



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 02:05 pm GMT

PDB ID : 1OXT  
Title : Crystal structure of GlcV, the ABC-ATPase of the glucose ABC transporter from *Sulfolobus solfataricus*  
Authors : Verdon, G.; Albers, S.V.; Dijkstra, B.W.; Driessen, A.J.; Thunnissen, A.M.  
Deposited on : 2003-04-03  
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](mailto: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.

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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

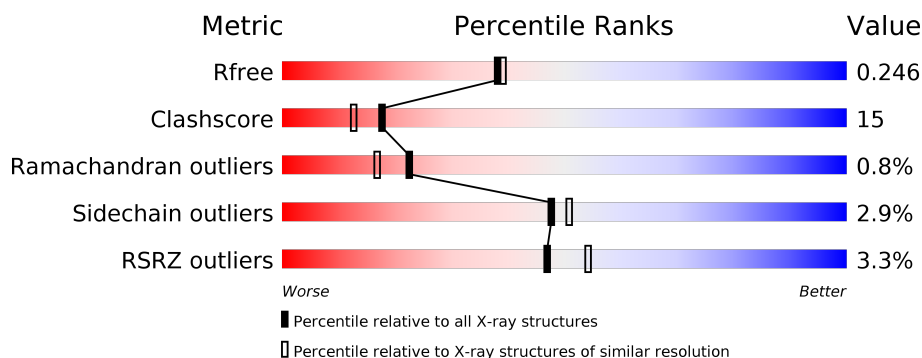
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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  $\geq 3$ , 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	353	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	B	353	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>18%</div> <div>.</div> </div> </div>
1	D	353	<div> <div>5%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8708 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 ABC transporter, ATP binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	5	0
			2702	1729	469	498	6			
1	B	352	Total	C	N	O	S	0	4	0
			2716	1742	471	497	6			
1	D	352	Total	C	N	O	S	0	1	0
			2643	1695	461	481	6			

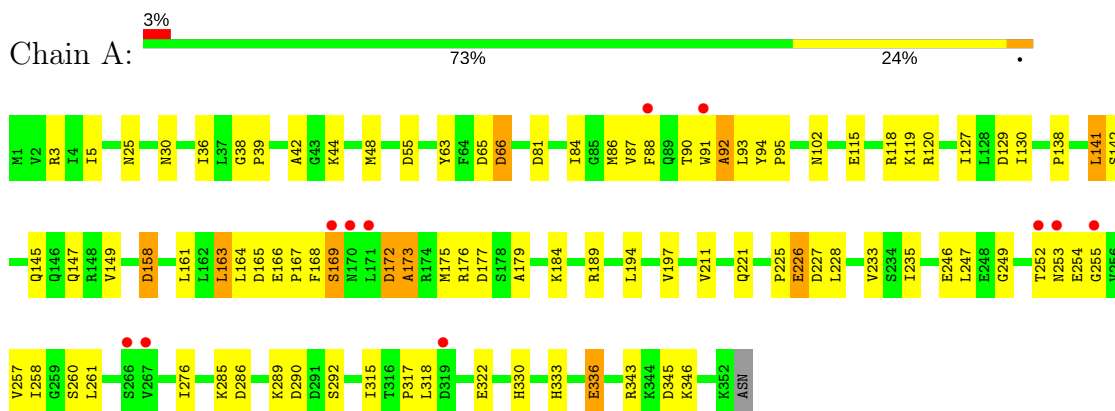
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	254	Total	O	0	4
			258	258		
2	B	230	Total	O	0	2
			232	232		
2	D	157	Total	O	0	0
			157	157		

