Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2025 – 05:28 AM EDT

PDB ID	:	2I5K / pdb_00002i5k
Title	:	Crystal structure of Ugp1p
Authors	:	Roeben, A.; Plitzko, J.M.; Koerner, R.; Boettcher, U.M.K.; Siegers, K.; Hayer-Hartl, M.; Bracher, A.
Deposited on	:	2006-08-25
Resolution	:	3.10 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 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:

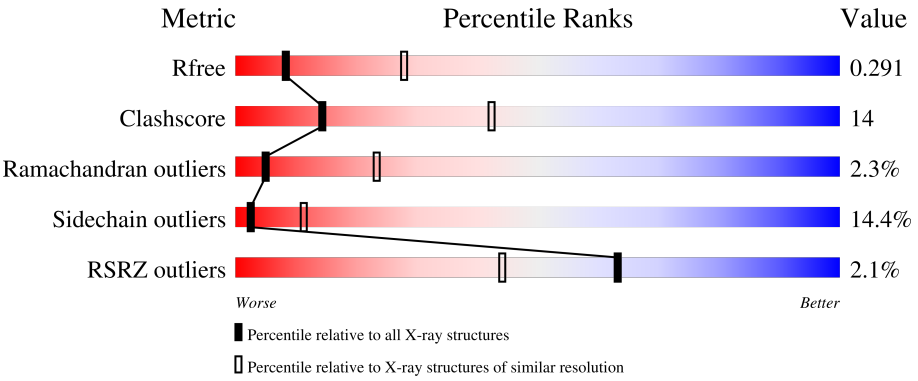
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	164625	1351 (3.10-3.10)
Clashscore	180529	1454 (3.10-3.10)
Ramachandran outliers	177936	1391 (3.10-3.10)
Sidechain outliers	177891	1391 (3.10-3.10)
RSRZ outliers	164620	1351 (3.10-3.10)

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 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 <=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	488	2% 65% 25% 5% 5%
1	B	488	2% 66% 24% 5% • 5%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6617 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 UTP--glucose-1-phosphate uridylyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3290	2077	567	638	8			
1	B	466	Total	C	N	O	S	0	0	0
			3317	2090	575	644	8			

- Molecule 2 is water.

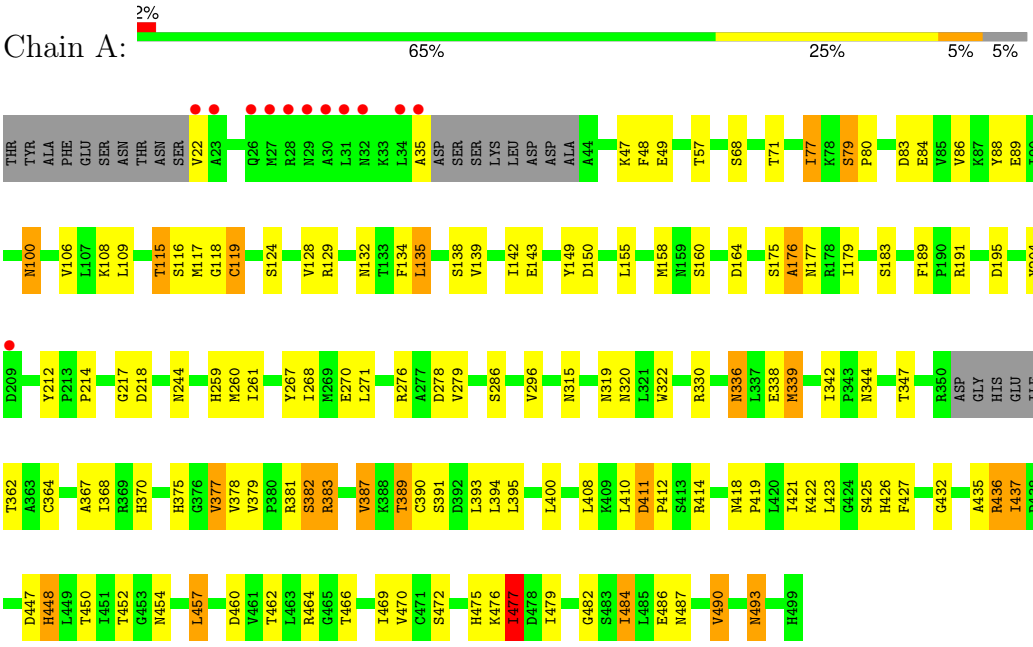
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	O	0	0
			4	4		
2	B	6	Total	O	0	0
			6	6		

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.

