



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:41 AM UTC

PDB ID : 3OTT / pdb_00003ott
Title : Crystal Structure of the extracellular domain of the putative one component system BT4673 from *B. thetaiotaomicron*
Authors : Zhang, Z.; Liu, Q.; Hendrickson, W.A.
Deposited on : 2010-09-13
Resolution : 2.30 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

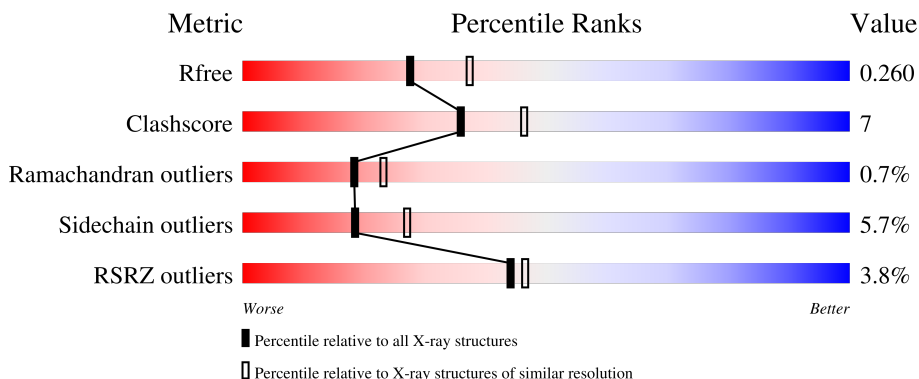
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	758	 6% 78% 16% ...
1	B	758	 % 80% 15% ..

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 12329 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.

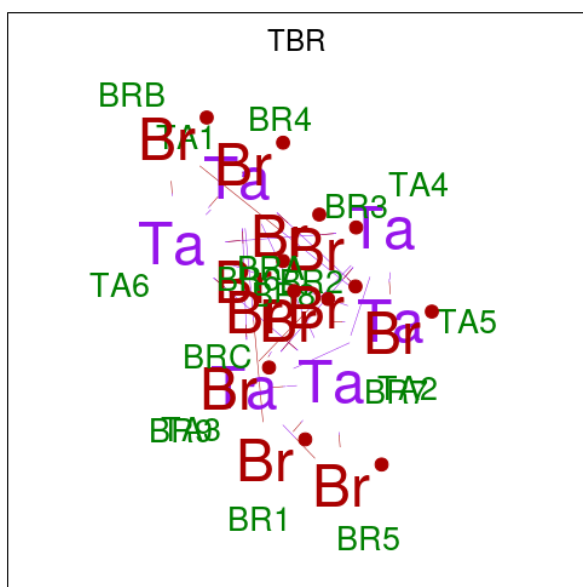
- Molecule 1 is a protein called Two-component system sensor histidine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	737	6002	3810	1030	1145	17	0	0	0
1	B	739	6011	3815	1028	1151	17	0	2	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	28	MET	-	expression tag	UNP Q89YQ8
A	29	GLU	-	expression tag	UNP Q89YQ8
A	778	LEU	-	expression tag	UNP Q89YQ8
A	779	GLU	-	expression tag	UNP Q89YQ8
A	780	HIS	-	expression tag	UNP Q89YQ8
A	781	HIS	-	expression tag	UNP Q89YQ8
A	782	HIS	-	expression tag	UNP Q89YQ8
A	783	HIS	-	expression tag	UNP Q89YQ8
A	784	HIS	-	expression tag	UNP Q89YQ8
A	785	HIS	-	expression tag	UNP Q89YQ8
B	28	MET	-	expression tag	UNP Q89YQ8
B	29	GLU	-	expression tag	UNP Q89YQ8
B	778	LEU	-	expression tag	UNP Q89YQ8
B	779	GLU	-	expression tag	UNP Q89YQ8
B	780	HIS	-	expression tag	UNP Q89YQ8
B	781	HIS	-	expression tag	UNP Q89YQ8
B	782	HIS	-	expression tag	UNP Q89YQ8
B	783	HIS	-	expression tag	UNP Q89YQ8
B	784	HIS	-	expression tag	UNP Q89YQ8
B	785	HIS	-	expression tag	UNP Q89YQ8

