



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:09 am GMT

PDB ID : 1SQJ
Title : Crystal Structure Analysis of Oligoxyloglucan reducing-end-specific cellobiohydrolase (OXG-RCBH)
Authors : Yaoi, K.; Kondo, H.; Noro, N.; Suzuki, M.; Tsuda, S.; Mitsuishi, Y.
Deposited on : 2004-03-19
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

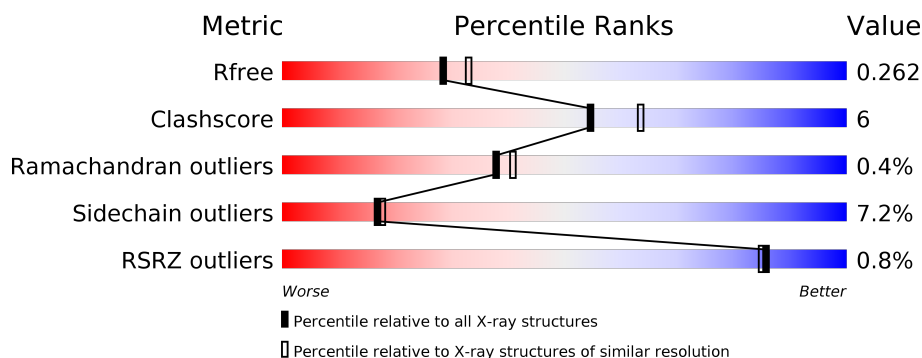
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	789	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; left: 0;">79%</div> <div style="position: absolute; top: 10px; right: 0;">16%</div> <div style="position: absolute; top: 10px; right: 0;">..</div> </div> </div>
1	B	789	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 10px; left: 0;">81%</div> <div style="position: absolute; top: 10px; right: 0;">14%</div> <div style="position: absolute; top: 10px; right: 0;">..</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11772 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 oligoxyloglucan reducing-end-specific cellobiohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total	C	N	O	S	0	0	0
			5853	3699	992	1143	19			
1	B	771	Total	C	N	O	S	0	0	0
			5856	3702	994	1141	19			

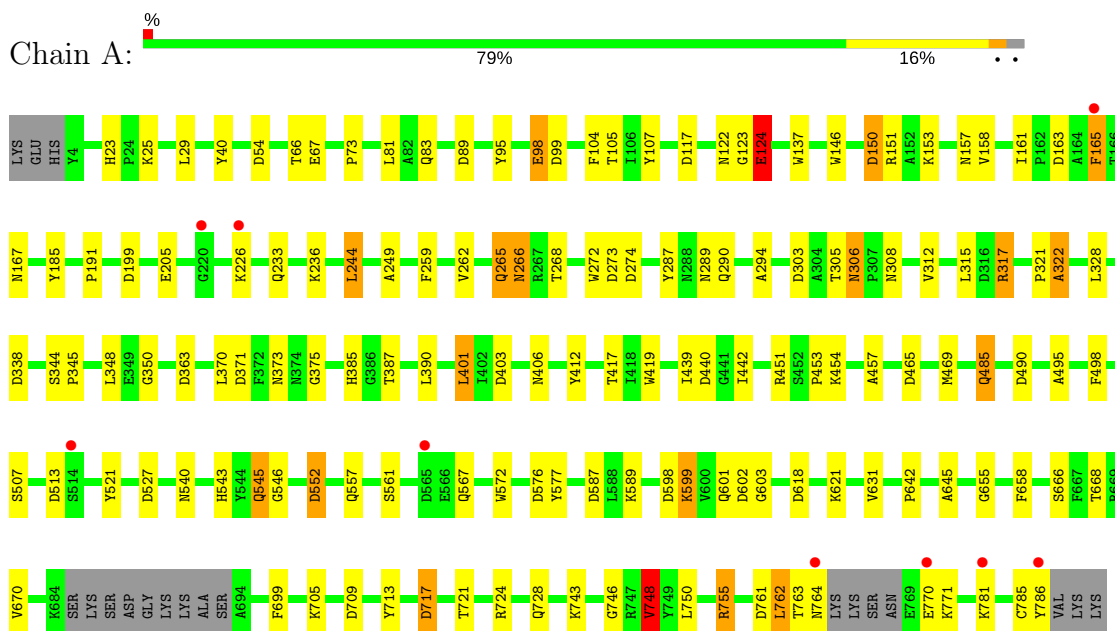
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	44	Total	O	0	0
			44	44		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: oligoxyloglucan reducing-end-specific cellobiohydrolase