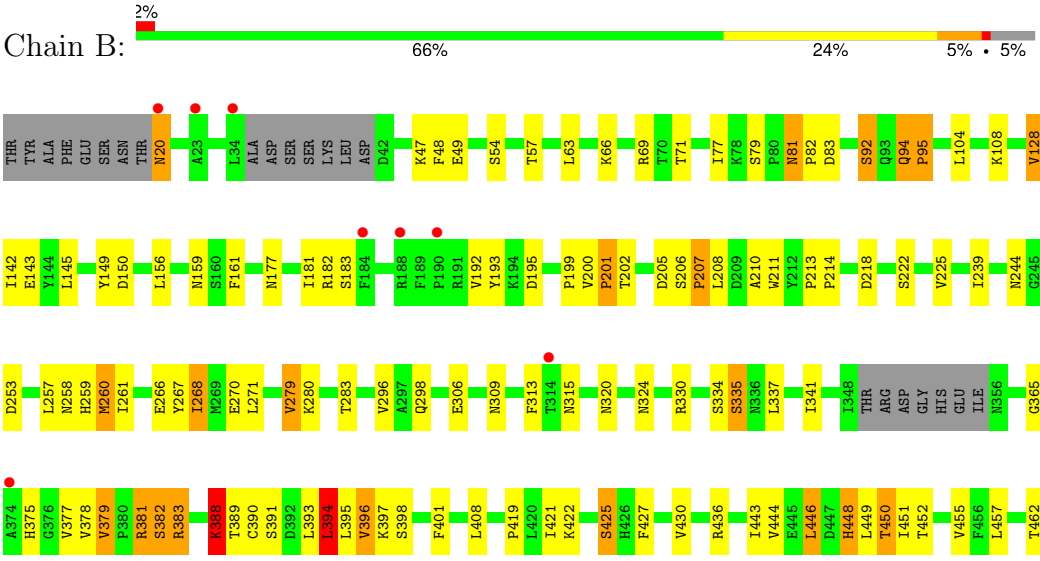
• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

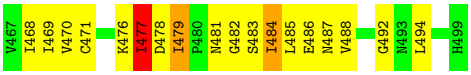
Chain A:



• Molecule 1: UTP--glucose-1-phosphate uridylyltransferase

Chain B:




V467
I468
I469
V470
C471
K476
T477
D478
I479
P480
N481
G482
S483
I484
L485
E486
N487
V488
G492
N493
L494
H499

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	110.19Å 147.44Å 167.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.10 19.99 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.99-3.10) 97.8 (19.99-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.85 (at 3.07Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.291 0.230 , 0.291	Depositor DCC
R_{free} test set	1262 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	78.8	Xtriage
Anisotropy	0.658	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 63.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6617	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.83	7/3349 (0.2%)	1.09	15/4587 (0.3%)
1	B	0.84	9/3377 (0.3%)	1.02	10/4622 (0.2%)
All	All	0.84	16/6726 (0.2%)	1.06	25/9209 (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	1
1	B	0	2
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	20	ASN	CA-CB	18.41	1.90	1.53
1	A	35	ALA	C-O	14.07	1.51	1.23
1	A	421	ILE	C-N	11.70	1.47	1.33
1	A	422	LYS	C-N	11.28	1.48	1.33
1	B	20	ASN	N-CA	10.31	1.65	1.46
1	B	422	LYS	C-N	10.09	1.47	1.33
1	B	482	GLY	C-O	8.91	1.37	1.24
1	A	22	VAL	N-CA	7.01	1.59	1.46
1	B	425	SER	CA-C	6.69	1.61	1.52
1	A	493	ASN	C-N	6.41	1.42	1.33
1	B	481	ASN	N-CA	6.32	1.53	1.46
1	A	22	VAL	CA-CB	6.28	1.71	1.54
1	B	425	SER	CA-CB	5.21	1.62	1.53
1	B	492	GLY	C-N	5.17	1.40	1.33
1	B	425	SER	C-O	5.16	1.30	1.24
1	A	423	LEU	C-O	5.01	1.29	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	79	SER	CA-C-N	8.94	129.02	119.90
1	A	79	SER	C-N-CA	8.94	129.02	119.90
1	A	206	SER	CA-C-N	7.78	129.57	119.84
1	A	206	SER	C-N-CA	7.78	129.57	119.84
1	A	426	HIS	N-CA-C	-6.91	104.96	113.19
1	A	418	ASN	CA-C-N	-6.80	112.98	119.85
1	A	418	ASN	C-N-CA	-6.80	112.98	119.85
1	B	81	ASN	CA-C-N	6.64	128.14	119.84
1	B	81	ASN	C-N-CA	6.64	128.14	119.84
1	A	342	ILE	CA-C-N	6.50	125.73	118.97
1	A	342	ILE	C-N-CA	6.50	125.73	118.97
1	B	483	SER	N-CA-CB	6.11	119.02	110.04
1	A	35	ALA	CA-C-O	-6.04	110.54	120.80
1	A	472	SER	N-CA-C	5.90	117.66	110.41
1	B	492	GLY	N-CA-C	5.58	118.75	110.60
1	B	394	LEU	N-CA-C	-5.57	104.84	111.69
1	A	119	CYS	N-CA-C	5.46	117.38	110.33
1	A	411	ASP	CA-C-N	5.26	125.31	119.32
1	A	411	ASP	C-N-CA	5.26	125.31	119.32
1	B	134	PHE	N-CA-C	-5.20	105.50	111.07
1	B	79	SER	CA-C-N	5.16	125.16	119.90
1	B	79	SER	C-N-CA	5.16	125.16	119.90
1	B	425	SER	CB-CA-C	-5.14	99.24	109.99
1	B	477	ILE	N-CA-C	5.13	115.24	107.75
1	A	477	ILE	N-CA-C	5.13	115.65	108.17

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	206	SER	Peptide
1	B	205	ASP	Peptide
1	B	388	LYS	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	3290	0	2957	84	0
1	B	3317	0	2978	91	0
2	A	4	0	0	0	0
2	B	6	0	0	0	0
All	All	6617	0	5935	174	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 14.