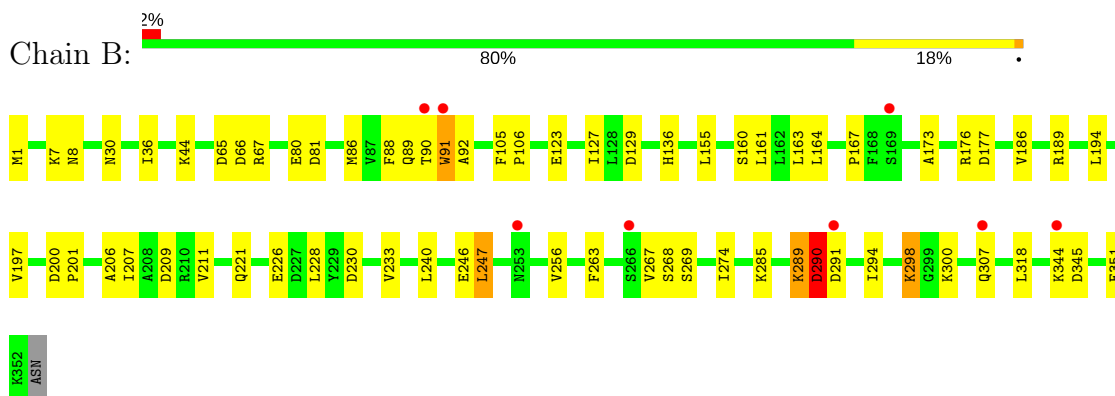
### 3 Residue-property plots

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.

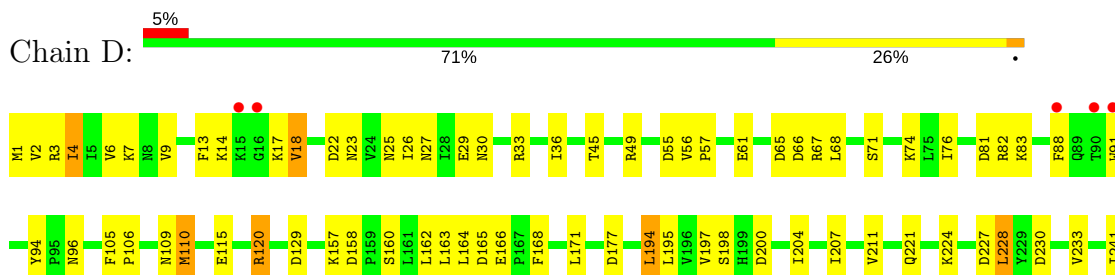
- Molecule 1: ABC transporter, ATP binding protein

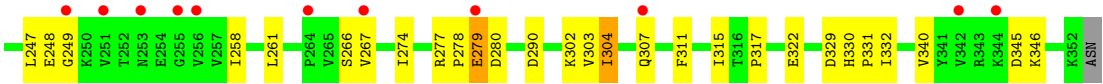


- Molecule 1: ABC transporter, ATP binding protein



- Molecule 1: ABC transporter, ATP binding protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.03Å 146.64Å 178.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.64 – 2.10 45.48 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.64-2.10) 95.4 (45.48-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.69 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.214 , 0.275 0.222 , 0.246	Depositor DCC
$R_{free}$ test set	3570 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 64.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8708	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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 54.51 % 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 3.6133e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> 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

### 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	0.36	0/2774	0.74	12/3752 (0.3%)
1	B	0.36	0/2782	0.71	11/3764 (0.3%)
1	D	0.31	0/2694	0.69	15/3642 (0.4%)
All	All	0.34	0/8250	0.71	38/11158 (0.3%)

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	55	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	290	ASP	CB-CG-OD2	6.13	123.81	118.30
1	D	65	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	200	ASP	CB-CG-OD2	5.65	123.39	118.30
1	D	129	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	158	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	345	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	280	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	345	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	129	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	66	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	81	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	65	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	22	ASP	CB-CG-OD2	5.33	123.10	118.30
1	D	227	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	66	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	81	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	177	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	329	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	158[A]	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	158[B]	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	227	ASP	CB-CG-OD2	5.27	123.04	118.30
1	D	200	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	172	ASP	CB-CG-OD2	5.23	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	165	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	291[A]	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	291[B]	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	65	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	230	ASP	CB-CG-OD2	5.16	122.94	118.30
1	D	230	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	177	ASP	CB-CG-OD2	5.15	122.94	118.30
1	D	345	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	81	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	290	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	66	ASP	CB-CG-OD2	5.08	122.88	118.30
1	D	177	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	286	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	129	ASP	CB-CG-OD2	5.04	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2702	0	2771	91	1
1	B	2716	0	2803	67	0
1	D	2643	0	2683	92	1
2	A	258	0	0	12	0
2	B	232	0	0	7	0
2	D	157	0	0	9	0
All	All	8708	0	8257	250	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 15.