- Molecule 2 is HEXATANTALUM DODECABROMIDE (CCD ID: TBR) (formula: Br₁₂Ta₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Br	Ta	0	0
			18	12	6		
2	B	1	Total	Br	Ta	0	0
			18	12	6		

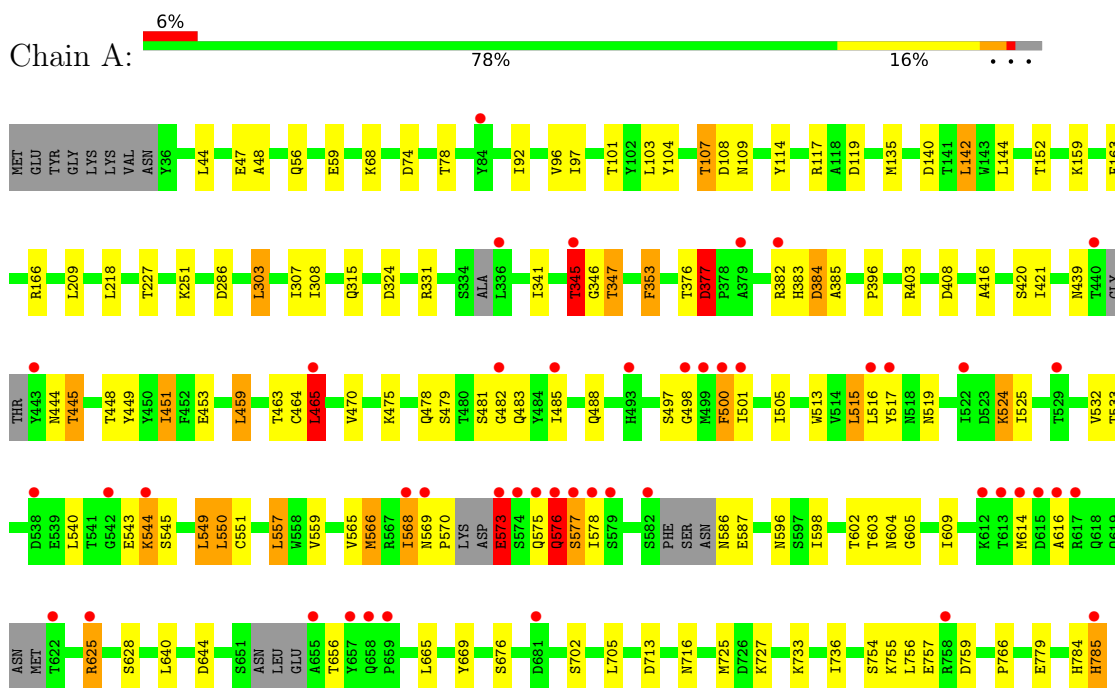
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	138	Total	O	0	0
			138	138		
3	B	142	Total	O	0	0
			142	142		

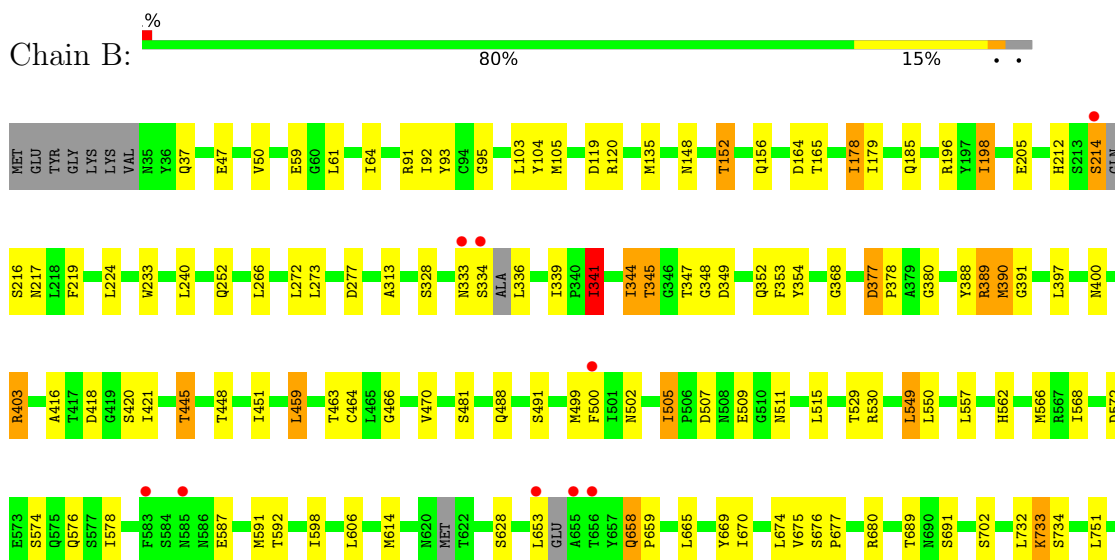
3 Residue-property plots [i](#)

