



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:58 pm BST

PDB ID : 1H3G
Title : Cyclomaltodextrinase from *Flavobacterium* sp. No. 92: from DNA sequence to protein structure
Authors : Fritzsche, H.B.; Schwede, T.; Jelakovic, S.; Schulz, G.E.
Deposited on : 2002-09-03
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

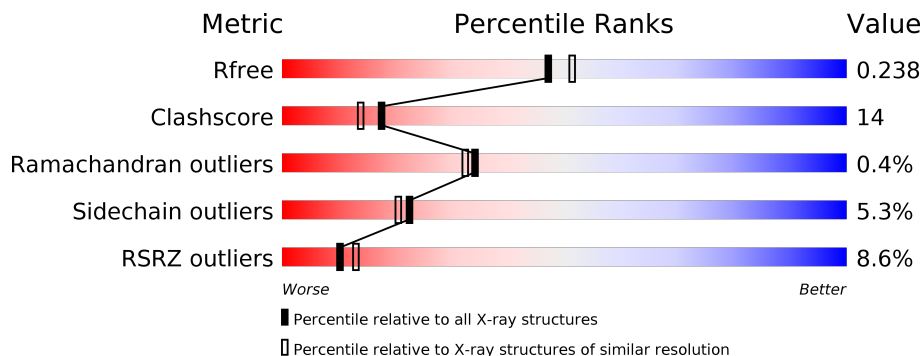
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	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 on 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	601	 6% 74% 21%
1	B	601	 10% 77% 20%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 10239 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 Cyclomalto-dextrinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	598	4771	3016	858	873	24	0	0	1
1	B	598	4771	3016	858	873	24	0	0	1

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	initiating methionine	UNP Q8KKG0
A	2	ALA	-	expression tag	UNP Q8KKG0
A	3	PRO	-	expression tag	UNP Q8KKG0
A	4	THR	-	expression tag	UNP Q8KKG0
A	5	ALA	-	expression tag	UNP Q8KKG0
B	1	MSE	-	initiating methionine	UNP Q8KKG0
B	2	ALA	-	expression tag	UNP Q8KKG0
B	3	PRO	-	expression tag	UNP Q8KKG0
B	4	THR	-	expression tag	UNP Q8KKG0
B	5	ALA	-	expression tag	UNP Q8KKG0

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

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

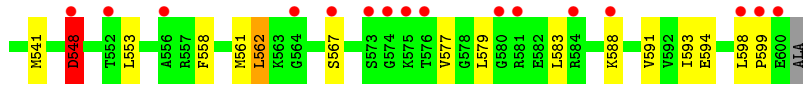
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	413	Total 413	O 413	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	280	Total 280	O 280	0	0



4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	181.34Å 181.34Å 231.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	21.10 – 2.10 20.72 – 2.08	Depositor EDS
% Data completeness (in resolution range)	91.6 (21.10-2.10) 91.6 (20.72-2.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.40 (at 2.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.223 0.208 , 0.238	Depositor DCC
R_{free} test set	1990 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for $-2/3^*h-1/3^*k+2/3^*l,-1/3^*h-2/3^*k-2/3^*l,2/3^*h-2/3^*k+1/3^*l$ 0.011 for $-h,1/3^*h-1/3^*k+2/3^*l,2/3^*h+4/3^*k+1/3^*l$ 0.009 for $-1/3^*h+1/3^*k-2/3^*l,-k,-4/3^*h-2/3^*k+1/3^*l$	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10239	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: 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	0.65	5/4881 (0.1%)	0.80	15/6581 (0.2%)
1	B	0.54	1/4881 (0.0%)	0.78	13/6581 (0.2%)
All	All	0.60	6/9762 (0.1%)	0.79	28/13162 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	443	MSE	SE-CE	-7.42	1.51	1.95
1	A	544	MSE	SE-CE	-6.34	1.58	1.95
1	A	422	MSE	SE-CE	-6.29	1.58	1.95
1	A	370	MSE	SE-CE	-5.89	1.60	1.95
1	A	130	MSE	SE-CE	-5.45	1.63	1.95
1	A	378	MSE	SE-CE	-5.43	1.63	1.95

