



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:35 AM UTC

PDB ID : 7P38 / pdb_00007p38
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

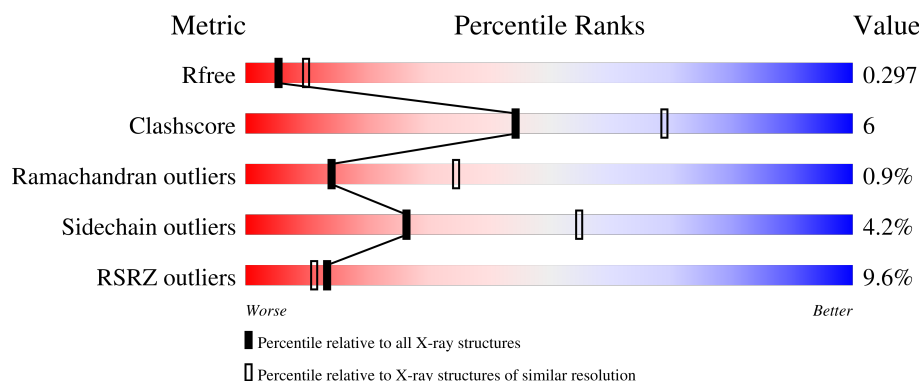
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	881	10% 79% 14% 6%
1	B	881	8% 78% 15% 6%

2 Entry composition

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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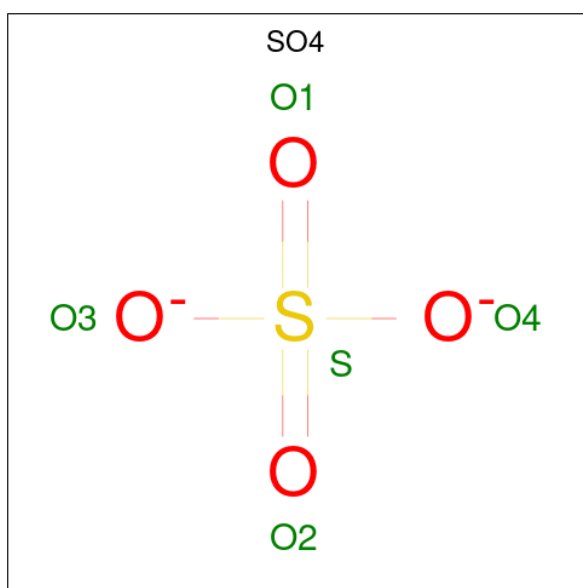
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Chain	Residue	Modelled	Actual	Comment	Reference
B	402	HIS	-	expression tag	UNP A0A1Z2RUH3
B	403	HIS	-	expression tag	UNP A0A1Z2RUH3
B	404	HIS	-	expression tag	UNP A0A1Z2RUH3
B	405	SER	-	expression tag	UNP A0A1Z2RUH3
B	406	ALA	-	expression tag	UNP A0A1Z2RUH3
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 (CCD ID: 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 (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