All (250) 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:D:204:ILE:CG2	1:D:211:VAL:HG21	1.72	1.18
1:D:110:MET:HA	1:D:110:MET:CE	1.81	1.10
1:B:344:LYS:HD2	1:B:344:LYS:O	1.53	1.09
1:D:110:MET:HA	1:D:110:MET:HE2	1.32	1.07
1:A:211:VAL:HG13	1:A:228:LEU:HD11	1.33	1.07
1:D:204:ILE:HG23	1:D:211:VAL:HG21	1.32	1.03
1:A:147:GLN:HE22	1:A:179:ALA:HB2	1.23	1.01
1:A:168:PHE:O	1:A:169:SER:O	1.81	0.99
1:D:3:ARG:C	1:D:4:ILE:HD12	1.83	0.98
1:D:304:ILE:H	1:D:304:ILE:HD13	1.27	0.96
1:D:115:GLU:HG2	2:D:482:HOH:O	1.66	0.95
1:B:294:ILE:HG13	1:B:344:LYS:HB2	1.47	0.95
1:D:204:ILE:HG23	1:D:211:VAL:CG2	1.97	0.94
1:B:289:LYS:HA	1:B:289:LYS:HE3	1.50	0.93
1:D:13:PHE:O	1:D:17:LYS:O	1.90	0.89
1:A:94:TYR:H	1:A:102:ASN:HD21	1.13	0.89
1:B:86:MET:HE3	2:B:529:HOH:O	1.71	0.89
1:A:167:PRO:HG2	1:A:168:PHE:CE1	2.08	0.88
1:D:162:LEU:HG	1:D:164:LEU:HD11	1.55	0.87
1:D:67:ARG:HD3	2:D:387:HOH:O	1.75	0.87
1:A:147:GLN:NE2	1:A:179:ALA:HB2	1.89	0.86
1:B:344:LYS:HD2	1:B:344:LYS:C	1.92	0.86
1:B:289:LYS:HE3	1:B:290:ASP:N	1.90	0.86
1:D:29:GLU:HG3	2:D:465:HOH:O	1.76	0.85
1:D:204:ILE:HG21	1:D:211:VAL:HG21	1.54	0.85
1:B:289:LYS:CA	1:B:289:LYS:HE3	2.07	0.84
1:A:175:MET:HA	2:A:534:HOH:O	1.77	0.84
1:A:211:VAL:HG13	1:A:228:LEU:CD1	2.08	0.84
1:D:302:LYS:HE2	2:D:446:HOH:O	1.75	0.83
1:A:167:PRO:HG2	1:A:168:PHE:CD1	2.12	0.83
1:B:289:LYS:CE	1:B:290:ASP:N	2.41	0.82
1:D:224:LYS:O	1:D:228:LEU:HD23	1.80	0.82
1:A:172:ASP:O	1:A:173:ALA:CB	2.28	0.81
1:A:184:LYS:HD2	2:A:588:HOH:O	1.80	0.80
1:B:289:LYS:HE3	1:B:290:ASP:H	1.44	0.78
1:A:211:VAL:CG1	1:A:228:LEU:HD11	2.12	0.78
1:B:209:ASP:OD1	2:B:509:HOH:O	2.03	0.77
1:D:194:LEU:HD13	1:D:194:LEU:C	2.04	0.77
1:A:211:VAL:CG1	1:A:228:LEU:CD1	2.63	0.77
1:B:246:GLU:C	1:B:247:LEU:HD13	2.05	0.76
1:D:194:LEU:HD13	1:D:195:LEU:N	2.01	0.75
1:A:285:LYS:HE2	1:A:336:GLU:HG2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TRP:O	1:A:93:LEU:N	2.19	0.75
1:A:48:MET:SD	1:A:163:LEU:HG	2.27	0.74
1:A:221:GLN:HE22	1:A:233:VAL:H	1.36	0.73
1:A:36:ILE:HB	1:A:197:VAL:HG12	1.71	0.72
1:B:7:LYS:HE2	1:B:8:ASN:HD21	1.54	0.72
1:A:86:MET:HE3	2:A:557:HOH:O	1.90	0.72
1:A:147:GLN:NE2	1:A:179:ALA:CB	2.54	0.71
1:D:304:ILE:H	1:D:304:ILE:CD1	2.04	0.71
1:B:90:THR:C	1:B:92:ALA:H	1.94	0.71
1:D:277:ARG:HB3	1:D:279:GLU:OE1	1.89	0.71
1:D:311:PHE:CE1	1:D:331:PRO:HD3	2.26	0.71
1:B:7:LYS:CD	1:B:8:ASN:ND2	2.54	0.71
1:B:88:PHE:O	1:B:91:TRP:HB3	1.92	0.69
1:A:94:TYR:N	1:A:102:ASN:HD21	1.88	0.69
1:A:173:ALA:HA	1:A:176:ARG:NE	2.07	0.69
1:B:91:TRP:O	1:B:91:TRP:CE3	2.46	0.69
1:D:110:MET:HE3	1:D:110:MET:HA	1.74	0.69
1:A:235:ILE:HD11	1:A:246:GLU:HG2	1.75	0.68
1:D:4:ILE:CD1	1:D:4:ILE:N	2.55	0.68
1:A:261:LEU:HD22	1:A:317:PRO:HG3	1.75	0.68