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ASP	CB-CG-OD2	7.80	125.32	118.30
1	B	187	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	431	ASP	CB-CG-OD2	6.35	124.01	118.30
1	A	155	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	61	ASP	CB-CG-OD2	6.21	123.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	258	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	31	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	371	ASP	CB-CG-OD2	5.89	123.61	118.30
1	B	465	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	135	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	135	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	537	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	401	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	311	ASP	CB-CG-OD2	5.38	123.15	118.30
1	B	499	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	31	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	401	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	548	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	200	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	311	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	360	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	80	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	265	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	548	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	429	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	238	ASP	CB-CG-OD2	5.05	122.84	118.30
1	B	74	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	598	LEU	Peptide

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	4771	0	4576	139	0
1	B	4771	0	4576	117	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
3	A	413	0	0	20	1
3	B	280	0	0	10	1
All	All	10239	0	9152	256	2

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 14.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:N	1:A:67:GLU:OE1	1.57	1.33
1:A:598:LEU:HG	1:A:599:PRO:CD	1.63	1.29
1:B:520:MSE:HE2	1:B:561:MSE:HG2	1.27	1.16
1:B:520:MSE:CE	1:B:561:MSE:HG2	1.82	1.09
1:A:435:MSE:HG2	1:A:544:MSE:HE3	1.18	1.08
1:B:398:LEU:HD11	1:B:443:MSE:HE1	1.37	1.06
1:A:598:LEU:HG	1:A:599:PRO:HD3	1.11	1.05
1:A:422:MSE:CE	3:A:2332:HOH:O	2.16	0.94
1:A:378:MSE:HE2	1:A:382:LEU:HG	1.49	0.94
1:A:67:GLU:H	1:A:67:GLU:CD	1.73	0.92
1:A:378:MSE:HE3	1:A:381:ALA:HB3	1.51	0.90
1:A:598:LEU:CG	1:A:599:PRO:CD	2.50	0.90
1:A:435:MSE:CG	1:A:544:MSE:HE3	2.01	0.89
1:B:520:MSE:HE2	1:B:561:MSE:CG	2.01	0.89
1:A:491:THR:HG22	1:A:494:GLN:H	1.41	0.84
1:B:520:MSE:HE3	1:B:522:PHE:CZ	2.13	0.83