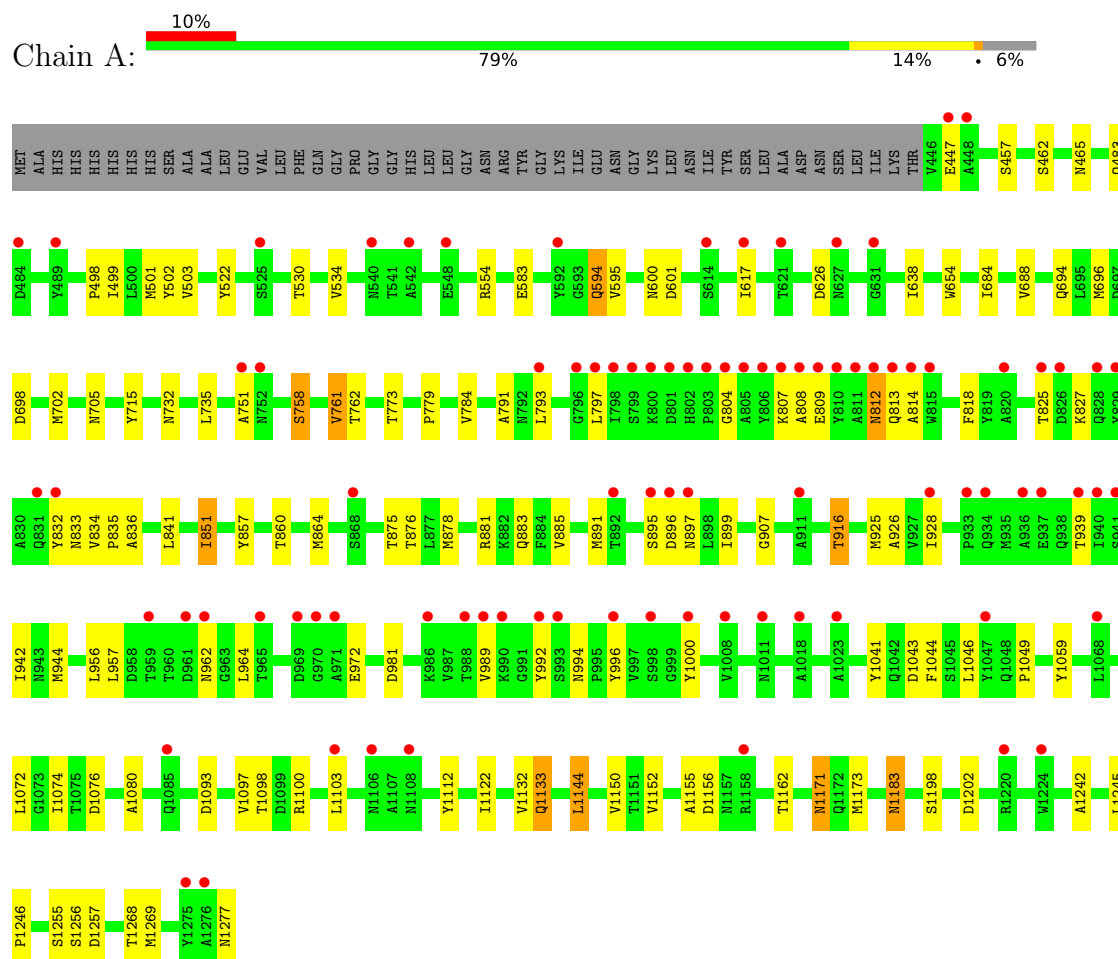
- Molecule 5 is water.

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

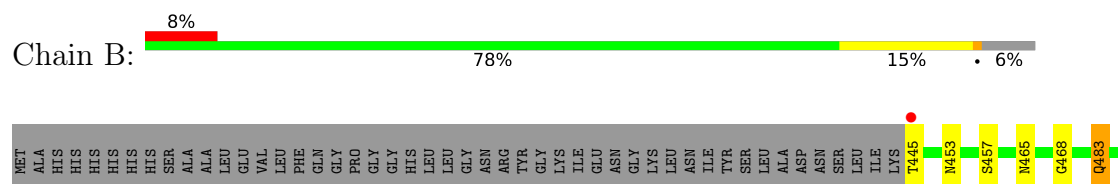
3 Residue-property plots [i](#)

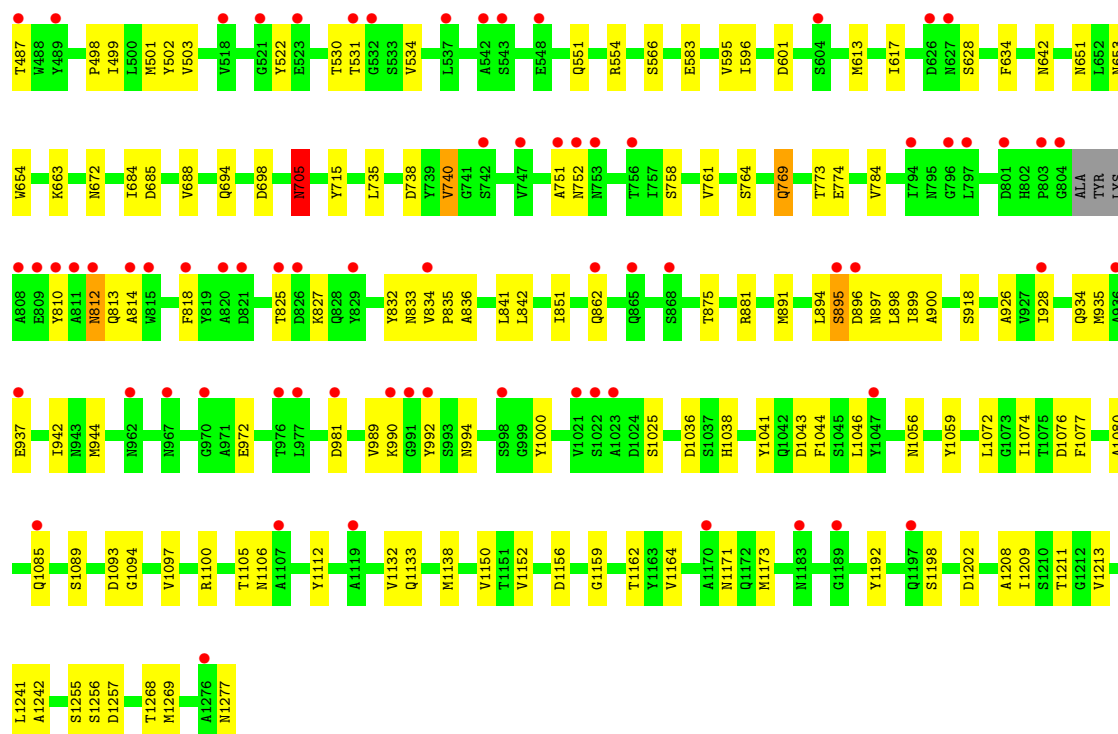
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Dextranucrase