- Molecule 1: oligoxyloglucan reducing-end-specific cellobiohydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.08Å 146.05Å 212.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 39.09 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.2 (20.00-2.20) 75.8 (39.09-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.251 0.224 , 0.262	Depositor DCC
R_{free} test set	4300 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11772	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.63	0/6032	0.87	26/8248 (0.3%)
1	B	0.63	0/6036	0.86	24/8254 (0.3%)
All	All	0.63	0/12068	0.86	50/16502 (0.3%)

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	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CB-CG-OD2	7.64	125.17	118.30
1	A	761	ASP	CB-CG-OD2	7.54	125.09	118.30
1	A	117	ASP	CB-CG-OD2	7.52	125.07	118.30
1	B	318	ASP	CB-CG-OD2	7.30	124.87	118.30
1	A	401	LEU	CA-CB-CG	7.22	131.91	115.30
1	A	465	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	33	ARG	NE-CZ-NH1	-6.92	116.84	120.30
1	B	587	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	422	ASP	CB-CG-OD2	6.76	124.38	118.30
1	B	618	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	576	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	587	ASP	CB-CG-OD2	6.60	124.24	118.30
1	B	717	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	609	ASP	CB-CG-OD2	6.51	124.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	150	ASP	CB-CG-OD2	6.48	124.13	118.30
1	A	363	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	513	ASP	CB-CG-OD2	6.25	123.93	118.30
1	B	602	ASP	CB-CG-OD2	6.23	123.90	118.30
1	B	709	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	717	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	647	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	552	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	513	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	602	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	440	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	324	ASP	CB-CG-OD2	5.85	123.56	118.30
1	A	99	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	552	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	124	GLU	CB-CA-C	5.78	121.96	110.40
1	B	117	ASP	CB-CG-OD2	5.67	123.41	118.30
1	B	199	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	709	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	527	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	43	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	273	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	338	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	331	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	199	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	527	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	662	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	33	ARG	NE-CZ-NH2	5.35	122.97	120.30
1	A	89	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	598	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	748	VAL	CB-CA-C	-5.24	101.45	111.40
1	A	165	PHE	N-CA-C	5.14	124.89	111.00
1	A	618	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	274	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	273	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	704	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	490	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	122	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	A	321	PRO	Peptide
1	B	122	ASN	Peptide
1	B	123	GLY	Peptide
1	B	321	PRO	Peptide