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: Two-component system sensor histidine kinase



- Molecule 1: Two-component system sensor histidine kinase



D759	S763	N764	R765	P766	I773	W777	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.17Å 88.17Å 432.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.27 – 2.30 39.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (39.27-2.30) 99.0 (39.27-2.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.29Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.195 , 0.253 0.204 , 0.260	Depositor DCC
R_{free} test set	3840 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtrriage
Anisotropy	0.275	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12329	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: TBR

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	1.03	4/6153 (0.1%)	1.03	9/8355 (0.1%)
1	B	1.16	3/6165 (0.0%)	1.14	17/8372 (0.2%)
All	All	1.10	7/12318 (0.1%)	1.08	26/16727 (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
1	B	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	614	MET	C-N	10.14	1.47	1.33
1	A	573	GLU	C-N	9.52	1.47	1.33
1	A	614	MET	C-O	6.47	1.32	1.24
1	B	313	ALA	CA-CB	6.31	1.61	1.53
1	A	587	GLU	N-CA	6.05	1.52	1.45
1	B	240	LEU	CA-C	5.85	1.59	1.52
1	B	64	ILE	CA-CB	5.10	1.60	1.54

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	GLU	N-CA-C	8.55	123.67	110.42
1	B	344	ILE	CA-C-N	8.43	137.65	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	344	ILE	C-N-CA	8.43	137.65	121.54
1	B	341	ILE	CB-CA-C	-8.30	98.82	112.26
1	A	345	THR	CB-CA-C	-8.14	99.47	110.79
1	B	164	ASP	N-CA-C	7.46	118.11	108.34
1	B	344	ILE	N-CA-C	7.39	124.71	109.34
1	A	444	ASN	N-CA-C	6.72	116.86	108.19
1	B	212	HIS	N-CA-C	6.69	118.57	111.28
1	B	403	ARG	NE-CZ-NH2	-6.28	113.55	119.20
1	B	148	ASN	N-CA-C	6.24	118.87	110.88
1	B	481	SER	N-CA-C	5.99	118.76	111.82
1	B	344	ILE	O-C-N	-5.98	115.10	122.57
1	A	353	PHE	N-CA-C	5.96	117.91	108.67
1	A	92	ILE	CB-CA-C	-5.80	102.95	110.84
1	B	219	PHE	CB-CA-C	-5.78	100.89	109.90
1	A	577	SER	N-CA-C	5.61	117.14	109.18
1	A	396	PRO	N-CA-C	5.58	120.06	111.57
1	A	117	ARG	CG-CD-NE	-5.42	100.08	112.00
1	A	576	GLN	N-CA-C	5.42	115.71	108.23
1	B	377	ASP	CA-C-N	5.37	125.08	119.82
1	B	377	ASP	C-N-CA	5.37	125.08	119.82
1	B	658	GLN	CA-C-N	5.18	125.11	119.78
1	B	658	GLN	C-N-CA	5.18	125.11	119.78
1	B	198	ILE	CA-C-N	-5.06	114.61	119.87
1	B	198	ILE	C-N-CA	-5.06	114.61	119.87

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	573	GLU	Mainchain
1	B	344	ILE	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	6002	0	5719	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6011	0	5748	76	0
2	A	18	0	0	2	0
2	B	18	0	0	1	0
3	A	138	0	0	1	0
3	B	142	0	0	4	0
All	All	12329	0	11467	171	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 7.