4 Data and refinement statistics

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) 100.0 (47.24-2.70)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 34.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.55	0/6652	0.77	1/9063 (0.0%)
1	B	0.56	0/6631	0.78	3/9034 (0.0%)
All	All	0.55	0/13283	0.78	4/18097 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	705	ASN	CB-CA-C	-6.12	103.38	110.17
1	A	705	ASN	CB-CA-C	-6.03	103.47	110.17
1	B	751	ALA	N-CA-C	-5.34	101.94	109.96
1	B	628	SER	N-CA-C	5.18	116.53	109.18

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	6510	0	6129	76	1
1	B	6491	0	6108	76	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	152	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 6.

All (152) 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:A:784:VAL:HG23	1:A:841:LEU:HD22	1.59	0.82
1:B:898:LEU:HD22	1:B:935:MET:HE1	1.60	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:B:613:MET:HE2	1:B:1159:GLY:HA3	1.65	0.77
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:A:878:MET:HE1	1:A:1074:ILE:HD11	1.76	0.66
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:B:596:ILE:CG2	1:B:613:MET:HE1	2.27	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:651:ASN:CG	1:B:1138:MET:HE2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:TRP:CZ2	1:A:1100:ARG:HG2	2.35	0.61
1:A:503:VAL:HG21	1:A:1269:MET:HE3	1.82	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:B:503:VAL:HG21	1:B:1269:MET:HE3	1.85	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
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:A:885:VAL:HG12	1:A:925:MET:HE2	1.88	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:596:ILE:HG21	1:B:613:MET:HE1	1.89	0.55
1:B:613:MET:HE3	1:B:634:PHE:CE2	2.42	0.54
1:B:596:ILE:HG22	1:B:613:MET:HE1	1.89	0.54
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:1085:GLN:CD	1:B:1094:GLY:HA2	2.34	0.53
1:A:600:ASN:ND2	1:A:1171:ASN:ND2	2.58	0.52
1:A:885:VAL:CG1	1:A:925:MET:HE2	2.40	0.52
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:499:ILE:HG23	1:B:1269:MET:HE1	1.93	0.51
1:B:684:ILE:HD12	1:B:688:VAL:HG21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:503:VAL:CG2	1:B:1269:MET:HE3	2.42	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:HE3	1:B:634:PHE:HE2	1.78	0.48
1:A:499:ILE:HG23	1:A:1269:MET:HE1	1.94	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
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:503:VAL:CG2	1:A:1269:MET:HE3	2.44	0.46
1:B:1043:ASP:OD1	1:B:1043:ASP:C	2.59	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:A:857:TYR:OH	1:A:864:MET:HE3	2.16	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:851:ILE:HD12	1:A:851:ILE:N	2.33	0.44
1:A:1043:ASP:OD1	1:A:1043:ASP:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1059:TYR:CZ	1:A:1112:TYR:HB2	2.52	0.44
1:B:891:MET:HE2	1:B:899:ILE:HD13	2.00	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:A:891:MET:HE2	1:A:899:ILE:HD13	1.99	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:812:ASN:OD1	1:B:812:ASN:C	2.61	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
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:B:651:ASN:HB3	1:B:1138:MET:HE2	2.02	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:595:VAL:HB	1:B:1152:VAL:HB	2.03	0.41
1:A:793:LEU:C	1:A:793:LEU:HD23	2.46	0.40
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:926:ALA:HB2	1:A:944:MET:HE1	2.02	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%)	12	32
1	B	826/881 (94%)	773 (94%)	46 (6%)	7 (1%)	16	37
All	All	1656/1762 (94%)	1549 (94%)	92 (6%)	15 (1%)	14	35