All (174) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:ASN:CA	1:B:20:ASN:CB	1.90	1.45
1:B:448:HIS:CE1	1:B:450:THR:HG22	1.85	1.11
1:B:448:HIS:HE1	1:B:450:THR:CG2	1.68	1.05
1:B:448:HIS:CE1	1:B:450:THR:CG2	2.45	0.96
1:A:436:ARG:HG2	1:A:436:ARG:HH11	1.34	0.93
1:B:94:GLN:CB	1:B:95:PRO:HD3	2.08	0.83
1:A:270:GLU:OE1	1:A:383:ARG:NH1	2.12	0.82
1:B:436:ARG:HG2	1:B:455:VAL:O	1.78	0.82
1:A:475:HIS:CD2	1:A:493:ASN:HD22	1.97	0.81
1:A:460:ASP:O	1:A:482:GLY:HA2	1.82	0.80
1:A:91:ILE:HD12	1:A:377:VAL:HG21	1.63	0.78
1:B:206:SER:HB2	1:B:207:PRO:HD2	1.65	0.77
1:A:84:GLU:OE1	1:A:286:SER:HB3	1.85	0.76
1:A:389:THR:HG22	1:A:391:SER:H	1.53	0.74
1:A:260:MET:HG3	1:A:268:ILE:HD12	1.72	0.72
1:B:63:LEU:O	1:B:66:LYS:HB3	1.90	0.72
1:B:477:ILE:HD11	1:B:479:ILE:HG13	1.73	0.71
1:B:201:PRO:HG3	1:B:211:TRP:CZ3	2.26	0.71
1:A:91:ILE:CD1	1:A:377:VAL:HG21	2.21	0.70
1:A:270:GLU:HG3	1:A:320:ASN:O	1.91	0.69
1:B:471:CYS:HB2	1:B:477:ILE:HG23	1.73	0.69
1:A:124:SER:O	1:A:134:PHE:HB2	1.93	0.69
1:A:466:THR:H	1:A:487:ASN:ND2	1.90	0.68
1:B:448:HIS:HE1	1:B:450:THR:HG21	1.59	0.68
1:A:339:MET:SD	1:A:367:ALA:HB2	2.33	0.68
1:A:387:VAL:HG12	1:A:387:VAL:O	1.91	0.68
1:B:393:LEU:O	1:B:397:LYS:HG3	1.94	0.68
1:B:466:THR:H	1:B:487:ASN:ND2	1.92	0.68
1:B:477:ILE:HD11	1:B:479:ILE:CD1	2.23	0.67
1:B:425:SER:C	1:B:427:PHE:H	2.02	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:GLU:H	1:A:370:HIS:CE1	2.13	0.67
1:A:432:GLY:O	1:A:436:ARG:HD2	1.95	0.67
1:B:253:ASP:HB2	1:B:383:ARG:NH2	2.10	0.66
1:A:436:ARG:HG2	1:A:436:ARG:NH1	2.10	0.66
1:B:104:LEU:HD22	1:B:257:LEU:HD22	1.78	0.65
1:A:270:GLU:CD	1:A:383:ARG:HH12	2.03	0.65
1:B:108:LYS:NZ	1:B:244:ASN:O	2.30	0.65
1:B:192:VAL:HG12	1:B:193:TYR:N	2.12	0.65
1:A:259:HIS:HE1	1:A:375:HIS:NE2	1.95	0.64
1:B:369:ARG:HG3	1:B:370:HIS:CD2	2.33	0.64
1:A:390:CYS:HA	1:A:393:LEU:HB2	1.79	0.63
1:B:20:ASN:CB	1:B:20:ASN:C	2.72	0.63
1:B:466:THR:H	1:B:487:ASN:HD22	1.45	0.63
1:A:464:ARG:HB2	1:A:486:GLU:HB2	1.82	0.62
1:B:477:ILE:HD11	1:B:479:ILE:CG1	2.30	0.61
1:A:475:HIS:CD2	1:A:493:ASN:ND2	2.69	0.61
1:B:192:VAL:HG12	1:B:193:TYR:H	1.66	0.60
1:A:454:ASN:ND2	1:A:476:LYS:HG3	2.17	0.60
1:B:259:HIS:HE1	1:B:375:HIS:NE2	2.00	0.59
1:B:484:ILE:HG12	1:B:484:ILE:O	2.01	0.59
1:B:201:PRO:HG3	1:B:211:TRP:HZ3	1.67	0.58
1:A:437:ILE:HD13	1:A:457:LEU:HD22	1.85	0.57
1:B:425:SER:C	1:B:427:PHE:N	2.61	0.56
1:B:381:ARG:O	1:B:382:SER:C	2.48	0.56
1:A:490:VAL:HG23	1:B:494:LEU:HD11	1.87	0.56