All (171) 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:616:ALA:HB2	3:A:799:HOH:O	1.47	1.14
1:A:107:THR:HG22	1:A:109:ASN:H	1.09	1.11
1:A:345:THR:HG23	1:A:385:ALA:HB3	1.15	1.08
1:A:345:THR:CG2	1:A:385:ALA:HB3	1.86	1.03
1:B:507:ASP:HB3	1:B:509:GLU:H	1.25	1.02
1:A:602:THR:HG22	1:A:605:GLY:O	1.65	0.96
1:B:502:ASN:HB2	1:B:515:LEU:HD12	1.51	0.89
1:B:333:ASN:HA	3:B:831:HOH:O	1.74	0.86
1:A:107:THR:HG22	1:A:109:ASN:N	1.90	0.84
1:A:420:SER:OG	1:A:445:THR:HG23	1.76	0.84
1:A:345:THR:HG23	1:A:385:ALA:CB	2.05	0.83
1:B:416:ALA:HB1	1:B:448:THR:HG22	1.62	0.82
1:B:732:LEU:O	1:B:733:LYS:CB	2.29	0.81
1:B:104:TYR:O	1:B:135:MET:HE1	1.82	0.80
1:A:331:ARG:NH1	1:A:713:ASP:OD1	2.16	0.79
1:A:47:GLU:HG3	1:A:68:LYS:HG3	1.65	0.76
1:A:346:GLY:HA2	1:A:347:THR:O	1.85	0.75
1:B:345:THR:HG22	1:B:347:THR:H	1.52	0.75
1:A:464:CYS:O	1:A:464:CYS:SG	2.44	0.75
1:A:513:TRP:CZ2	1:A:524:LYS:HD3	2.22	0.75
1:A:586:ASN:N	1:A:604:ASN:HD21	1.85	0.74
1:B:334:SER:HB2	1:B:336:LEU:N	2.04	0.73
1:B:152:THR:HG22	3:B:895:HOH:O	1.89	0.73
1:A:566:MET:HE3	1:A:568:ILE:HD11	1.71	0.72
1:B:670:ILE:HD12	1:B:675:VAL:HG21	1.70	0.72
1:A:602:THR:HG23	1:A:604:ASN:H	1.56	0.71
1:A:565:VAL:HG21	1:A:609:ILE:HD13	1.74	0.70
1:B:591:MET:HE2	1:B:598:ILE:HD11	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:732:LEU:O	1:B:733:LYS:HB2	1.92	0.69
1:A:420:SER:OG	1:A:445:THR:CG2	2.42	0.68
1:B:341:ILE:O	1:B:345:THR:HB	1.94	0.68
1:A:525:ILE:HG12	1:A:532:VAL:HG22	1.77	0.66
1:B:119:ASP:OD2	1:B:676:SER:HB2	1.96	0.66
1:B:214:SER:HG	1:B:216:SER:N	1.95	0.65
1:B:152:THR:HG21	3:B:6:HOH:O	1.98	0.64
1:A:56:GLN:OE1	1:A:315:GLN:HG2	1.99	0.63
1:B:198:ILE:HD11	1:B:205:GLU:HB2	1.80	0.62
1:B:420:SER:OG	1:B:445:THR:HG23	1.98	0.62
1:A:463:THR:HG22	1:A:465:LEU:H	1.64	0.62
1:A:481:SER:O	1:A:483:GLN:N	2.33	0.62
1:A:602:THR:HG23	1:A:604:ASN:N	2.15	0.61
1:A:114:TYR:OH	1:A:119:ASP:OD1	2.18	0.61
1:A:403:ARG:NH2	1:B:156:GLN:O	2.33	0.61
1:A:549:LEU:HD23	1:A:559:VAL:HG22	1.81	0.60
1:A:498:GLY:HA3	1:A:500:PHE:CE2	2.36	0.60
1:B:566:MET:CE	1:B:568:ILE:HD11	2.32	0.59
1:A:513:TRP:CE2	1:A:524:LYS:HD3	2.37	0.59
1:A:602:THR:HG22	1:A:605:GLY:H	1.68	0.59
1:B:334:SER:CB	1:B:336:LEU:N	2.66	0.59
1:A:565:VAL:HG21	1:A:609:ILE:CD1	2.31	0.59
1:B:95:GLY:HA2	1:B:135:MET:CE	2.32	0.58
1:B:390:MET:HE3	1:B:391:GLY:H	1.68	0.58
1:A:568:ILE:HA	1:A:575:GLN:HB2	1.85	0.58
1:A:377:ASP:O	1:A:383:HIS:ND1	2.37	0.57
1:B:591:MET:HE2	1:B:598:ILE:CD1	2.34	0.57
1:B:416:ALA:CB	1:B:448:THR:HG22	2.34	0.56
1:A:107:THR:CG2	1:A:109:ASN:H	2.01	0.56
1:A:500:PHE:O	1:A:517:TYR:HB3	2.06	0.55
1:A:602:THR:CG2	1:A:605:GLY:H	2.19	0.55