1:A:435:MSE:HG2	1:A:544:MSE:CE	2.07	0.83
1:A:541:MSE:HE2	1:A:593:ILE:HD12	1.60	0.83
1:A:181:HIS:HD2	1:A:183:TYR:H	1.25	0.82
1:B:251:HIS:HD2	1:B:315:TYR:OH	1.63	0.82
1:A:137:ARG:NH1	3:A:2109:HOH:O	2.13	0.82
1:B:548:ASP:OD2	3:B:2270:HOH:O	1.98	0.81
1:A:4:THR:HG23	1:A:6:ILE:H	1.48	0.79
1:A:598:LEU:HG	1:A:599:PRO:HD2	1.64	0.79
1:A:518:ARG:HB3	1:A:518:ARG:HH11	1.47	0.79
1:B:532:PHE:CD1	1:B:561:MSE:HG3	2.18	0.78
1:B:370:MSE:CE	1:B:448:GLN:HE21	1.98	0.77
1:A:334:ARG:CB	1:A:334:ARG:HH11	1.99	0.75
1:A:481:LYS:HE2	1:A:481:LYS:HA	1.70	0.74
1:B:263:GLN:HE21	1:B:267:GLU:HG3	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ALA:CB	1:B:142:ARG:HB2	2.17	0.74
1:B:398:LEU:CD1	1:B:443:MSE:HE1	2.15	0.73
1:B:520:MSE:HE3	1:B:522:PHE:CE2	2.23	0.73
1:A:370:MSE:CE	1:A:413:PHE:CD2	2.72	0.72
1:A:353:GLN:HE21	1:A:405:PRO:HD2	1.54	0.72
1:B:143:HIS:ND1	1:B:472:ASP:OD1	2.16	0.71
1:B:491:THR:O	1:B:495:ARG:HG3	1.90	0.71
1:A:491:THR:HG21	3:A:2364:HOH:O	1.89	0.71
1:B:353:GLN:HE21	1:B:405:PRO:HD2	1.55	0.71
1:A:280:ASP:OD1	3:A:2216:HOH:O	2.09	0.70
1:B:398:LEU:HD11	1:B:443:MSE:CE	2.18	0.70
1:A:378:MSE:HE2	1:A:382:LEU:CG	2.21	0.70
1:A:382:LEU:CD2	1:A:435:MSE:HE2	2.22	0.69
1:B:226:LYS:HB2	1:B:226:LYS:NZ	2.07	0.69
1:B:181:HIS:HD2	1:B:183:TYR:H	1.39	0.69
1:A:341:GLU:OE1	3:A:2254:HOH:O	2.11	0.68
1:B:151:ILE:HG21	1:B:203:ARG:HH12	1.58	0.68
1:B:370:MSE:CE	1:B:448:GLN:NE2	2.56	0.68
1:B:370:MSE:HE1	1:B:448:GLN:HE21	1.59	0.68
1:A:422:MSE:HE2	3:A:2332:HOH:O	1.86	0.67
1:A:365:HIS:ND1	3:A:2279:HOH:O	2.27	0.67
1:B:520:MSE:HE1	1:B:561:MSE:HG2	1.70	0.67
1:A:137:ARG:NH1	3:A:2108:HOH:O	2.26	0.66
1:A:598:LEU:CG	1:A:599:PRO:HD2	2.22	0.66
1:A:591:VAL:CG1	1:A:593:ILE:HG13	2.25	0.66
1:A:35:MSE:HA	1:A:35:MSE:HE2	1.77	0.65
1:A:581:ARG:HB2	1:A:581:ARG:NH1	2.11	0.64
1:B:134:ALA:HB3	1:B:142:ARG:HB2	1.78	0.64
1:B:226:LYS:HB2	1:B:226:LYS:HZ2	1.62	0.64
1:B:226:LYS:CB	1:B:226:LYS:NZ	2.61	0.64
1:B:548:ASP:N	1:B:548:ASP:OD2	2.31	0.63
1:A:35:MSE:HE1	1:A:80:ASP:CB	2.29	0.62
1:B:408:GLN:NE2	3:B:2222:HOH:O	2.22	0.62
1:A:422:MSE:HE3	1:A:453:ASP:OD2	2.00	0.62
1:B:191:ILE:O	3:B:2123:HOH:O	2.16	0.62
1:A:35:MSE:HE1	1:A:79:GLY:C	2.20	0.61
1:A:370:MSE:HE2	1:A:413:PHE:CD2	2.35	0.61
1:B:136:ARG:HA	1:B:143:HIS:CD2	2.35	0.61
1:A:378:MSE:CE	1:A:381:ALA:HB3	2.28	0.61
1:A:197:SER:HB2	1:A:199:GLU:OE2	2.01	0.61
1:A:221:LEU:HD21	1:A:296:ASN:HD21	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:SER:O	1:B:385:THR:N	2.35	0.60
1:A:511:GLN:HE22	1:A:538:LYS:NZ	2.00	0.59
1:A:398:LEU:HD11	1:A:443:MSE:SE	2.52	0.59
1:B:538:LYS:NZ	1:B:594:GLU:OE1	2.28	0.58
