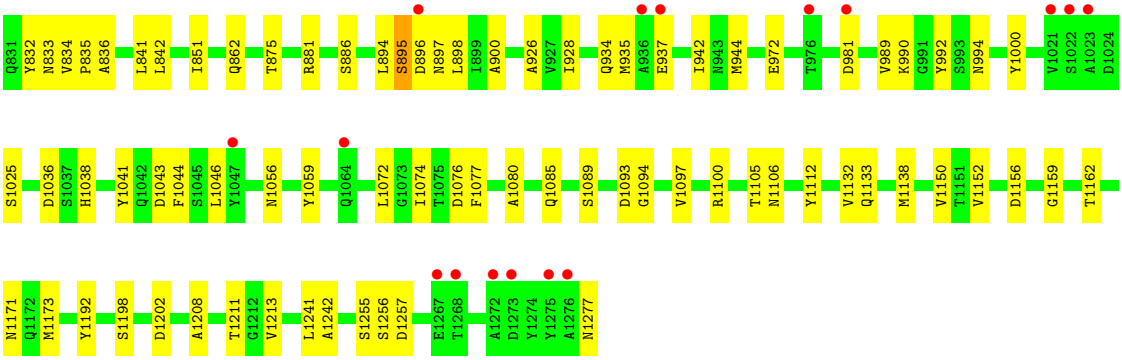


• Molecule 1: Dextransucrase

Chain B:






Q831 Y832 N833 V834 P835 A836 L841 L842 I851 Q862 T875 R881 S886 L894 S895 D896 N897 L898 I899 A900 A926 Y927 I928 Q934 M935 A936 E937 I942 N943 M944 E972 T976 D981 V989 K990 G991 Y992 S993 N994 Y1000 V1021 S1022 A1023 D1024
S1025 D1036 S1037 H1038 Y1041 Q1042 D1043 F1044 S1045 L1046 Y1047 N1056 Y1059 Q1064 L1072 G1073 I1074 T1075 D1076 F1077 A1080 Q1085 S1089 D1093 G1094 V1097 R1100 T1105 N1106 Y1112 V1132 Q1133 M1138 V1150 T1151 V1152 D1156 G1159 T1162
N1171 Q1172 M1173 Y1192 S1198 D1202 A1208 T1211 G1212 V1213 L1241 A1242 S1255 S1256 D1257 E1267 T1268 A1272 D1273 Y1274 Y1275 A1276 N1277

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	107.35Å 134.50Å 147.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.24 – 2.70 47.24 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.24-2.70) 99.9 (47.24-2.70)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0210	Depositor
R, R_{free}	0.260 , 0.299 0.259 , 0.297	Depositor DCC
R_{free} test set	2962 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.3	Xtriage
Anisotropy	1.498	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	13114	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.93 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.9510e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4, CA

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	0.40	0/6652	0.59	0/9063
1	B	0.41	0/6631	0.60	0/9034
All	All	0.41	0/13283	0.59	0/18097

There are no bond length outliers.

There are no bond angle outliers.

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	6510	0	6129	69	1
1	B	6491	0	6108	66	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	B	6	0	8	0	0
5	A	50	0	0	0	0
5	B	45	0	0	0	0
All	All	13114	0	12245	135	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 5.