1:A:784:HIS:O	1:A:785:HIS:HB2	2.07	0.54
1:B:352:GLN:O	1:B:368:GLY:HA3	2.08	0.54
1:A:451:ILE:HD11	1:A:459:LEU:HG	1.89	0.54
1:A:315:GLN:HG3	2:A:1:TBR:BRC	2.64	0.53
1:A:97:ILE:HG12	1:A:103:LEU:HD23	1.90	0.53
1:A:119:ASP:OD2	1:A:676:SER:HB2	2.08	0.53
1:A:505:ILE:HG21	1:A:551:CYS:HB2	1.92	0.52
1:B:689:THR:HG22	1:B:691:SER:H	1.75	0.52
1:A:470:VAL:HB	1:A:488:GLN:HB2	1.92	0.52
1:B:591:MET:CE	1:B:598:ILE:HD11	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:LYS:H	1:A:544:LYS:HD2	1.75	0.51
1:B:390:MET:HE3	1:B:391:GLY:N	2.25	0.51
1:A:159:LYS:HE2	1:B:587:GLU:OE2	2.11	0.51
1:A:96:VAL:HG12	1:A:135:MET:HE3	1.91	0.51
1:A:96:VAL:HG12	1:A:135:MET:CE	2.41	0.50
1:A:104:TYR:O	1:A:135:MET:HE1	2.10	0.50
1:B:389:ARG:HB2	1:B:400:ASN:OD1	2.10	0.50
1:B:463:THR:HG22	1:B:464:CYS:O	2.11	0.50
1:A:550:LEU:HD12	1:A:550:LEU:C	2.36	0.50
1:A:341:ILE:HG13	1:A:644:ASP:C	2.37	0.50
1:A:140:ASP:OD2	1:B:354:TYR:OH	2.25	0.49
1:B:507:ASP:HB2	1:B:511:ASN:H	1.77	0.49
1:A:44:LEU:HD23	1:A:78:THR:HG21	1.94	0.49
1:B:502:ASN:HB2	1:B:515:LEU:CD1	2.33	0.49
1:B:224:LEU:HD21	1:B:266:LEU:HG	1.95	0.49
1:B:764:ASN:C	1:B:766:PRO:HD3	2.38	0.49
1:A:97:ILE:HG12	1:A:103:LEU:CD2	2.42	0.49
1:A:716:ASN:CG	1:A:755:LYS:HE3	2.38	0.49
1:A:251:LYS:NZ	1:A:286:ASP:OD1	2.43	0.48
1:A:449:TYR:CE1	1:A:464:CYS:HB2	2.48	0.48
1:B:566:MET:HE3	1:B:568:ILE:HD11	1.93	0.48
1:A:408:ASP:HB2	1:A:453:GLU:OE2	2.13	0.48
1:B:732:LEU:O	1:B:733:LYS:HB3	2.10	0.48
1:B:515:LEU:C	1:B:515:LEU:HD13	2.38	0.48
1:B:347:THR:HG22	1:B:349:ASP:H	1.79	0.48
1:B:47:GLU:O	1:B:47:GLU:HG3	2.13	0.47
1:A:565:VAL:CG2	1:A:609:ILE:HD13	2.43	0.47
1:B:185:GLN:NE2	1:B:196:ARG:HD2	2.29	0.47
1:A:303:LEU:HD11	1:A:308:ILE:HD11	1.97	0.47
1:A:516:LEU:HB3	1:A:519:ASN:HB3	1.95	0.47
1:A:142:LEU:HD13	1:A:144:LEU:HD21	1.97	0.47
1:B:403:ARG:HD2	1:B:418:ASP:OD1	2.15	0.47
1:B:578:ILE:HG12	1:B:614:MET:HE2	1.97	0.47
1:A:733:LYS:HB2	1:A:736:ILE:HD12	1.97	0.47
1:B:529:THR:O	1:B:530:ARG:HB2	2.15	0.47
1:A:640:LEU:HD12	1:A:640:LEU:N	2.30	0.46
1:B:59:GLU:HA	2:B:2:TBR:BR8	2.71	0.46
1:A:346:GLY:HA2	1:A:347:THR:C	2.40	0.46
1:A:353:PHE:O	1:A:628:SER:HB2	2.15	0.46
1:A:603:THR:O	1:A:625:ARG:HG2	2.16	0.46
1:B:50:VAL:HG11	1:B:91[A]:ARG:HH21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:MET:HB3	1:B:598:ILE:HD11	1.98	0.46
1:A:577:SER:O	1:A:578:ILE:HG23	2.16	0.46
1:B:763:SER:OG	1:B:764:ASN:N	2.49	0.46
1:A:550:LEU:HD12	1:A:550:LEU:O	2.15	0.46
1:B:421:ILE:HG22	1:B:448:THR:HG21	1.98	0.46
1:B:669:TYR:HB2	1:B:702:SER:HB2	1.97	0.46
1:B:95:GLY:HA2	1:B:135:MET:HE1	1.97	0.46
1:A:107:THR:CG2	1:A:108:ASP:N	2.78	0.46
1:B:463:THR:HG22	1:B:466:GLY:H	1.81	0.46