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	5853	0	5490	66	0
1	B	5856	0	5498	72	0
2	A	19	0	0	0	0
2	B	44	0	0	0	0
All	All	11772	0	10988	136	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 (136) 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:290:GLN:HE22	1:A:322:ALA:HB3	1.06	1.08
1:B:647:ASP:OD2	1:B:659:HIS:HE1	1.48	0.96
1:A:205:GLU:OE1	1:B:198:HIS:HE1	1.49	0.93
1:A:290:GLN:NE2	1:A:322:ALA:HB3	1.85	0.91
1:A:385:HIS:HD2	1:A:387:THR:H	1.18	0.90
1:B:60:ASP:OD2	1:B:784:HIS:HD2	1.63	0.82
1:A:631:VAL:HG21	1:A:655:GLY:HA3	1.63	0.81
1:A:545:GLN:HE21	1:A:545:GLN:H	1.28	0.80
1:B:167:ASN:HD22	1:B:169:ILE:H	1.30	0.79
1:A:303:ASP:OD1	1:A:305:THR:HG22	1.82	0.79
1:A:543:HIS:HE1	1:A:546:GLY:O	1.66	0.78
1:A:23:HIS:HD2	1:A:25:LYS:H	1.30	0.78
1:A:205:GLU:OE1	1:B:198:HIS:CE1	2.38	0.74
1:B:672:THR:HG23	1:B:704:ASP:O	1.88	0.74
1:A:294:ALA:O	1:A:317:ARG:HD3	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:VAL:HG23	1:B:275:ILE:HG13	1.71	0.71
1:B:747:ARG:HD3	1:B:761:ASP:OD1	1.91	0.70
1:B:167:ASN:ND2	1:B:169:ILE:H	1.90	0.69
1:B:727:ASP:OD1	1:B:730:HIS:HD2	1.77	0.67
1:A:385:HIS:CD2	1:A:387:THR:H	2.07	0.67
1:B:240:THR:HG22	1:B:243:PHE:H	1.59	0.67
1:B:518:ARG:HD3	1:B:539:MET:O	1.96	0.66
1:B:647:ASP:OD2	1:B:659:HIS:CE1	2.40	0.66
1:A:266:ASN:HD22	1:A:268:THR:H	1.44	0.65
1:A:567:GLN:HE22	1:A:572:TRP:HE1	1.44	0.64
1:A:23:HIS:CD2	1:A:25:LYS:H	2.13	0.64
1:A:557:GLN:NE2	1:A:603:GLY:HA2	2.15	0.62
1:A:345:PRO:HG2	1:A:348:LEU:HD11	1.81	0.61
1:B:683:PRO:HA	1:B:696:SER:HA	1.83	0.61
1:B:553:ALA:O	1:B:554:SER:HB3	2.01	0.61
1:A:454:LYS:HE3	1:A:642:PRO:O	2.01	0.60
1:B:167:ASN:HD21	1:B:170:GLY:H	1.49	0.60
1:B:641:ASN:HD22	1:B:643:TRP:H	1.51	0.58
1:A:545:GLN:NE2	1:A:545:GLN:H	1.97	0.58
1:B:553:ALA:O	1:B:554:SER:CB	2.52	0.57
1:A:185:TYR:CE2	1:A:244:LEU:HD21	2.39	0.57
1:B:660:SER:HB2	1:B:666:SER:O	2.05	0.56
1:B:98:GLU:OE1	1:B:151:ARG:NH2	2.38	0.56
1:B:60:ASP:OD2	1:B:784:HIS:CD2	2.51	0.56
1:B:262:VAL:CG2	1:B:275:ILE:HG13	2.36	0.55
1:B:322:ALA:HA	1:B:350:GLY:O	2.06	0.55
1:B:406:ASN:HD21	1:B:408:GLU:HB2	1.71	0.55
1:B:132:ASN:C	1:B:132:ASN:HD22	2.11	0.55
1:A:262:VAL:HG21	1:A:312:VAL:HG11	1.88	0.54