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 ⓘ

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%)	674 (96%)	28 (4%)	28	56
1	B	701/741 (95%)	670 (96%)	31 (4%)	25	53
All	All	1403/1482 (95%)	1344 (96%)	59 (4%)	26	55

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	447	GLU
1	A	465	ASN
1	A	522	TYR
1	A	583	GLU
1	A	594	GLN
1	A	601	ASP
1	A	626	ASP
1	A	698	ASP
1	A	758	SER
1	A	761	VAL
1	A	773	THR
1	A	797	LEU
1	A	851	ILE
1	A	883	GLN
1	A	916	THR
1	A	939	THR
1	A	962	ASN
1	A	981	ASP
1	A	1097	VAL
1	A	1098	THR
1	A	1133	GLN
1	A	1144	LEU
1	A	1150	VAL
1	A	1171	ASN
1	A	1183	ASN
1	A	1198	SER
1	A	1268	THR

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Mol	Chain	Res	Type
1	A	1277	ASN
1	B	445	THR
1	B	457	SER
1	B	483	GLN
1	B	487	THR
1	B	522	TYR
1	B	531	THR
1	B	566	SER
1	B	583	GLU
1	B	601	ASP
1	B	698	ASP
1	B	705	ASN
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	918	SER
1	B	934	GLN
1	B	981	ASP
1	B	1025	SER
1	B	1089	SER
1	B	1097	VAL
1	B	1150	VAL
1	B	1164	VAL
1	B	1171	ASN
1	B	1198	SER
1	B	1209	ILE
1	B	1268	THR
1	B	1277	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	594	GLN
1	A	602	ASN
1	A	618	ASN
1	A	619	ASN
1	A	767	ASN
1	A	831	GLN