1:B:94:GLN:CB	1:B:95:PRO:CD	2.83	0.55
1:A:410:LEU:HD21	1:A:414:ARG:HB3	1.89	0.55
1:B:77:ILE:HG13	1:B:77:ILE:O	2.06	0.55
1:B:448:HIS:CE1	1:B:450:THR:HG21	2.34	0.55
1:A:142:ILE:HD11	1:A:179:ILE:CB	2.37	0.55
1:B:129:ARG:NH1	1:B:396:VAL:O	2.40	0.54
1:B:159:ASN:HD21	1:B:183:SER:HB2	1.72	0.54
1:A:436:ARG:NH1	1:A:436:ARG:CG	2.66	0.54
1:A:214:PRO:HG2	1:A:218:ASP:OD1	2.09	0.52
1:B:446:LEU:HD11	1:B:449:LEU:HB2	1.90	0.52
1:B:222:SER:HA	1:B:225:VAL:HB	1.91	0.52
1:B:253:ASP:HB2	1:B:383:ARG:HH21	1.73	0.52
1:A:124:SER:HB2	1:A:135:LEU:HD22	1.91	0.52
1:A:115:THR:O	1:A:118:GLY:N	2.40	0.52
1:A:100:ASN:ND2	1:A:100:ASN:H	2.07	0.52
1:B:270:GLU:OE1	1:B:383:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:CG	1:A:268:ILE:HD12	2.40	0.51
1:B:128:VAL:O	1:B:397:LYS:HE2	2.09	0.51
1:B:419:PRO:HB3	1:B:446:LEU:O	2.10	0.51
1:A:191:ARG:HE	1:A:212:TYR:HB3	1.75	0.51
1:A:336:ASN:ND2	1:A:370:HIS:HB3	2.25	0.51
1:B:81:ASN:O	1:B:83:ASP:N	2.44	0.51
1:A:149:TYR:O	1:A:150:ASP:HB2	2.10	0.51
1:A:387:VAL:O	1:A:387:VAL:CG1	2.60	0.50
1:A:381:ARG:O	1:A:382:SER:C	2.55	0.50
1:A:400:LEU:HD11	1:A:414:ARG:HD3	1.93	0.50
1:B:383:ARG:HH11	1:B:383:ARG:HG3	1.77	0.50
1:B:389:THR:HG22	1:B:391:SER:H	1.77	0.50
1:B:477:ILE:HD11	1:B:479:ILE:HD12	1.91	0.50
1:B:208:LEU:C	1:B:210:ALA:H	2.20	0.50
1:A:394:LEU:C	1:A:394:LEU:HD23	2.37	0.50
1:A:47:LYS:C	1:A:49:GLU:H	2.19	0.50
1:B:47:LYS:C	1:B:49:GLU:H	2.20	0.49
1:A:484:ILE:HG22	1:A:484:ILE:O	2.12	0.49
1:A:270:GLU:OE2	1:A:320:ASN:HB3	2.12	0.49
1:B:401:PHE:CD1	1:B:408:LEU:HB3	2.48	0.49
1:A:217:GLY:HA2	1:A:364:CYS:N	2.27	0.48
1:A:466:THR:O	1:A:487:ASN:HA	2.13	0.48
1:A:400:LEU:HD21	1:A:419:PRO:HD3	1.95	0.48
1:B:465:GLY:HA3	1:B:487:ASN:HD21	1.78	0.48
1:A:469:ILE:HG12	1:A:490:VAL:HG13	1.95	0.48
1:B:464:ARG:O	1:B:486:GLU:HA	2.13	0.48
1:A:129:ARG:O	1:A:132:ASN:HB2	2.13	0.47
1:A:115:THR:HA	1:A:119:CYS:O	2.13	0.47
1:B:258:ASN:O	1:B:261:ILE:HG22	2.14	0.47
1:B:390:CYS:HA	1:B:393:LEU:HB2	1.96	0.47
1:B:206:SER:O	1:B:207:PRO:C	2.58	0.47
1:B:391:SER:OG	1:B:421:ILE:HG22	2.14	0.47
1:A:448:HIS:O	1:A:466:THR:HA	2.15	0.47
1:B:451:ILE:HA	1:B:469:ILE:O	2.14	0.47
1:B:214:PRO:HB2	1:B:218:ASP:HB2	1.97	0.47
1:A:189:PHE:CD1	1:A:214:PRO:HG3	2.50	0.46
1:B:334:SER:O	1:B:335:SER:C	2.59	0.46
1:A:410:LEU:HD23	1:A:411:ASP:O	2.16	0.46
1:B:69:ARG:O	1:B:69:ARG:HG3	2.16	0.46
1:B:270:GLU:HB2	1:B:320:ASN:HB2	1.97	0.46
1:A:175:SER:O	1:A:176:ALA:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PHE:CZ	1:B:211:TRP:HB2	2.51	0.46