1:B:246:GLU:O	1:B:247:LEU:HD13	1.93	0.68
1:D:2:VAL:HG13	1:D:4:ILE:HD11	1.74	0.68
1:B:289:LYS:CE	1:B:290:ASP:H	2.03	0.68
1:B:289:LYS:HE2	1:B:290:ASP:N	2.08	0.68
1:D:4:ILE:N	1:D:4:ILE:HD12	2.04	0.67
1:A:221:GLN:NE2	1:A:233:VAL:H	1.92	0.67
1:A:333:HIS:ND1	2:A:426:HOH:O	2.28	0.67
1:A:30:ASN:OD1	2:A:502:HOH:O	2.13	0.66
1:D:162:LEU:HG	1:D:164:LEU:CD1	2.25	0.66
1:D:30:ASN:ND2	2:D:465:HOH:O	2.28	0.66
1:D:110:MET:CA	1:D:110:MET:CE	2.68	0.66
1:A:211:VAL:HG11	1:A:228:LEU:HD12	1.78	0.66
1:D:109:ASN:O	1:D:110:MET:HE3	1.95	0.66
1:A:252:THR:OG1	1:A:257:VAL:CG2	2.43	0.66
1:D:163:LEU:C	1:D:164:LEU:HD12	2.17	0.64
1:D:88:PHE:O	1:D:91:TRP:HB3	1.97	0.64
1:D:33:ARG:NH2	2:D:379:HOH:O	2.30	0.64
1:B:91:TRP:O	1:B:91:TRP:HE3	1.80	0.64
1:A:173:ALA:H	1:A:176:ARG:HG3	1.62	0.63
1:A:147:GLN:HE22	1:A:179:ALA:CB	2.04	0.63
1:A:252:THR:OG1	1:A:257:VAL:HG23	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD23	1:B:194:LEU:C	2.19	0.63
1:B:221:GLN:HE22	1:B:233:VAL:H	1.46	0.63
1:B:1:MET:HE1	2:B:441:HOH:O	1.97	0.63
1:D:228:LEU:N	1:D:228:LEU:HD22	2.13	0.63
1:A:3:ARG:HD3	2:A:554:HOH:O	1.97	0.63
1:D:194:LEU:CD1	1:D:194:LEU:C	2.67	0.63
1:B:226:GLU:CD	1:B:226:GLU:H	2.01	0.63
1:A:94:TYR:H	1:A:102:ASN:ND2	1.93	0.62
1:B:267:VAL:O	1:B:269:SER:N	2.32	0.62
1:A:167:PRO:CG	1:A:168:PHE:CE1	2.83	0.61
1:B:7:LYS:HE2	1:B:8:ASN:ND2	2.16	0.60
1:D:91:TRP:CD2	1:D:91:TRP:O	2.54	0.60
1:A:172:ASP:O	1:A:173:ALA:HB2	2.00	0.60
1:B:289:LYS:CA	1:B:289:LYS:CE	2.77	0.60
1:A:194:LEU:C	1:A:194:LEU:HD23	2.22	0.59
1:D:17:LYS:O	1:D:18:VAL:HB	2.01	0.59
1:B:211:VAL:HG13	1:B:228:LEU:HD22	1.84	0.59
1:D:164:LEU:HD12	1:D:164:LEU:N	2.18	0.59
1:A:173:ALA:HA	1:A:176:ARG:HE	1.68	0.59
1:A:211:VAL:CG1	1:A:228:LEU:HD12	2.33	0.59
1:D:221:GLN:HE22	1:D:233:VAL:H	1.52	0.58
1:B:289:LYS:HE3	1:B:289:LYS:C	2.22	0.58
1:B:289:LYS:O	1:B:290:ASP:HB2	2.04	0.58
1:B:136:HIS:HE1	2:B:559:HOH:O	1.87	0.57
1:D:247:LEU:HB3	1:D:258:ILE:CD1	2.34	0.57
1:B:221:GLN:NE2	1:B:233:VAL:H	2.02	0.57
1:A:87:VAL:HB	1:A:164:LEU:CD2	2.35	0.57
1:A:172:ASP:O	1:A:173:ALA:HB3	2.03	0.56
1:B:256:VAL:HG21	1:B:274:ILE:HD11	1.88	0.56
1:D:105:PHE:HB3	1:D:106:PRO:HD3	1.88	0.56
1:D:228:LEU:N	1:D:228:LEU:CD2	2.69	0.56
1:D:247:LEU:HD12	1:D:322:GLU:HB3	1.87	0.56
1:D:120:ARG:HD3	1:D:120:ARG:O	2.06	0.56
1:D:221:GLN:HG2	1:D:228:LEU:CD1	2.36	0.56
1:A:161:LEU:HG	1:A:163:LEU:HD13	1.86	0.56
1:D:278:PRO:HD2	1:D:279:GLU:OE1	2.07	0.55
1:B:211:VAL:CG1	1:B:228:LEU:HD22	2.36	0.55
1:D:88:PHE:O	1:D:91:TRP:CD1	2.59	0.55
1:D:304:ILE:N	1:D:304:ILE:CD1	2.67	0.55
1:D:88:PHE:O	1:D:91:TRP:HD1	1.89	0.55
1:B:67:ARG:NE	2:B:418:HOH:O	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ILE:CD1	1:A:149:VAL:HG22	2.36	0.54