1:A:66:PRO:N	1:A:67:GLU:OE1	2.35	0.58
1:A:378:MSE:HE2	1:A:382:LEU:CD2	2.33	0.58
1:B:151:ILE:HG21	1:B:203:ARG:NH1	2.17	0.58
1:B:142:ARG:HD2	1:B:179:SER:OG	2.04	0.58
1:B:173:ASN:O	1:B:179:SER:HB2	2.03	0.58
1:B:567:SER:HB2	1:B:577:VAL:O	2.04	0.58
1:B:32:ILE:HD12	1:B:35:MSE:HG3	1.86	0.58
1:A:130:MSE:HE2	1:A:194:ARG:NH2	2.19	0.58
1:B:532:PHE:CG	1:B:561:MSE:HG3	2.39	0.57
1:B:151:ILE:HD13	1:B:203:ARG:HH11	1.69	0.57
1:A:408:GLN:NE2	3:A:2309:HOH:O	2.17	0.57
1:A:518:ARG:CB	1:A:518:ARG:HH11	2.14	0.57
1:A:581:ARG:CB	1:A:581:ARG:NH1	2.67	0.57
1:B:67:GLU:CD	1:B:67:GLU:H	2.08	0.57
1:A:32:ILE:HD12	1:A:35:MSE:HG3	1.87	0.57
1:A:541:MSE:CE	1:A:593:ILE:HD12	2.32	0.57
1:A:154:LEU:HD22	1:A:213:MSE:HE1	1.86	0.56
1:B:251:HIS:CD2	1:B:315:TYR:OH	2.53	0.56
1:B:85:ARG:NH1	3:B:2052:HOH:O	2.37	0.56
1:B:329:MSE:HE1	1:B:335:LEU:HD23	1.86	0.56
1:A:363:THR:HA	3:A:2271:HOH:O	2.04	0.56
1:A:69:GLN:HG3	1:A:70:PRO:HD2	1.88	0.56
1:A:130:MSE:HE1	1:A:174:ASP:HB2	1.87	0.55
1:A:581:ARG:CB	1:A:581:ARG:HH11	2.19	0.55
1:B:166:TRP:CD1	1:B:166:TRP:C	2.79	0.55
1:B:502:ARG:HD2	3:B:2250:HOH:O	2.07	0.55
1:A:251:HIS:HD2	1:A:315:TYR:OH	1.90	0.54
1:B:344:THR:O	3:B:2188:HOH:O	2.18	0.54
1:A:167:PRO:HD2	1:A:216:ILE:O	2.08	0.54
1:B:398:LEU:HD21	1:B:443:MSE:HE1	1.89	0.54
1:B:35:MSE:CE	1:B:84:GLU:HG2	2.38	0.53
1:A:276:GLU:CD	1:A:276:GLU:H	2.12	0.53
1:A:166:TRP:C	1:A:166:TRP:CD1	2.78	0.53
1:B:536:LYS:H	1:B:536:LYS:HE3	1.74	0.53
1:A:181:HIS:CD2	1:A:183:TYR:H	2.16	0.53
1:A:171:VAL:HG22	1:A:187:ASP:O	2.09	0.52
1:A:200:ASP:OD1	1:A:203:ARG:NH2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD21	1:A:296:ASN:ND2	2.24	0.52
1:A:35:MSE:CA	1:A:35:MSE:HE2	2.37	0.52
1:A:8:HIS:HB2	1:A:28:HIS:HB3	1.91	0.52
1:B:67:GLU:OE1	1:B:67:GLU:N	2.41	0.52
1:B:472:ASP:HB3	1:B:477:TRP:CZ3	2.45	0.52
1:A:532:PHE:CE2	1:A:541:MSE:HB2	2.44	0.52
1:A:563:LYS:HG3	1:A:598:LEU:HD11	1.92	0.52
1:A:581:ARG:HB3	1:A:581:ARG:HH11	1.75	0.51
1:B:296:ASN:ND2	1:B:324:TYR:OH	2.30	0.51
1:A:491:THR:HG23	1:A:493:GLN:H	1.75	0.51
1:A:415:GLY:HA3	3:A:2317:HOH:O	2.09	0.51
1:A:173:ASN:O	1:A:179:SER:HB2	2.10	0.51
1:B:74:ASP:OD1	1:B:87:ARG:NH1	2.43	0.50
1:A:190:ARG:CZ	1:A:193:PRO:HG3	2.42	0.50
1:B:168:THR:HB	1:B:169:PRO:CD	2.42	0.50
1:B:329:MSE:HE1	1:B:335:LEU:HB3	1.94	0.50
1:B:530:VAL:HG11	1:B:541:MSE:HE3	1.94	0.50
1:A:414:GLY:HA3	1:A:422:MSE:HE2	1.92	0.49
1:A:581:ARG:HB2	1:A:581:ARG:CZ	2.41	0.49
1:B:598:LEU:HB3	1:B:599:PRO:CD	2.43	0.49
1:A:130:MSE:HE1	1:A:174:ASP:CB	2.43	0.49
1:A:378:MSE:HE1	1:A:391:LEU:HD21	1.93	0.49
1:B:167:PRO:HB2	1:B:170:LEU:HD11	1.95	0.49
1:B:329:MSE:HA	1:B:329:MSE:HE2	1.94	0.49