1:B:107:TYR:CE2	1:B:153:LYS:HG3	2.42	0.53
1:B:132:ASN:HD22	1:B:134:ASN:H	1.56	0.53
1:A:567:GLN:NE2	1:A:572:TRP:HE1	2.06	0.53
1:A:717:ASP:OD2	1:A:721:THR:OG1	2.23	0.52
1:A:453:PRO:HG2	1:A:457:ALA:O	2.09	0.52
1:A:543:HIS:CE1	1:A:546:GLY:O	2.55	0.52
1:B:552:ASP:OD1	1:B:553:ALA:O	2.29	0.51
1:B:699:PHE:CE1	1:B:714:ARG:HG3	2.45	0.51
1:A:107:TYR:CZ	1:A:153:LYS:HG2	2.46	0.51
1:B:683:PRO:CA	1:B:696:SER:HA	2.41	0.51
1:A:521:TYR:CE1	1:A:577:TYR:HB3	2.47	0.50
1:B:132:ASN:ND2	1:B:134:ASN:H	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:GLN:HE22	1:A:603:GLY:HA2	1.75	0.50
1:B:498:PHE:CD1	1:B:554:SER:HA	2.46	0.50
1:A:375:GLY:HA3	1:A:485:GLN:NE2	2.26	0.50
1:A:25:LYS:HD2	1:A:73:PRO:O	2.11	0.50
1:A:322:ALA:HA	1:A:350:GLY:O	2.12	0.50
1:B:557:GLN:OE1	1:B:603:GLY:HA2	2.12	0.50
1:A:631:VAL:CG2	1:A:655:GLY:HA3	2.38	0.49
1:B:183:THR:OG1	1:B:198:HIS:HD2	1.95	0.49
1:A:370:LEU:HD21	1:A:417:THR:HG21	1.95	0.49
1:B:185:TYR:CE2	1:B:244:LEU:HD11	2.47	0.49
1:A:287:TYR:HB3	1:A:322:ALA:HB2	1.95	0.48
1:B:167:ASN:C	1:B:167:ASN:HD22	2.16	0.48
1:A:123:GLY:HA3	1:A:236:LYS:HE2	1.96	0.48
1:B:167:ASN:ND2	1:B:170:GLY:H	2.10	0.48
1:B:518:ARG:CD	1:B:539:MET:O	2.62	0.47
1:A:54:ASP:OD2	1:A:755:ARG:NH1	2.47	0.47
1:B:95:TYR:HB3	1:B:104:PHE:CD2	2.49	0.47
1:A:137:TRP:CZ3	1:A:158:VAL:HG21	2.49	0.47
1:B:309:ARG:HA	1:B:329:SER:O	2.15	0.47
1:A:150:ASP:HB2	1:A:153:LYS:HE2	1.96	0.47
1:B:750:LEU:N	1:B:750:LEU:HD12	2.30	0.46
1:B:124:GLU:OE2	1:B:124:GLU:HA	2.14	0.46
1:B:140:THR:O	1:B:170:GLY:HA3	2.15	0.46
1:A:439:ILE:O	1:A:439:ILE:HG13	2.15	0.46
1:A:699:PHE:CE2	1:A:748:VAL:HG22	2.51	0.46
1:A:287:TYR:CB	1:A:322:ALA:HB2	2.46	0.46
1:A:403:ASP:HB3	1:A:406:ASN:O	2.15	0.46
1:B:699:PHE:CZ	1:B:714:ARG:HG3	2.51	0.46
1:B:43:ASP:HB2	1:B:50:ILE:CD1	2.46	0.45
1:A:266:ASN:ND2	1:A:268:THR:H	2.13	0.45
1:B:715:SER:HB2	1:B:722:TRP:CE3	2.51	0.45
1:B:641:ASN:ND2	1:B:643:TRP:H	2.15	0.45
1:B:454:LYS:NZ	1:B:496:GLY:O	2.37	0.45
1:B:454:LYS:HE3	1:B:642:PRO:O	2.17	0.45
1:A:306:ASN:HD22	1:A:306:ASN:C	2.19	0.45
1:A:294:ALA:O	1:A:317:ARG:CD	2.61	0.44
1:B:498:PHE:HD1	1:B:554:SER:HA	1.82	0.44