All (135) 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:B:653:ASN:HD21	1:B:1192:TYR:H	1.23	0.86
1:A:881:ARG:HG3	1:A:885:VAL:HG21	1.59	0.83
1:B:784:VAL:HG23	1:B:841:LEU:HD22	1.60	0.83
1:B:898:LEU:HD22	1:B:935:MET:HE1	1.60	0.82
1:A:784:VAL:HG23	1:A:841:LEU:HD22	1.59	0.82
1:B:862:GLN:HE21	1:B:1056:ASN:HD22	1.27	0.81
1:A:600:ASN:HD22	1:A:1171:ASN:HD21	1.29	0.81
1:A:881:ARG:O	1:A:885:VAL:HG22	1.81	0.80
1:A:957:LEU:HD21	1:A:964:LEU:HD22	1.71	0.72
1:B:928:ILE:HD11	1:B:942:ILE:HD11	1.71	0.71
1:B:972:GLU:OE1	1:B:990:LYS:HE3	1.89	0.71
1:A:1183:ASN:HD22	1:A:1183:ASN:N	1.89	0.71
1:B:453:ASN:HD21	1:B:551:GLN:HE22	1.37	0.70
1:B:740:VAL:HG13	1:B:764:SER:HB2	1.71	0.70
1:B:694:GLN:NE2	1:B:1202:ASP:OD1	2.23	0.70
1:A:600:ASN:HD22	1:A:1171:ASN:ND2	1.90	0.68
1:A:1122:ILE:HG23	1:A:1132:VAL:HG11	1.77	0.67
1:B:894:LEU:HD11	1:B:900:ALA:HB2	1.78	0.65
1:B:1208:ALA:HB3	1:B:1211:THR:HG22	1.79	0.64
1:A:878:MET:CE	1:A:1074:ILE:HD11	2.28	0.63
1:A:907:GLY:O	1:A:916:THR:HG22	1.97	0.63
1:B:928:ILE:HD11	1:B:942:ILE:CD1	2.28	0.63
1:A:885:VAL:HG23	1:A:885:VAL:O	1.99	0.63
1:A:860:THR:O	1:A:1049:PRO:HG3	2.00	0.62
1:B:654:TRP:CZ2	1:B:1100:ARG:HG2	2.35	0.62
1:A:654:TRP:CZ2	1:A:1100:ARG:HG2	2.35	0.61
1:B:881:ARG:NH2	1:B:1036:ASP:O	2.34	0.60
1:A:694:GLN:NE2	1:A:1202:ASP:OD1	2.29	0.60
1:B:972:GLU:OE1	1:B:990:LYS:HG3	2.01	0.59
1:B:738:ASP:OD2	1:B:740:VAL:HG22	2.03	0.59
1:A:957:LEU:CD2	1:A:964:LEU:HD22	2.32	0.58
1:B:812:ASN:O	1:B:814:ALA:N	2.37	0.58
1:A:994:ASN:HD22	1:A:996:TYR:H	1.51	0.58
1:A:758:SER:O	1:A:761:VAL:HG12	2.04	0.57
1:A:594:GLN:NE2	1:A:1155:ALA:O	2.38	0.57
1:B:705:ASN:HD22	1:B:705:ASN:N	2.03	0.57
1:A:812:ASN:O	1:A:814:ALA:N	2.38	0.56
1:A:638:ILE:HD13	1:A:1144:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1103:LEU:N	1:A:1103:LEU:HD12	2.20	0.56
1:A:807:LYS:O	1:A:809:GLU:N	2.38	0.56
1:A:732:ASN:ND2	1:A:779:PRO:HD2	2.20	0.56
1:A:600:ASN:ND2	1:A:1171:ASN:HD21	2.01	0.56
1:B:895:SER:O	1:B:897:ASN:N	2.39	0.56
1:B:1211:THR:HG23	1:B:1213:VAL:H	1.70	0.55
1:A:895:SER:O	1:A:897:ASN:N	2.39	0.55
1:A:881:ARG:CG	1:A:885:VAL:HG21	2.35	0.55
1:A:994:ASN:ND2	1:A:996:TYR:H	2.04	0.55
1:B:1038:HIS:HD2	1:B:1076:ASP:OD1	1.90	0.54
1:A:498:PRO:HG2	1:A:501:MET:HG3	1.90	0.53
1:B:1041:TYR:HB2	1:B:1074:ILE:HG12	1.91	0.53
1:B:596:ILE:HG22	1:B:613:MET:HE3	1.91	0.53
1:A:600:ASN:ND2	1:A:1171:ASN:ND2	2.58	0.52
1:A:878:MET:HE1	1:A:1074:ILE:HD11	1.90	0.52
1:A:885:VAL:CG1	1:A:925:MET:HE2	2.40	0.51
1:A:833:ASN:HB3	1:A:836:ALA:HB3	1.92	0.51
1:B:833:ASN:HB3	1:B:836:ALA:HB3	1.91	0.51
1:B:1255:SER:O	1:B:1257:ASP:N	2.43	0.51
1:B:1044:PHE:CG	1:B:1080:ALA:HB2	2.46	0.51
1:B:498:PRO:HG2	1:B:501:MET:HG3	1.92	0.51
1:B:684:ILE:HD12	1:B:688:VAL:HG21	1.93	0.50
1:A:1122:ILE:HG23	1:A:1132:VAL:CG1	2.41	0.50
1:A:1255:SER:O	1:A:1257:ASP:N	2.44	0.50
1:A:1044:PHE:CG	1:A:1080:ALA:HB2	2.46	0.50
1:B:613:MET:HE1	1:B:1159:GLY:HA3	1.94	0.50
1:B:1208:ALA:HB3	1:B:1211:THR:CG2	2.40	0.50
1:A:684:ILE:HD12	1:A:688:VAL:HG21	1.94	0.49
1:B:827:LYS:HB2	1:B:832:TYR:CE1	2.46	0.49
1:A:827:LYS:HB2	1:A:832:TYR:CE1	2.46	0.49