1:A:598:LEU:CB	1:A:599:PRO:HD2	2.43	0.49
1:B:5:ALA:HB1	1:B:84:GLU:HG3	1.94	0.49
1:A:334:ARG:HB2	1:A:334:ARG:HH11	1.77	0.49
1:B:163:THR:HA	1:B:213:MSE:HG2	1.95	0.49
1:B:532:PHE:CE2	1:B:541:MSE:HB2	2.48	0.49
1:B:134:ALA:HB1	1:B:142:ARG:H	1.78	0.48
1:B:385:THR:O	3:B:2209:HOH:O	2.20	0.48
1:B:374:LEU:HD21	1:B:443:MSE:HE2	1.94	0.48
1:B:536:LYS:H	1:B:536:LYS:CE	2.24	0.48
1:A:199:GLU:H	1:A:199:GLU:CD	2.16	0.48
1:A:370:MSE:HE2	1:A:413:PHE:CE2	2.48	0.48
1:A:168:THR:HB	1:A:169:PRO:CD	2.44	0.48
1:A:334:ARG:HB3	1:A:334:ARG:HH11	1.76	0.48
1:B:221:LEU:HD21	1:B:296:ASN:HD21	1.79	0.48
1:B:9:MSE:HG2	1:B:86:TYR:CZ	2.48	0.48
1:B:434:ARG:CD	3:B:2228:HOH:O	2.61	0.48
1:A:171:VAL:HG21	1:A:188:HIS:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LEU:HD22	1:A:435:MSE:HE2	1.94	0.48
1:A:536:LYS:NZ	3:A:2391:HOH:O	2.47	0.48
1:A:35:MSE:HE1	1:A:80:ASP:HB3	1.95	0.48
1:B:353:GLN:NE2	1:B:406:GLU:H	2.11	0.48
1:A:598:LEU:CB	1:A:599:PRO:CD	2.92	0.47
1:B:217:GLN:NE2	1:B:305:LEU:HD11	2.28	0.47
1:B:166:TRP:HZ3	1:B:448:GLN:NE2	2.11	0.47
1:A:35:MSE:HB3	1:A:77:PHE:HB3	1.96	0.47
1:A:518:ARG:CG	1:A:518:ARG:HH11	2.27	0.47
1:A:511:GLN:HE22	1:A:538:LYS:HZ1	1.62	0.47
1:B:370:MSE:HB3	1:B:372:PHE:CE2	2.49	0.47
1:B:8:HIS:HB2	1:B:28:HIS:HB3	1.96	0.47
1:B:370:MSE:HG3	1:B:413:PHE:CE2	2.49	0.47
1:B:311:ASP:O	1:B:312:THR:C	2.53	0.47
1:A:77:PHE:O	1:A:83:SER:HA	2.15	0.47
1:B:46:LEU:HD21	1:B:60:VAL:HG13	1.96	0.47
1:A:130:MSE:HE3	1:A:174:ASP:OD1	2.14	0.46
1:A:34:ARG:C	1:A:35:MSE:HE2	2.36	0.46
1:B:226:LYS:CB	1:B:226:LYS:HZ3	2.27	0.46
1:B:579:LEU:HD23	1:B:583:LEU:HD13	1.98	0.46
1:B:203:ARG:HA	3:B:2133:HOH:O	2.15	0.46
1:B:520:MSE:CE	1:B:522:PHE:CZ	2.94	0.46
1:B:34:ARG:NH1	1:B:34:ARG:HB3	2.31	0.46
1:A:558:PHE:HB2	1:A:562:LEU:HD22	1.98	0.45
1:A:66:PRO:CD	1:A:67:GLU:OE1	2.65	0.45
1:B:87:ARG:HG2	1:B:87:ARG:HH11	1.81	0.45
1:A:4:THR:HG23	1:A:6:ILE:N	2.24	0.45
1:B:217:GLN:HE21	1:B:305:LEU:HD11	1.81	0.45
1:A:66:PRO:HD2	1:A:67:GLU:OE1	2.17	0.45
1:B:398:LEU:CG	1:B:443:MSE:HE1	2.47	0.45
1:A:441:MSE:HE1	1:A:447:PRO:HB2	1.99	0.45
1:A:337:MSE:H	1:A:367:PRO:HG2	1.82	0.45
1:A:35:MSE:HE1	1:A:80:ASP:HB2	1.98	0.45
1:A:435:MSE:HE1	1:A:546:ASN:OD1	2.17	0.45
1:A:106:GLY:HA2	1:A:515:HIS:CD2	2.52	0.45
1:B:593:ILE:N	1:B:593:ILE:HD12	2.32	0.44
1:A:464:ARG:NH1	3:A:2341:HOH:O	2.32	0.44
1:B:171:VAL:HG22	1:B:187:ASP:O	2.16	0.44
1:A:422:MSE:HE1	3:A:2332:HOH:O	1.99	0.44
1:B:372:PHE:N	1:B:373:PRO:CD	2.80	0.44
1:A:553:LEU:HD22	1:A:553:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:THR:HB	1:A:562:LEU:HD23	1.98	0.43
1:B:258:ASP:HA	1:B:259:PRO:HD3	1.90	0.43