1:B:132:ASN:HD21	1:B:134:ASN:HB2	1.82	0.44
1:B:750:LEU:CD1	1:B:750:LEU:N	2.81	0.44
1:A:95:TYR:HB3	1:A:104:PHE:CD1	2.53	0.44
1:B:608:THR:HG23	1:B:638:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:ASP:HB3	1:B:406:ASN:O	2.18	0.43
1:A:124:GLU:OE1	1:A:124:GLU:HA	2.18	0.43
1:B:162:PRO:HD3	1:B:204:TRP:HB2	2.01	0.43
1:A:631:VAL:HG13	1:A:658:PHE:CZ	2.54	0.43
1:A:746:GLY:HA3	1:A:762:LEU:HD22	2.01	0.43
1:A:785:CYS:O	1:A:786:TYR:CB	2.67	0.43
1:A:265:GLN:HG3	1:A:272:TRP:CE2	2.54	0.42
1:A:495:ALA:HB3	1:A:498:PHE:O	2.18	0.42
1:B:123:GLY:HA2	1:B:172:THR:O	2.19	0.42
1:B:346:SER:CB	1:B:347:ASN:HD22	2.33	0.42
1:B:473:ASP:OD2	1:B:476:LYS:HG3	2.18	0.42
1:A:713:TYR:CE2	1:A:724:ARG:HD3	2.54	0.42
1:B:283:SER:HA	1:B:284:PRO:C	2.39	0.42
1:B:318:ASP:OD2	1:B:319:PRO:HA	2.20	0.42
1:B:290:GLN:OE1	1:B:322:ALA:HB3	2.20	0.42
1:A:249:ALA:HA	1:A:259:PHE:O	2.20	0.42
1:B:470:LYS:NZ	1:B:527:ASP:OD2	2.44	0.42
1:B:81:LEU:HB2	1:B:95:TYR:HB2	2.01	0.42
1:A:306:ASN:HD21	1:A:308:ASN:HB2	1.84	0.42
1:B:11:ILE:HG21	1:B:445:ASN:ND2	2.35	0.42
1:B:43:ASP:HB2	1:B:50:ILE:HD12	2.02	0.42
1:B:98:GLU:CD	1:B:151:ARG:HH22	2.23	0.42
1:A:371:ASP:OD1	1:A:373:ASN:N	2.45	0.41
1:A:743:LYS:HB2	1:A:743:LYS:HE2	1.91	0.41
1:A:98:GLU:OE1	1:A:151:ARG:NH2	2.50	0.41
1:B:540:ASN:HD22	1:B:542:SER:H	1.68	0.41
1:B:637:MET:HA	1:B:638:PRO:HD3	1.89	0.41
1:A:66:THR:HG23	1:A:83:GLN:NE2	2.36	0.41
1:A:601:GLN:HB2	1:A:645:ALA:HB1	2.02	0.41
1:A:412:TYR:CZ	1:A:419:TRP:HB2	2.54	0.41
1:B:161:ILE:HA	1:B:162:PRO:HD3	1.97	0.41
1:B:571:PRO:HG2	1:B:595:VAL:HG11	2.02	0.41
1:A:191:PRO:HD3	1:A:233:GLN:OE1	2.20	0.41
1:A:771:LYS:HB3	1:A:771:LYS:HE3	1.86	0.41
1:A:146:TRP:NE1	1:A:157:ASN:ND2	2.64	0.41
1:B:123:GLY:CA	1:B:172:THR:O	2.69	0.41
1:A:40:TYR:CE1	1:A:442:ILE:HA	2.56	0.41
1:B:35:ASP:HB3	1:B:120:ARG:HD2	2.04	0.40
1:A:454:LYS:HD2	1:A:599:LYS:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	764/789 (97%)	720 (94%)	40 (5%)	4 (0%)	32	34
1	B	765/789 (97%)	727 (95%)	36 (5%)	2 (0%)	44	49
All	All	1529/1578 (97%)	1447 (95%)	76 (5%)	6 (0%)	38	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	PHE
1	A	322	ALA
1	B	322	ALA
1	A	124	GLU
1	A	289	ASN
1	B	124	GLU