1:A:540:LEU:HD11	1:A:566:MET:HE2	1.98	0.45
1:A:705:LEU:C	1:A:705:LEU:HD12	2.41	0.45
1:A:416:ALA:HB1	1:A:448:THR:HG22	1.98	0.45
1:B:388:TYR:HB3	1:B:397:LEU:HG	1.97	0.45
1:A:566:MET:CE	1:A:568:ILE:HD11	2.44	0.45
1:B:470:VAL:HB	1:B:488:GLN:HB2	1.97	0.45
1:A:421:ILE:HG22	1:A:448:THR:HG21	1.97	0.45
1:A:74:ASP:OD1	1:A:74:ASP:C	2.57	0.45
1:A:152:THR:HG23	1:A:163:PHE:HE1	1.82	0.45
1:A:557:LEU:HD13	1:A:570:PRO:HG3	1.98	0.45
1:B:347:THR:HG22	1:B:348:GLY:N	2.32	0.45
1:B:380:GLY:HA2	3:B:819:HOH:O	2.16	0.45
1:B:451:ILE:HD11	1:B:459:LEU:HG	1.98	0.45
1:A:543:GLU:C	1:A:545:SER:H	2.25	0.44
1:B:92:ILE:HG23	1:B:105:MET:HB3	1.98	0.44
1:A:59:GLU:HA	2:A:1:TBR:BR1	2.72	0.44
1:A:565:VAL:HG22	1:A:578:ILE:HD11	1.99	0.44
1:B:658:GLN:HA	1:B:659:PRO:HD2	1.77	0.44
1:A:544:LYS:HD2	1:A:544:LYS:N	2.34	0.43
1:B:591:MET:CE	1:B:598:ILE:CD1	2.96	0.43
1:A:47:GLU:CG	1:A:48:ALA:N	2.81	0.43
1:B:572:ASP:CG	1:B:574:SER:HB2	2.44	0.43
1:A:345:THR:O	1:A:347:THR:HB	2.19	0.43
1:A:382:ARG:O	1:A:384:ASP:N	2.47	0.43
1:B:119:ASP:OD2	1:B:677:PRO:HD2	2.19	0.42
1:B:562:HIS:NE2	1:B:587:GLU:HG2	2.34	0.42
1:A:376:THR:O	1:A:383:HIS:HA	2.18	0.42
1:A:463:THR:HG22	1:A:464:CYS:N	2.34	0.42
1:B:421:ILE:CG2	1:B:448:THR:HG21	2.50	0.42
1:A:586:ASN:N	1:A:604:ASN:ND2	2.61	0.42
1:A:754:SER:OG	1:A:766:PRO:HB3	2.19	0.42
1:A:459:LEU:HD12	1:A:459:LEU:HA	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:TYR:HB2	1:A:702:SER:HB2	2.01	0.42
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.87	0.42
1:A:515:LEU:C	1:A:515:LEU:HD13	2.44	0.42
1:B:178:ILE:HG13	1:B:179:ILE:N	2.34	0.42
1:A:307:ILE:HB	1:A:324:ASP:HB2	2.00	0.42
1:A:569:ASN:OD1	1:A:569:ASN:C	2.64	0.41
1:A:209:LEU:HB2	1:A:218:LEU:HD21	2.02	0.41
1:A:569:ASN:H	1:A:575:GLN:HG2	1.85	0.41
1:B:353:PHE:O	1:B:628:SER:HB2	2.21	0.41
1:A:119:ASP:O	1:A:119:ASP:CG	2.63	0.41
1:A:576:GLN:CD	1:A:576:GLN:N	2.78	0.41
1:B:505:ILE:HG13	1:B:549:LEU:HD13	2.02	0.41
1:B:91[A]:ARG:HD3	1:B:93:TYR:CE1	2.56	0.41
1:B:566:MET:HE2	1:B:568:ILE:HD11	2.02	0.41
1:B:233:TRP:CE2	1:B:272:LEU:HG	2.56	0.40
1:B:377:ASP:HA	1:B:378:PRO:HD2	1.88	0.40
1:B:390:MET:CE	1:B:391:GLY:N	2.84	0.40
1:A:451:ILE:CD1	1:A:459:LEU:HG	2.50	0.40
1:B:491:SER:HB2	1:B:499:MET:SD	2.61	0.40
1:A:451:ILE:HD11	1:A:459:LEU:CG	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	723/758 (95%)	677 (94%)	38 (5%)	8 (1%)	11 13
1	B	731/758 (96%)	698 (96%)	31 (4%)	2 (0%)	36 46
All	All	1454/1516 (96%)	1375 (95%)	69 (5%)	10 (1%)	18 23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	384	ASP
1	A	482	GLY
1	A	656	THR
1	A	347	THR
1	A	439	ASN
1	B	345	THR
1	B	733	LYS
1	A	465	LEU
1	A	101	THR
1	A	377	ASP