1:A:211:ARG:HG3	1:A:211:ARG:HH11	1.83	0.43
1:B:217:GLN:HB2	1:B:305:LEU:CD1	2.48	0.43
1:B:313:TYR:CZ	1:B:366:LEU:HD22	2.53	0.43
1:B:398:LEU:HD21	1:B:443:MSE:CE	2.49	0.43
1:B:8:HIS:HD2	1:B:28:HIS:ND1	2.15	0.43
1:A:372:PHE:N	1:A:373:PRO:CD	2.81	0.43
1:A:354:ARG:CZ	1:A:367:PRO:HB3	2.48	0.43
1:B:423:PHE:CD1	1:B:456:LEU:HD22	2.53	0.43
1:A:190:ARG:NH2	1:A:193:PRO:HG3	2.34	0.43
1:B:346:VAL:HB	1:B:347:PRO:HD3	2.01	0.43
1:B:558:PHE:HB2	1:B:562:LEU:HD22	1.99	0.43
1:B:190:ARG:CZ	1:B:193:PRO:HG3	2.48	0.43
1:B:311:ASP:OD1	1:B:312:THR:HG23	2.19	0.43
1:A:35:MSE:CE	1:A:80:ASP:HB2	2.49	0.43
1:A:62:LEU:N	1:A:62:LEU:HD12	2.33	0.43
1:B:464:ARG:HG2	1:B:464:ARG:H	1.56	0.43
1:B:431:ASP:HB3	1:B:588:LYS:O	2.18	0.43
1:A:346:VAL:N	1:A:347:PRO:CD	2.83	0.42
1:A:358:ASN:ND2	3:A:2274:HOH:O	2.43	0.42
1:A:8:HIS:HD2	1:A:28:HIS:ND1	2.16	0.42
1:B:346:VAL:N	1:B:347:PRO:CD	2.82	0.42
1:B:221:LEU:HD21	1:B:296:ASN:ND2	2.35	0.42
1:B:328:LEU:HD23	1:B:337:MSE:SE	2.69	0.42
1:B:130:MSE:HE3	1:B:174:ASP:HA	2.01	0.42
1:A:434:ARG:HG3	1:A:500:LEU:HD21	2.01	0.42
1:A:413:PHE:HB3	1:A:448:GLN:NE2	2.35	0.42
1:A:154:LEU:HD22	1:A:213:MSE:CE	2.50	0.42
1:A:422:MSE:HE3	1:A:453:ASP:CG	2.39	0.42
1:A:591:VAL:HG13	1:A:593:ILE:HG13	1.99	0.42
1:B:99:GLN:NE2	1:B:334:ARG:HD2	2.35	0.42
1:B:258:ASP:OD2	1:B:259:PRO:HD2	2.20	0.41
1:B:591:VAL:HB	1:B:593:ILE:CD1	2.51	0.41
1:A:487:GLY:HA2	1:A:490:LEU:HD22	2.01	0.41
1:B:351:ARG:HA	1:B:358:ASN:HD21	1.85	0.41
1:B:9:MSE:HG2	1:B:86:TYR:CE1	2.55	0.41
1:A:353:GLN:HE22	1:A:404:TYR:HB3	1.86	0.41
1:B:504:LEU:HA	1:B:504:LEU:HD12	1.89	0.41
1:B:535:ASN:HB2	1:B:536:LYS:NZ	2.36	0.41
1:A:495:ARG:NE	3:A:2366:HOH:O	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:GLN:HB2	1:B:305:LEU:HD13	2.02	0.41
1:A:242:TYR:HA	3:A:2191:HOH:O	2.20	0.41
1:B:434:ARG:HD2	3:B:2228:HOH:O	2.20	0.41
1:A:168:THR:HB	1:A:169:PRO:HD2	2.02	0.41
1:A:24:GLN:NE2	3:A:2017:HOH:O	2.51	0.41
1:B:165:LEU:HB2	1:B:213:MSE:CE	2.51	0.41
1:B:246:PHE:CG	1:B:276:GLU:HG2	2.56	0.41
1:B:398:LEU:CD2	1:B:443:MSE:HE1	2.51	0.41
1:A:170:LEU:HD13	1:A:201:PHE:CE1	2.56	0.41
1:A:374:LEU:HD12	1:A:374:LEU:HA	1.94	0.41
1:A:387:GLU:HG3	3:A:2290:HOH:O	2.20	0.41
1:A:253:ARG:O	1:A:256:VAL:HG22	2.22	0.40
1:A:242:TYR:CD2	1:A:247:VAL:HB	2.56	0.40
1:A:435:MSE:HE3	1:A:544:MSE:CE	2.51	0.40
1:A:41:TYR:HA	1:A:42:PRO:HD3	1.91	0.40
1:A:102:GLY:HA2	1:A:306:SER:O	2.22	0.40
1:A:413:PHE:N	1:A:413:PHE:CD2	2.89	0.40
1:B:548:ASP:HB3	1:B:588:LYS:HE3	2.02	0.40
1:A:311:ASP:O	1:A:312:THR:C	2.60	0.40
1:A:329:MSE:SE	1:A:337:MSE:HE2	2.72	0.40
1:A:560:GLU:HG2	3:A:2400:HOH:O	2.21	0.40