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	608/625 (97%)	564 (93%)	44 (7%)	17	18
1	B	609/625 (97%)	565 (93%)	44 (7%)	17	18
All	All	1217/1250 (97%)	1129 (93%)	88 (7%)	17	18

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	67	GLU
1	A	81	LEU
1	A	98	GLU
1	A	105	THR
1	A	124	GLU
1	A	161	ILE
1	A	163	ASP
1	A	167	ASN
1	A	226	LYS
1	A	244	LEU
1	A	265	GLN
1	A	266	ASN
1	A	306	ASN
1	A	315	LEU
1	A	317	ARG
1	A	328	LEU
1	A	344	SER
1	A	390	LEU
1	A	401	LEU
1	A	451	ARG
1	A	469	MET
1	A	485	GLN
1	A	507	SER
1	A	540	ASN
1	A	545	GLN
1	A	552	ASP
1	A	561	SER
1	A	589	LYS
1	A	599	LYS
1	A	621	LYS
1	A	666	SER
1	A	668	THR
1	A	670	VAL
1	A	705	LYS
1	A	728	GLN
1	A	748	VAL
1	A	750	LEU
1	A	755	ARG
1	A	762	LEU
1	A	763	THR
1	A	764	ASN
1	A	770	GLU

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Mol	Chain	Res	Type
1	A	781	LYS
1	B	3	HIS
1	B	7	LYS
1	B	33	ARG
1	B	67	GLU
1	B	98	GLU
1	B	124	GLU
1	B	132	ASN
1	B	149	SER
1	B	156	THR
1	B	167	ASN
1	B	179	GLU
1	B	180	ARG
1	B	226	LYS
1	B	240	THR
1	B	262	VAL
1	B	406	ASN
1	B	451	ARG
1	B	469	MET
1	B	518	ARG
1	B	540	ASN
1	B	552	ASP
1	B	554	SER
1	B	565	ASP
1	B	567	GLN
1	B	596	LEU
1	B	641	ASN
1	B	666	SER
1	B	668	THR
1	B	669	ARG
1	B	674	ASN
1	B	684	LYS
1	B	685	SER
1	B	693	SER
1	B	696	SER
1	B	708	SER
1	B	723	THR
1	B	728	GLN
1	B	737	MET
1	B	744	VAL
1	B	747	ARG
1	B	750	LEU

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Mol	Chain	Res	Type
1	B	761	ASP
1	B	771	LYS
1	B	780	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	83	GLN
1	A	198	HIS
1	A	242	ASN
1	A	265	GLN
1	A	266	ASN
1	A	290	GLN
1	A	306	ASN
1	A	308	ASN
1	A	377	GLN
1	A	385	HIS
1	A	485	GLN
1	A	510	HIS
1	A	540	ASN
1	A	543	HIS
1	A	545	GLN
1	A	557	GLN
1	A	567	GLN
1	A	601	GLN
1	A	764	ASN
1	A	784	HIS
1	B	132	ASN
1	B	134	ASN
1	B	167	ASN
1	B	198	HIS
1	B	242	ASN
1	B	341	GLN
1	B	347	ASN
1	B	357	ASN
1	B	377	GLN
1	B	406	ASN
1	B	438	GLN
1	B	445	ASN
1	B	540	ASN
1	B	641	ASN

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Mol	Chain	Res	Type
1	B	659	HIS
1	B	674	ASN
1	B	718	ASN
1	B	728	GLN
1	B	730	HIS
1	B	784	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](#)

There are no ligands in this entry.

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	770/789 (97%)	-0.19	9 (1%) 79 77	25, 36, 48, 63	0
1	B	771/789 (97%)	-0.25	4 (0%) 90 90	23, 34, 55, 65	0
All	All	1541/1578 (97%)	-0.22	13 (0%) 86 85	23, 35, 53, 65	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	764	ASN	3.2
1	B	3	HIS	3.1
1	B	685	SER	3.0
1	B	568	ALA	3.0
1	A	786	TYR	2.4
1	A	770	GLU	2.4
1	A	781	LYS	2.3
1	A	514	SER	2.3
1	A	226	LYS	2.3
1	A	565	ASP	2.2
1	A	165	PHE	2.1
1	B	707	GLY	2.1
1	A	220	GLY	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.