1:A:530:THR:O	1:A:534:VAL:HG22	2.12	0.49
1:B:502:TYR:CE1	1:B:554:ARG:HD3	2.47	0.49
1:A:761:VAL:HG13	1:A:762:THR:HG23	1.95	0.48
1:A:875:THR:HG22	1:A:1072:LEU:HD22	1.95	0.48
1:A:1041:TYR:HB2	1:A:1074:ILE:HG12	1.95	0.48
1:B:937:GLU:HA	1:B:990:LYS:HG2	1.94	0.48
1:B:613:MET:CE	1:B:1159:GLY:HA3	2.44	0.48
1:B:1085:GLN:CD	1:B:1094:GLY:HA2	2.34	0.48
1:A:502:TYR:CE1	1:A:554:ARG:HD3	2.49	0.48
1:B:842:LEU:HD21	1:B:851:ILE:HD11	1.96	0.47
1:B:875:THR:HG22	1:B:1072:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:ASN:HD22	1:B:468:GLY:H	1.61	0.47
1:B:761:VAL:CG1	1:B:769:GLN:HB2	2.44	0.47
1:A:1183:ASN:HD22	1:A:1183:ASN:H	1.61	0.47
1:B:989:VAL:HG12	1:B:1000:TYR:CZ	2.50	0.47
1:A:989:VAL:HG12	1:A:1000:TYR:CZ	2.50	0.47
1:B:653:ASN:ND2	1:B:1192:TYR:H	2.02	0.47
1:A:1156:ASP:HB3	1:A:1162:THR:HG21	1.97	0.46
1:B:1156:ASP:HB3	1:B:1162:THR:HG21	1.97	0.46
1:B:530:THR:O	1:B:534:VAL:HG22	2.14	0.46
1:A:814:ALA:O	1:A:818:PHE:N	2.49	0.46
1:A:1173:MET:HG2	1:A:1242:ALA:HB2	1.98	0.45
1:B:1077:PHE:HB3	1:B:1132:VAL:HG13	1.98	0.45
1:B:814:ALA:O	1:B:818:PHE:N	2.48	0.45
1:B:1076:ASP:HB3	1:B:1133:GLN:HE22	1.81	0.45
1:B:1173:MET:HG2	1:B:1242:ALA:HB2	1.99	0.45
1:B:705:ASN:N	1:B:705:ASN:ND2	2.64	0.45
1:B:1059:TYR:CZ	1:B:1112:TYR:HB2	2.52	0.44
1:A:885:VAL:HG12	1:A:925:MET:HE2	2.00	0.44
1:A:851:ILE:HD12	1:A:851:ILE:N	2.33	0.44
1:A:1059:TYR:CZ	1:A:1112:TYR:HB2	2.52	0.44
1:A:834:VAL:N	1:A:835:PRO:CD	2.81	0.44
1:B:642:ASN:ND2	1:B:651:ASN:HD21	2.15	0.44
1:B:1046:LEU:HD22	1:B:1093:ASP:OD2	2.18	0.44
1:A:885:VAL:CG1	1:A:925:MET:CE	2.96	0.43
1:A:1183:ASN:N	1:A:1183:ASN:ND2	2.61	0.43
1:A:1245:LEU:HB3	1:A:1246:PRO:HD2	1.98	0.43
1:B:834:VAL:N	1:B:835:PRO:CD	2.81	0.43
1:A:715:TYR:HB3	1:A:735:LEU:HB2	2.00	0.43
1:B:761:VAL:HG11	1:B:769:GLN:HB2	2.00	0.43
1:B:684:ILE:HD12	1:B:688:VAL:CG2	2.49	0.43
1:A:457:SER:OG	1:A:462:SER:OG	2.10	0.42
1:B:715:TYR:HB3	1:B:735:LEU:HB2	2.01	0.42
1:A:876:THR:HG22	1:A:956:LEU:HD21	2.02	0.42
1:A:972:GLU:HG2	1:A:992:TYR:OH	2.20	0.42
1:B:926:ALA:HB2	1:B:944:MET:SD	2.60	0.42
1:A:928:ILE:HD11	1:A:942:ILE:HD13	2.01	0.42
1:B:651:ASN:HB3	1:B:1138:MET:CE	2.50	0.42
1:B:663:LYS:H	1:B:672:ASN:HD21	1.67	0.42
1:A:926:ALA:HB2	1:A:944:MET:SD	2.60	0.42
1:A:1076:ASP:HB3	1:A:1133:GLN:OE1	2.20	0.42
1:B:825:THR:HG23	1:B:994:ASN:CA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:851:ILE:N	1:A:851:ILE:CD1	2.83	0.41
1:B:685:ASP:O	1:B:688:VAL:HG22	2.21	0.41
1:A:825:THR:HG23	1:A:994:ASN:CA	2.51	0.41
1:A:791:ALA:HB2	1:A:1046:LEU:HD12	2.03	0.41
1:A:1046:LEU:HD22	1:A:1093:ASP:OD2	2.21	0.41
1:B:972:GLU:HG2	1:B:992:TYR:OH	2.21	0.41
1:B:1043:ASP:OD1	1:B:1043:ASP:C	2.59	0.41
1:A:1043:ASP:C	1:A:1043:ASP:OD1	2.59	0.41
1:B:595:VAL:HB	1:B:1152:VAL:HB	2.03	0.41
1:A:595:VAL:HB	1:A:1152:VAL:HB	2.03	0.40
1:A:696:MET:HB3	1:A:702:MET:SD	2.61	0.40
1:A:1044:PHE:CD1	1:A:1080:ALA:HB2	2.56	0.40
1:B:715:TYR:CE1	1:B:1133:GLN:HG2	2.56	0.40
1:B:825:THR:HG23	1:B:994:ASN:HA	2.02	0.40
1:B:1105:THR:HG22	1:B:1106:ASN:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:GLN:OE1	1:B:483:GLN:NE2[1_455]	1.95	0.25