All (2) 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)
3:B:2193:HOH:O	3:B:2218:HOH:O[12_555]	0.98	1.22
3:A:2263:HOH:O	3:A:2293:HOH:O[12_555]	1.75	0.45

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	596/601 (99%)	580 (97%)	14 (2%)	2 (0%)	41	41
1	B	596/601 (99%)	569 (96%)	24 (4%)	3 (0%)	29	26
All	All	1192/1202 (99%)	1149 (96%)	38 (3%)	5 (0%)	34	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	B	384	LYS
1	A	244	GLY
1	B	243	GLY
1	B	464	ARG

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	492/469 (105%)	462 (94%)	30 (6%)	18	16
1	B	492/469 (105%)	470 (96%)	22 (4%)	27	27
All	All	984/938 (105%)	932 (95%)	52 (5%)	22	20

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	36	GLU
1	A	46	LEU
1	A	51	ARG
1	A	63	GLU
1	A	67	GLU
1	A	69	GLN
1	A	76	VAL
1	A	87	ARG
1	A	90	LEU
1	A	91	LEU

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Mol	Chain	Res	Type
1	A	95	GLN
1	A	170	LEU
1	A	194	ARG
1	A	253	ARG
1	A	276	GLU
1	A	290	ASN
1	A	334	ARG
1	A	435	MSE
1	A	436	ASN
1	A	448	GLN
1	A	464	ARG
1	A	490	LEU
1	A	491	THR
1	A	518	ARG
1	A	521	HIS
1	A	536	LYS
1	A	562	LEU
1	A	581	ARG
1	A	584	ARG
1	B	7	GLU
1	B	21	LYS
1	B	46	LEU
1	B	61	ASP
1	B	87	ARG
1	B	90	LEU
1	B	91	LEU
1	B	94	GLU
1	B	135	ASP
1	B	171	VAL
1	B	194	ARG
1	B	199	GLU
1	B	226	LYS
1	B	436	ASN
1	B	448	GLN
1	B	492	SER
1	B	504	LEU
1	B	521	HIS
1	B	536	LYS
1	B	548	ASP
1	B	553	LEU
1	B	562	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	99	GLN
1	A	111	GLN
1	A	181	HIS
1	A	217	GLN
1	A	251	HIS
1	A	296	ASN
1	A	353	GLN
1	A	358	ASN
1	A	436	ASN
1	A	448	GLN
1	A	498	GLN
1	A	511	GLN
1	A	521	HIS
1	B	8	HIS
1	B	20	HIS
1	B	99	GLN
1	B	111	GLN
1	B	181	HIS
1	B	217	GLN
1	B	251	HIS
1	B	257	GLN
1	B	263	GLN
1	B	296	ASN
1	B	353	GLN
1	B	358	ASN
1	B	436	ASN
1	B	448	GLN
1	B	493	GLN
1	B	521	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 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 [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	574/601 (95%)	0.40	36 (6%) 20 24	18, 26, 38, 52	0
1	B	574/601 (95%)	0.64	63 (10%) 5 7	22, 30, 43, 53	0