1:A:226:GLU:OE1	1:A:226:GLU:N	2.29	0.54
1:B:127:ILE:HG21	1:B:189:ARG:CZ	2.37	0.54
1:B:201:PRO:HG3	1:B:240:LEU:O	2.08	0.54
1:B:256:VAL:HG11	1:B:274:ILE:CG1	2.37	0.54
1:D:3:ARG:O	1:D:4:ILE:HD12	2.06	0.54
1:D:304:ILE:N	1:D:304:ILE:HD13	2.05	0.54
1:B:89:GLN:O	1:B:91:TRP:CD1	2.60	0.54
1:B:256:VAL:HG11	1:B:274:ILE:HG13	1.89	0.54
1:A:260:SER:HB3	1:A:318:LEU:HB2	1.89	0.54
1:A:330:HIS:HB2	2:A:479:HOH:O	2.07	0.53
1:B:105:PHE:HB3	1:B:106:PRO:HD3	1.91	0.53
1:A:130:ILE:HD12	1:A:149:VAL:HG22	1.90	0.53
1:B:161:LEU:HD21	1:B:163:LEU:HD21	1.90	0.53
1:B:206:ALA:C	1:B:207:ILE:HD13	2.30	0.53
1:B:289:LYS:CE	1:B:289:LYS:C	2.77	0.53
1:D:228:LEU:H	1:D:228:LEU:CD2	2.22	0.53
1:A:290:ASP:CG	1:A:292:SER:HG	2.11	0.52
1:A:225:PRO:HD2	1:A:226:GLU:OE1	2.08	0.52
1:D:55:ASP:OD1	1:D:56:VAL:N	2.40	0.52
1:A:91:TRP:O	1:A:92:ALA:C	2.46	0.52
1:A:315:ILE:HD12	1:A:315:ILE:C	2.31	0.51
1:B:211:VAL:HG13	1:B:228:LEU:CD2	2.40	0.51
1:D:221:GLN:NE2	1:D:233:VAL:H	2.07	0.51
1:A:142:SER:H	1:A:145:GLN:NE2	2.10	0.50
1:A:141:LEU:HG	1:A:145:GLN:HB3	1.92	0.50
1:A:173:ALA:CA	1:A:176:ARG:HE	2.24	0.50
1:B:269:SER:HB2	1:B:351:GLU:HG3	1.94	0.50
1:A:184:LYS:NZ	2:A:588:HOH:O	2.45	0.50
1:B:7:LYS:CE	1:B:8:ASN:ND2	2.75	0.50
1:A:253:ASN:O	1:A:255:GLY:N	2.40	0.50
1:B:90:THR:C	1:B:92:ALA:N	2.63	0.49
1:D:248:GLU:O	1:D:258:ILE:HD13	2.11	0.49
1:D:261:LEU:HG	1:D:317:PRO:HB3	1.94	0.49
1:B:173:ALA:HB2	1:B:176:ARG:NH1	2.28	0.49
1:B:189:ARG:NH2	2:B:400:HOH:O	2.46	0.49
1:D:96:ASN:O	1:D:96:ASN:OD1	2.30	0.49
1:A:226:GLU:H	1:A:226:GLU:CD	2.06	0.48
1:D:221:GLN:HG2	1:D:228:LEU:HD11	1.95	0.48
1:A:115:GLU:HG3	1:A:119:LYS:HE3	1.95	0.48
1:A:252:THR:OG1	1:A:257:VAL:HG21	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:GLU:CB	2:D:474:HOH:O	2.61	0.48
1:A:118:ARG:HG3	2:A:508:HOH:O	2.13	0.48
1:D:68:LEU:CD2	1:D:76:ILE:HD12	2.44	0.48
1:D:164:LEU:CD1	1:D:164:LEU:N	2.77	0.48
1:A:184:LYS:CD	2:A:588:HOH:O	2.47	0.48
1:D:45:THR:O	1:D:49:ARG:HG3	2.14	0.48
1:D:36:ILE:HB	1:D:197:VAL:HG12	1.97	0.47
1:D:1:MET:HB2	1:D:160:SER:HB2	1.96	0.47
1:A:120:ARG:NH2	1:A:158[A]:ASP:OD1	2.47	0.47
1:A:235:ILE:CD1	1:A:246:GLU:HG2	2.43	0.47
1:D:91:TRP:O	1:D:91:TRP:CE3	2.68	0.47
1:A:141:LEU:HD21	1:A:149:VAL:HG21	1.96	0.47
1:D:315:ILE:CD1	1:D:340:VAL:HG22	2.45	0.47
1:B:7:LYS:HD2	1:B:8:ASN:ND2	2.29	0.46
1:D:3:ARG:NH1	1:D:29:GLU:OE2	2.48	0.46
1:A:221:GLN:HE22	1:A:233:VAL:N	2.10	0.46
1:A:249:GLY:HA3	1:A:258:ILE:HG12	1.96	0.46
1:D:14:LYS:HB3	2:D:377:HOH:O	2.14	0.46
1:D:7:LYS:HB3	1:D:7:LYS:HE3	1.39	0.46
1:D:247:LEU:HB3	1:D:258:ILE:HD12	1.97	0.46
1:D:82:ARG:O	1:D:83:LYS:HB2	2.15	0.46
1:D:71:SER:O	1:D:74:LYS:HB3	2.16	0.46
1:D:110:MET:SD	1:D:157:LYS:HE3	2.55	0.46
1:A:84:ILE:HG21	1:A:163:LEU:HD22	1.97	0.46