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	830/881 (94%)	776 (94%)	46 (6%)	8 (1%)	15	37
1	B	826/881 (94%)	773 (94%)	46 (6%)	7 (1%)	19	43
All	All	1656/1762 (94%)	1549 (94%)	92 (6%)	15 (1%)	17	40

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	751	ALA
1	A	808	ALA
1	A	813	GLN
1	B	813	GLN
1	B	896	ASP
1	A	896	ASP
1	B	752	ASN
1	B	1241	LEU
1	A	804	GLY
1	A	812	ASN
1	B	895	SER
1	A	617	ILE
1	A	1256	SER
1	B	617	ILE
1	B	1256	SER

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	702/741 (95%)	673 (96%)	29 (4%)	30	59
1	B	701/741 (95%)	673 (96%)	28 (4%)	31	60
All	All	1403/1482 (95%)	1346 (96%)	57 (4%)	30	59

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	GLU
1	A	465	ASN
1	A	566	SER
1	A	583	GLU
1	A	594	GLN
1	A	601	ASP
1	A	626	ASP
1	A	698	ASP
1	A	715	TYR

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Mol	Chain	Res	Type
1	A	758	SER
1	A	759	ASN
1	A	761	VAL
1	A	769	GLN
1	A	773	THR
1	A	883	GLN
1	A	886	SER
1	A	916	THR
1	A	939	THR
1	A	962	ASN
1	A	981	ASP
1	A	994	ASN
1	A	1088	GLU
1	A	1097	VAL
1	A	1133	GLN
1	A	1150	VAL
1	A	1171	ASN
1	A	1183	ASN
1	A	1198	SER
1	A	1277	ASN
1	B	445	THR
1	B	457	SER
1	B	483	GLN
1	B	566	SER
1	B	569	GLN
1	B	583	GLU
1	B	601	ASP
1	B	698	ASP
1	B	705	ASN
1	B	715	TYR
1	B	740	VAL
1	B	758	SER
1	B	769	GLN
1	B	773	THR
1	B	774	GLU
1	B	810	TYR
1	B	812	ASN
1	B	813	GLN
1	B	886	SER
1	B	934	GLN
1	B	981	ASP
1	B	1025	SER