All	All	1148/1202 (95%)	0.52	99 (8%) 10 13	18, 28, 42, 53	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	600	GLU	12.8
1	A	599	PRO	8.3
1	A	600	GLU	7.4
1	A	385	THR	7.1
1	B	548	ASP	7.1
1	B	462	LYS	6.5
1	B	386	GLY	6.4
1	B	464	ARG	6.3
1	A	386	GLY	6.0
1	B	599	PRO	5.9
1	B	244	GLY	5.5
1	A	598	LEU	5.3
1	B	581	ARG	5.0
1	B	385	THR	4.8
1	B	245	LYS	4.6
1	B	481	LYS	4.5
1	B	463	GLY	4.3
1	A	581	ARG	4.3
1	A	80	ASP	4.2
1	B	80	ASP	4.1
1	B	135	ASP	3.9
1	B	461	VAL	3.9
1	B	478	ALA	3.9
1	B	81	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	598	LEU	3.8
1	A	387	GLU	3.8
1	B	3	PRO	3.8
1	B	134	ALA	3.7
1	A	95	GLN	3.5
1	B	387	GLU	3.5
1	B	133	GLN	3.5
1	B	564	GLY	3.5
1	B	246	PHE	3.4
1	A	464	ARG	3.4
1	B	388	GLU	3.3
1	B	247	VAL	3.3
1	A	245	LYS	3.3
1	A	584	ARG	3.3
1	B	384	LYS	3.2
1	A	548	ASP	3.2
1	B	465	ASP	3.2
1	B	176	ALA	3.2
1	A	463	GLY	3.1
1	B	138	HIS	3.1
1	B	573	SER	3.1
1	A	536	LYS	3.1
1	B	177	ALA	3.0
1	B	243	GLY	3.0
1	A	246	PHE	3.0
1	A	388	GLU	3.0
1	B	178	TYR	3.0
1	B	128	ALA	3.0
1	B	584	ARG	3.0
1	B	30	ARG	2.8
1	B	276	GLU	2.8
1	A	479	GLY	2.8
1	B	482	ALA	2.7
1	A	243	GLY	2.7
1	B	67	GLU	2.6
1	B	488	ALA	2.6
1	A	129	GLY	2.6
1	B	487	GLY	2.6
1	B	552	THR	2.6
1	B	567	SER	2.5
1	B	574	GLY	2.4
1	B	263	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	556	ALA	2.4
1	B	281	LEU	2.4
1	B	79	GLY	2.4
1	A	481	LYS	2.4
1	A	30	ARG	2.3
1	B	575	LYS	2.3
1	A	222	SER	2.3
1	A	578	GLY	2.3
1	B	580	GLY	2.3
1	B	34	ARG	2.3
1	B	526	GLU	2.3
1	A	564	GLY	2.2
1	B	479	GLY	2.2
1	B	495	ARG	2.2
1	A	81	GLY	2.2
1	A	67	GLU	2.2
1	B	428	GLU	2.2
1	A	240	ILE	2.1
1	B	477	TRP	2.1
1	A	276	GLU	2.1
1	B	588	LYS	2.1
1	A	530	VAL	2.1
1	B	431	ASP	2.1
1	A	478	ALA	2.1
1	B	576	THR	2.1
1	A	462	LYS	2.1
1	B	78	LYS	2.1
1	A	133	GLN	2.1
1	A	263	GLN	2.1
1	A	349	VAL	2.1
1	B	129	GLY	2.1
1	B	61	ASP	2.0
1	A	384	LYS	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
2	CA	B	700	1/1	0.98	0.08	41,41,41,41	0
2	CA	A	701	1/1	0.98	0.06	35,35,35,35	0
2	CA	B	701	1/1	0.98	0.03	40,40,40,40	0
2	CA	A	700	1/1	0.98	0.20	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.