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Mol	Chain	Res	Type
1	A	837	GLN
1	A	862	GLN
1	A	897	ASN
1	A	948	HIS
1	A	994	ASN
1	A	1071	ASN
1	A	1171	ASN
1	A	1183	ASN
1	A	1185	GLN
1	A	1277	ASN
1	B	461	ASN
1	B	464	ASN
1	B	465	ASN
1	B	551	GLN
1	B	602	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	767	ASN
1	B	780	ASN
1	B	862	GLN
1	B	934	GLN
1	B	938	GLN
1	B	982	ASN
1	B	1038	HIS
1	B	1071	ASN
1	B	1085	GLN
1	B	1133	GLN
1	B	1161	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	1302	-	4,4,4	0.40	0	6,6,6	0.18	0
4	GOL	B	1302	-	5,5,5	0.42	0	5,5,5	0.20	0
3	SO4	B	1303	-	4,4,4	0.47	0	6,6,6	0.23	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
4	GOL	B	1302	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1302	GOL	O1-C1-C2-C3
4	B	1302	GOL	C1-C2-C3-O3
4	B	1302	GOL	O1-C1-C2-O2
4	B	1302	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	832/881 (94%)	0.95	89 (10%) 11 9	26, 36, 65, 83	0
1	B	830/881 (94%)	0.93	71 (8%) 16 13	26, 35, 55, 70	0
All	All	1662/1762 (94%)	0.94	160 (9%) 13 11	26, 35, 60, 83	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	810	TYR	7.4
1	A	808	ALA	6.3
1	A	627	ASN	6.1
1	A	806	TYR	6.1
1	A	804	GLY	5.8
1	B	1023	ALA	5.7
1	B	808	ALA	5.5
1	A	803	PRO	5.0
1	A	801	ASP	4.6
1	A	807	LYS	4.5
1	A	810	TYR	4.5
1	A	805	ALA	4.4
1	B	896	ASP	4.4
1	A	936	ALA	4.4
1	B	752	ASN	4.3
1	B	797	LEU	4.3
1	A	809	GLU	4.2
1	B	937	GLU	3.9
1	A	812	ASN	3.8
1	B	753	ASN	3.7
1	A	489	TYR	3.7
1	A	797	LEU	3.6
1	B	804	GLY	3.6
1	B	1276	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	803	PRO	3.6
1	A	1085	GLN	3.5
1	A	800	LYS	3.5
1	A	752	ASN	3.4
1	A	826	ASP	3.4
1	A	897	ASN	3.4
1	A	820	ALA	3.4
1	B	751	ALA	3.4
1	A	811	ALA	3.3
1	B	809	GLU	3.3
1	A	998	SER	3.3
1	A	1008	VAL	3.2
1	A	796	GLY	3.2
1	A	1023	ALA	3.2
1	A	1011	ASN	3.1
1	A	802	HIS	3.1
1	B	936	ALA	3.1
1	B	990	LYS	3.1
1	A	751	ALA	3.0
1	B	627	ASN	3.0
1	A	448	ALA	3.0
1	A	990	LYS	3.0
1	A	962	ASN	2.9
1	A	992	TYR	2.9
1	B	489	TYR	2.9
1	A	933	PRO	2.9
1	B	1047	TYR	2.9
1	A	1108	ASN	2.9
1	B	829	TYR	2.9
1	A	813	GLN	2.9
1	B	1022	SER	2.9
1	A	832	TYR	2.8
1	A	814	ALA	2.8
1	B	976	THR	2.8
1	A	892	THR	2.8
1	B	518	VAL	2.8
1	A	798	ILE	2.8
1	A	993	SER	2.7
1	A	1000	TYR	2.7
1	B	814	ALA	2.7
1	B	991	GLY	2.7
1	B	1085	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1047	TYR	2.7
1	A	793	LEU	2.7
1	A	937	GLU	2.7
1	B	1183	ASN	2.7
1	A	621	THR	2.7
1	B	532	GLY	2.6
1	A	540	ASN	2.6
1	A	542	ALA	2.6
1	A	1276	ALA	2.6
1	B	542	ALA	2.6
1	A	970	GLY	2.6
1	B	531	THR	2.6
1	B	1021	VAL	2.6
1	A	959	THR	2.5
1	B	895	SER	2.5
1	A	799	SER	2.5
1	B	977	LEU	2.5
1	B	747	VAL	2.5
1	A	934	GLN	2.5
1	A	1106	ASN	2.5
1	B	818	PHE	2.5
1	B	537	LEU	2.4
1	A	484	ASP	2.4
1	B	796	GLY	2.4
1	B	756	THR	2.4
1	B	523	GLU	2.4
1	B	811	ALA	2.4
1	A	941	SER	2.4
1	A	986	LYS	2.4
1	A	631	GLY	2.4
1	B	865	GLN	2.4
1	B	812	ASN	2.3
1	A	896	ASP	2.3
1	B	742	SER	2.3
1	B	928	ILE	2.3
1	B	826	ASP	2.3
1	B	868	SER	2.3
1	B	521	GLY	2.3
1	A	548	GLU	2.3
1	A	895	SER	2.3
1	A	1158	ARG	2.3
1	A	940	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	965	THR	2.3
1	B	626	ASP	2.3
1	B	487	THR	2.2
1	B	821	ASP	2.2
1	B	1189	GLY	2.2
1	A	971	ALA	2.2
1	B	820	ALA	2.2
1	A	825	THR	2.2
1	A	939	THR	2.2
1	B	825	THR	2.2
1	B	992	TYR	2.2
1	B	970	GLY	2.2
1	B	445	THR	2.2
1	A	1275	TYR	2.2
1	A	831	GLN	2.2
1	A	614	SER	2.2
1	B	548	GLU	2.2
1	B	967	ASN	2.2
1	B	998	SER	2.2
1	A	911	ALA	2.1
1	B	1107	ALA	2.1
1	B	962	ASN	2.1
1	A	1068	LEU	2.1
1	A	617	ILE	2.1
1	A	961	ASP	2.1
1	B	801	ASP	2.1
1	B	981	ASP	2.1
1	A	868	SER	2.1
1	B	604	SER	2.1
1	A	1220	ARG	2.1
1	A	988	THR	2.1
1	A	828	GLN	2.1
1	B	1119	ALA	2.1
1	A	447	GLU	2.1
1	B	862	GLN	2.1
1	A	592	TYR	2.1
1	A	815	TRP	2.1
1	B	815	TRP	2.1
1	A	829	TYR	2.1
1	A	989	VAL	2.1
1	A	969	ASP	2.0
1	A	1018	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1197	GLN	2.0
1	A	928	ILE	2.0
1	A	996	TYR	2.0
1	B	1170	ALA	2.0
1	A	525	SER	2.0
1	B	543	SER	2.0
1	A	1224	TRP	2.0
1	A	1103	LEU	2.0
1	B	794	ILE	2.0
1	B	834	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	1303	5/5	0.79	0.18	47,47,48,48	0
4	GOL	B	1302	6/6	0.81	0.17	22,22,22,22	0
2	CA	A	1301	1/1	0.87	0.08	30,30,30,30	0
3	SO4	A	1302	5/5	0.89	0.14	46,46,47,47	0
2	CA	B	1301	1/1	0.92	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.