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Mol	Chain	Res	Type
1	B	1089	SER
1	B	1097	VAL
1	B	1150	VAL
1	B	1171	ASN
1	B	1198	SER
1	B	1277	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	GLN
1	A	602	ASN
1	A	619	ASN
1	A	831	GLN
1	A	837	GLN
1	A	897	ASN
1	A	948	HIS
1	A	967	ASN
1	A	994	ASN
1	A	1085	GLN
1	A	1171	ASN
1	A	1183	ASN
1	A	1185	GLN
1	A	1277	ASN
1	B	461	ASN
1	B	465	ASN
1	B	551	GLN
1	B	618	ASN
1	B	619	ASN
1	B	642	ASN
1	B	653	ASN
1	B	672	ASN
1	B	705	ASN
1	B	711	ASN
1	B	780	ASN
1	B	862	GLN
1	B	934	GLN
1	B	982	ASN
1	B	1038	HIS
1	B	1085	GLN
1	B	1133	GLN
1	B	1277	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	832/881 (94%)	0.66	53 (6%)	19	18	26, 36, 65, 83	0
1	B	830/881 (94%)	0.64	47 (5%)	23	22	26, 35, 55, 70	0
All	All	1662/1762 (94%)	0.65	100 (6%)	21	20	26, 35, 60, 83	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	810	TYR	8.1
1	A	806	TYR	6.0
1	B	1023	ALA	5.5
1	A	804	GLY	5.4
1	A	627	ASN	5.2
1	B	753	ASN	5.1
1	A	801	ASP	4.9
1	A	810	TYR	4.9
1	B	797	LEU	4.8
1	A	808	ALA	4.7
1	B	896	ASP	4.4
1	A	826	ASP	4.4
1	B	829	TYR	4.3
1	A	829	TYR	4.0
1	B	751	ALA	3.8
1	A	809	GLU	3.8
1	B	489	TYR	3.8
1	B	937	GLU	3.8
1	A	798	ILE	3.6
1	A	797	LEU	3.6
1	A	805	ALA	3.6
1	A	936	ALA	3.6
1	A	803	PRO	3.5
1	B	826	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	796	GLY	3.4
1	A	752	ASN	3.4
1	B	752	ASN	3.4
1	A	489	TYR	3.4
1	A	796	GLY	3.3
1	A	757	ILE	3.2
1	B	799	SER	3.2
1	A	832	TYR	3.0
1	A	992	TYR	3.0
1	B	1272	ALA	3.0
1	B	627	ASN	2.9
1	A	892	THR	2.9
1	B	801	ASP	2.9
1	B	815	TRP	2.8
1	A	821	ASP	2.8
1	A	894	LEU	2.8
1	A	981	ASP	2.8
1	A	1000	TYR	2.8
1	A	1023	ALA	2.7
1	B	769	GLN	2.7
1	B	1047	TYR	2.7
1	A	896	ASP	2.7
1	A	1275	TYR	2.7
1	B	798	ILE	2.7
1	B	812	ASN	2.7
1	B	830	ALA	2.6
1	B	1022	SER	2.6
1	A	982	ASN	2.6
1	A	897	ASN	2.5
1	A	1197	GLN	2.5
1	A	751	ALA	2.5
1	B	818	PHE	2.5
1	A	1011	ASN	2.5
1	B	809	GLU	2.5
1	B	445	THR	2.5
1	A	828	GLN	2.5
1	A	1085	GLN	2.5
1	B	509	VAL	2.5
1	A	799	SER	2.5
1	A	448	ALA	2.5
1	B	936	ALA	2.5
1	B	803	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	976	THR	2.4
1	B	520	HIS	2.4
1	B	550	ALA	2.4
1	A	1025	SER	2.4
1	B	664	LEU	2.3
1	B	1064	GLN	2.3
1	B	1273	ASP	2.3
1	A	794	ILE	2.3
1	A	937	GLU	2.3
1	B	823	LYS	2.3
1	A	520	HIS	2.3
1	A	830	ALA	2.3
1	A	621	THR	2.2
1	A	1272	ALA	2.2
1	A	1276	ALA	2.2
1	B	800	LYS	2.2
1	A	753	ASN	2.2
1	A	993	SER	2.2
1	B	1021	VAL	2.2
1	B	828	GLN	2.2
1	B	1275	TYR	2.1
1	B	1267	GLU	2.1
1	B	794	ILE	2.1
1	A	812	ASN	2.1
1	A	988	THR	2.1
1	B	756	THR	2.1
1	A	938	GLN	2.1
1	A	813	GLN	2.0
1	B	813	GLN	2.0
1	A	1246	PRO	2.0
1	A	820	ALA	2.0
1	B	1268	THR	2.0
1	B	981	ASP	2.0
1	B	1276	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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
4	GOL	B	1302	6/6	0.74	0.27	22,22,22,22	0
2	CA	A	1301	1/1	0.79	0.15	30,30,30,30	0
3	SO4	B	1303	5/5	0.81	0.25	47,47,48,48	0
2	CA	B	1301	1/1	0.90	0.15	21,21,21,21	0
3	SO4	A	1302	5/5	0.90	0.20	46,46,47,47	0

6.5 Other polymers (i)

There are no such residues in this entry.