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	658/676 (97%)	618 (94%)	40 (6%)	17	24
1	B	660/676 (98%)	625 (95%)	35 (5%)	20	30
All	All	1318/1352 (98%)	1243 (94%)	75 (6%)	18	27

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	THR
1	A	142	LEU
1	A	166	ARG
1	A	227	THR
1	A	303	LEU
1	A	345	THR
1	A	377	ASP
1	A	445	THR
1	A	451	ILE
1	A	459	LEU
1	A	465	LEU
1	A	475	LYS
1	A	478	GLN
1	A	479	SER

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Mol	Chain	Res	Type
1	A	485	ILE
1	A	497	SER
1	A	500	PHE
1	A	501	ILE
1	A	515	LEU
1	A	524	LYS
1	A	533	THR
1	A	544	LYS
1	A	549	LEU
1	A	550	LEU
1	A	557	LEU
1	A	566	MET
1	A	568	ILE
1	A	573	GLU
1	A	576	GLN
1	A	596	ASN
1	A	598	ILE
1	A	625	ARG
1	A	665	LEU
1	A	725	MET
1	A	727	LYS
1	A	756	LEU
1	A	757	GLU
1	A	759	ASP
1	A	779	GLU
1	A	785	HIS
1	B	37	GLN
1	B	61	LEU
1	B	103	LEU
1	B	120	ARG
1	B	152	THR
1	B	165	THR
1	B	178	ILE
1	B	214	SER
1	B	217	ASN
1	B	252	GLN
1	B	273	LEU
1	B	277	ASP
1	B	328	SER
1	B	339	ILE
1	B	341	ILE
1	B	389	ARG