1:D:221:GLN:CD	1:D:228:LEU:HD13	2.36	0.46
1:A:127:ILE:HG21	1:A:189:ARG:CZ	2.45	0.45
1:A:87:VAL:HB	1:A:164:LEU:HD23	1.98	0.45
1:D:9:VAL:HG13	1:D:57:PRO:HB3	1.99	0.45
1:D:168:PHE:O	1:D:171:LEU:HB2	2.17	0.45
1:A:130:ILE:HD13	1:A:149:VAL:CG2	2.46	0.45
1:A:94:TYR:HB3	2:A:359:HOH:O	2.16	0.45
1:D:224:LYS:O	1:D:228:LEU:CD2	2.57	0.45
1:A:38:GLY:O	1:A:44:LYS:CE	2.65	0.45
1:B:7:LYS:HD3	1:B:8:ASN:ND2	2.30	0.44
1:D:330:HIS:HA	1:D:331:PRO:HD2	1.88	0.44
1:D:303:VAL:HG22	1:D:304:ILE:N	2.32	0.44
1:A:142:SER:H	1:A:145:GLN:HE21	1.65	0.44
1:A:39:PRO:HD2	1:A:42:ALA:HB2	1.98	0.44
1:D:168:PHE:CE2	1:D:207:ILE:CD1	3.01	0.44
1:B:80:GLU:H	1:B:80:GLU:CD	2.21	0.43
1:D:247:LEU:HB2	1:D:274:ILE:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:ILE:CD1	1:D:340:VAL:CG2	2.96	0.43
1:D:68:LEU:HD23	1:D:76:ILE:HD12	1.98	0.43
1:A:91:TRP:O	1:A:93:LEU:HG	2.17	0.43
1:A:173:ALA:N	1:A:176:ARG:HE	2.16	0.43
1:B:36:ILE:HB	1:B:197:VAL:HG12	2.00	0.43
1:A:290:ASP:OD1	1:A:292:SER:OG	2.35	0.43
1:D:204:ILE:HD12	1:D:211:VAL:HG22	2.00	0.43
1:D:91:TRP:CG	1:D:91:TRP:O	2.71	0.43
1:B:298:LYS:HD3	1:B:318:LEU:HD22	2.00	0.43
1:A:166:GLU:N	1:A:167:PRO:CD	2.81	0.43
1:A:66:ASP:OD1	1:A:66:ASP:N	2.52	0.42
1:D:249:GLY:HA3	1:D:258:ILE:HG12	2.01	0.42
1:A:290:ASP:CG	1:A:292:SER:OG	2.58	0.42
1:B:123:GLU:O	1:B:127:ILE:HG13	2.19	0.42
1:B:86:MET:CE	2:B:529:HOH:O	2.46	0.42
1:A:317:PRO:HD3	1:A:322:GLU:O	2.20	0.42
1:D:166:GLU:HG2	1:D:198:SER:HA	2.01	0.42
1:D:94:TYR:OH	2:D:476:HOH:O	2.21	0.42
1:D:6:VAL:O	1:D:25:ASN:HA	2.20	0.42
1:A:119:LYS:HD2	2:A:428:HOH:O	2.19	0.41
1:A:343:ARG:HB2	1:A:346:LYS:HB2	2.03	0.41
1:B:164:LEU:HB3	1:B:167:PRO:HG3	2.02	0.41
1:D:26:ILE:HG13	1:D:27:ASN:N	2.35	0.41
1:D:241:ILE:HG13	1:D:241:ILE:O	2.20	0.41
1:A:94:TYR:HA	1:A:95:PRO:HD2	1.93	0.41
1:B:1:MET:CE	1:B:160:SER:HA	2.50	0.41
1:A:276:ILE:O	1:A:276:ILE:HG23	2.20	0.41
1:A:88:PHE:CD2	1:A:165:ASP:HB3	2.55	0.41
1:D:110:MET:HE2	1:D:110:MET:CA	2.22	0.41
1:A:5:ILE:HB	1:A:63:TYR:HB2	2.01	0.41
1:B:256:VAL:HB	1:B:263:PHE:HB2	2.02	0.41
1:B:7:LYS:HD3	1:B:7:LYS:C	2.41	0.41
1:B:89:GLN:C	1:B:91:TRP:H	2.24	0.41
1:B:247:LEU:HD13	1:B:247:LEU:N	2.32	0.41
1:B:300:LYS:HB2	1:B:300:LYS:HE2	1.85	0.41
1:D:331:PRO:O	1:D:332:ILE:HD13	2.20	0.41
1:A:173:ALA:HB2	1:A:176:ARG:HH21	1.85	0.41
1:A:235:ILE:CG1	1:A:246:GLU:HG2	2.50	0.41
1:A:138:PRO:O	1:A:141:LEU:HB2	2.21	0.41
1:D:204:ILE:HD12	1:D:211:VAL:CG2	2.50	0.41
1:A:211:VAL:HG11	1:A:228:LEU:CD1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LYS:HB2	1:B:44:LYS:HE2	1.87	0.40
1:B:7:LYS:HD2	1:B:8:ASN:HD22	1.86	0.40
1:B:155:LEU:HD11	1:B:186:VAL:HG11	2.02	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:25:ASN:ND2	1:D:96:ASN:ND2[1_545]	1.97	0.23