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Mol	Chain	Res	Type
1	B	390	MET
1	B	445	THR
1	B	459	LEU
1	B	500	PHE
1	B	505	ILE
1	B	549	LEU
1	B	550	LEU
1	B	557	LEU
1	B	576	GLN
1	B	592	THR
1	B	606	LEU
1	B	653	LEU
1	B	665	LEU
1	B	674	LEU
1	B	680	ARG
1	B	734	SER
1	B	751	LEU
1	B	759	ASP
1	B	773	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	148	ASN
1	A	249	GLN
1	A	269	ASN
1	A	278	ASN
1	A	310	ASN
1	A	315	GLN
1	A	337	GLN
1	A	404	HIS
1	A	458	GLN
1	A	478	GLN
1	A	488	GLN
1	A	650	HIS
1	A	658	GLN
1	A	716	ASN
1	A	730	ASN
1	A	748	ASN
1	A	782	HIS
1	A	783	HIS

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Mol	Chain	Res	Type
1	B	230	GLN
1	B	242	GLN
1	B	310	ASN
1	B	315	GLN
1	B	383	HIS
1	B	433	HIS
1	B	435	ASN
1	B	508	ASN
1	B	575	GLN
1	B	586	ASN
1	B	730	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TBR	B	2	-	0,36,36	-	-	-		
2	TBR	A	1	-	0,36,36	-	-	-		

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.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	TBR	1	0
2	A	1	TBR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	737/758 (97%)	0.08	47 (6%) 25 27	12, 32, 91, 120	6 (0%)
1	B	739/758 (97%)	-0.34	9 (1%) 76 77	10, 24, 47, 83	2 (0%)
All	All	1476/1516 (97%)	-0.13	56 (3%) 44 46	10, 27, 80, 120	8 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	785	HIS	4.5
1	B	653	LEU	4.4
1	A	440	THR	4.1
1	A	655	ALA	4.1
1	A	615	ASP	3.8
1	B	583	PHE	3.8
1	A	499	MET	3.5
1	A	500	PHE	3.5
1	A	614	MET	3.4
1	A	574	SER	3.2
1	B	655	ALA	3.1
1	A	616	ALA	3.1
1	A	576	GLN	3.0
1	A	345	THR	3.0
1	A	516	LEU	2.9
1	A	517	TYR	2.8
1	A	613	THR	2.6
1	B	333	ASN	2.6
1	A	758	ARG	2.6
1	B	585	ASN	2.6
1	A	657	TYR	2.6
1	A	568	ILE	2.6
1	B	214	SER	2.6
1	A	658	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	538	ASP	2.6
1	A	482	GLY	2.6
1	A	443	TYR	2.6
1	A	579	SER	2.5
1	A	577	SER	2.5
1	B	334	SER	2.5
1	A	544	LYS	2.5
1	A	622	THR	2.4
1	A	522	ILE	2.4
1	A	612	LYS	2.4
1	A	617	ARG	2.4
1	A	573	GLU	2.4
1	A	84	TYR	2.4
1	A	382	ARG	2.4
1	A	379	ALA	2.3
1	B	500	PHE	2.3
1	A	582	SER	2.3
1	A	681	ASP	2.3
1	A	493	HIS	2.3
1	A	485	ILE	2.3
1	A	336	LEU	2.2
1	A	569	ASN	2.2
1	A	542	GLY	2.2
1	A	465	LEU	2.2
1	A	529	THR	2.2
1	A	575	GLN	2.1
1	A	498	GLY	2.1
1	A	625	ARG	2.1
1	A	659	PRO	2.0
1	B	656	THR	2.0
1	A	501	ILE	2.0
1	A	578	ILE	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
2	TBR	A	1	18/18	0.94	0.07	44,51,54,56	18
2	TBR	B	2	18/18	0.98	0.04	30,40,44,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.