## 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	355/353 (101%)	341 (96%)	10 (3%)	4 (1%)	17	11
1	B	354/353 (100%)	344 (97%)	7 (2%)	3 (1%)	22	17
1	D	351/353 (99%)	336 (96%)	14 (4%)	1 (0%)	44	44
All	All	1060/1059 (100%)	1021 (96%)	31 (3%)	8 (1%)	22	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ALA
1	A	169	SER
1	A	254	GLU
1	B	268	SER
1	A	173	ALA
1	B	290	ASP
1	B	91	TRP
1	D	18	VAL

### 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	297/307 (97%)	290 (98%)	7 (2%)	54	59
1	B	298/307 (97%)	292 (98%)	6 (2%)	60	66
1	D	279/307 (91%)	267 (96%)	12 (4%)	33	32
All	All	874/921 (95%)	849 (97%)	25 (3%)	48	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	141	LEU
1	A	163	LEU
1	A	226	GLU
1	A	247	LEU
1	A	289	LYS
1	A	336	GLU
1	B	30	ASN
1	B	247	LEU
1	B	285	LYS
1	B	289	LYS
1	B	298	LYS
1	B	307	GLN
1	D	4	ILE
1	D	23	ASN
1	D	110	MET
1	D	120	ARG
1	D	194	LEU
1	D	228	LEU
1	D	266	SER
1	D	267	VAL
1	D	279	GLU
1	D	304	ILE
1	D	307	GLN
1	D	346	LYS



Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	102	ASN
1	A	145	GLN
1	A	147	GLN
1	A	221	GLN
1	A	307	GLN
1	B	8	ASN
1	B	23	ASN
1	B	27	ASN
1	B	30	ASN
1	B	109	ASN
1	B	136	HIS
1	B	221	GLN
1	B	236	GLN
1	B	307	GLN
1	D	187	GLN
1	D	221	GLN
1	D	307	GLN

### 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	352/353 (99%)	0.01	11 (3%) 49 56	8, 20, 38, 88	0
1	B	352/353 (99%)	-0.02	8 (2%) 61 66	9, 21, 41, 120	0
1	D	352/353 (99%)	0.28	16 (4%) 34 40	7, 20, 37, 96	0
All	All	1056/1059 (99%)	0.09	35 (3%) 47 54	7, 20, 39, 120	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	ASN	19.1
1	B	91	TRP	15.8
1	B	90	THR	8.7
1	A	171	LEU	8.0
1	A	91	TRP	7.2
1	D	91	TRP	6.7
1	D	90	THR	6.1
1	B	266	SER	4.4
1	D	249	GLY	4.3
1	D	16	GLY	4.1
1	D	251	VAL	3.3
1	A	169	SER	3.1
1	B	307	GLN	3.1
1	A	252	THR	2.8
1	B	291[A]	ASP	2.8
1	D	253	ASN	2.7
1	D	267	VAL	2.6
1	D	342	VAL	2.6
1	A	88	PHE	2.5
1	D	264	PRO	2.5
1	A	267	VAL	2.5
1	B	253	ASN	2.4
1	B	344	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	2.4
1	D	256	VAL	2.4
1	D	15	LYS	2.3
1	D	88	PHE	2.3
1	B	169	SER	2.3
1	D	307	GLN	2.3
1	A	255	GLY	2.3
1	D	255	GLY	2.3
1	D	344	LYS	2.2
1	A	266	SER	2.2
1	A	253	ASN	2.1
1	D	279	GLU	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.