1:A:339:MET:HE2	1:A:339:MET:HB2	1.90	0.46
1:B:192:VAL:CG1	1:B:193:TYR:N	2.79	0.46
1:A:100:ASN:H	1:A:100:ASN:HD22	1.64	0.45
1:A:115:THR:C	1:A:117:MET:H	2.24	0.45
1:B:393:LEU:HD23	1:B:393:LEU:HA	1.83	0.45
1:A:425:SER:C	1:A:427:PHE:H	2.24	0.45
1:A:77:ILE:O	1:A:77:ILE:HG13	2.16	0.45
1:B:258:ASN:HA	1:B:261:ILE:HG22	1.98	0.45
1:A:244:ASN:ND2	1:A:319:ASN:HB3	2.32	0.45
1:B:213:PRO:HA	1:B:214:PRO:HD3	1.80	0.45
1:A:88:TYR:O	1:A:89:GLU:C	2.60	0.45
1:A:109:LEU:HD12	1:A:244:ASN:HA	1.99	0.44
1:A:432:GLY:O	1:A:435:ALA:HB3	2.17	0.44
1:B:471:CYS:HB2	1:B:477:ILE:CG2	2.44	0.44
1:A:109:LEU:HD23	1:A:158:MET:HE2	1.99	0.44
1:B:266:GLU:HA	1:B:324:ASN:HB2	1.99	0.44
1:B:450:THR:HG23	1:B:468:ILE:HG12	1.98	0.44
1:A:270:GLU:CD	1:A:322:TRP:HE1	2.26	0.44
1:A:411:ASP:HA	1:A:412:PRO:HD2	1.81	0.44
1:B:271:LEU:O	1:B:378:VAL:HA	2.18	0.44
1:B:268:ILE:HG23	1:B:377:VAL:HG12	1.99	0.44
1:B:279:VAL:HG23	1:B:280:LYS:N	2.33	0.44
1:B:71:THR:HG23	1:B:298:GLN:C	2.43	0.44
1:B:149:TYR:O	1:B:150:ASP:C	2.61	0.44
1:B:129:ARG:HD2	1:B:408:LEU:HD11	2.00	0.43
1:B:394:LEU:C	1:B:394:LEU:HD23	2.43	0.43
1:A:129:ARG:HD2	1:A:408:LEU:HD11	1.99	0.43
1:B:465:GLY:HA3	1:B:487:ASN:ND2	2.33	0.43
1:B:388:LYS:HB3	1:B:388:LYS:HE3	1.87	0.43
1:A:437:ILE:CD1	1:A:457:LEU:HD22	2.47	0.43
1:A:139:VAL:O	1:A:143:GLU:HB2	2.18	0.43
1:A:91:ILE:O	1:A:92:SER:C	2.61	0.42
1:A:205:ASP:O	1:A:206:SER:C	2.61	0.42
1:A:244:ASN:HD21	1:A:319:ASN:HB3	1.84	0.42
1:B:398:SER:HB2	1:B:443:ILE:HG12	2.01	0.42
1:A:212:TYR:OH	1:A:360:LEU:O	2.31	0.42
1:A:466:THR:H	1:A:487:ASN:HD22	1.64	0.42
1:B:246:ASP:OD2	1:B:388:LYS:NZ	2.52	0.42
1:B:448:HIS:C	1:B:448:HIS:ND1	2.77	0.42
1:B:218:ASP:O	1:B:218:ASP:CG	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:SER:C	1:A:427:PHE:N	2.78	0.42
1:B:260:MET:HG3	1:B:268:ILE:HD12	2.02	0.41
1:B:477:ILE:HD12	1:B:478:ASP:C	2.45	0.41
1:A:142:ILE:HD12	1:A:143:GLU:N	2.34	0.41
1:A:439:HIS:O	1:A:440:ILE:C	2.63	0.41
1:A:204:TYR:CD1	1:A:205:ASP:HB2	2.56	0.41
1:B:192:VAL:CG1	1:B:193:TYR:H	2.31	0.41
1:B:477:ILE:O	1:B:477:ILE:HG13	2.21	0.41
1:A:79:SER:HA	1:A:80:PRO:HD2	1.74	0.41
1:A:338:GLU:O	1:A:370:HIS:HE1	2.02	0.41
1:B:267:TYR:OH	1:B:365:GLY:HA2	2.20	0.41
1:B:379:VAL:HB	1:B:383:ARG:HD3	2.01	0.41
1:A:115:THR:C	1:A:117:MET:N	2.78	0.41
1:B:283:THR:HG21	1:B:313:PHE:HD1	1.86	0.41
1:A:160:SER:O	1:A:164:ASP:HB2	2.21	0.41
1:A:477:ILE:HD13	1:A:477:ILE:HG21	1.65	0.41
1:A:271:LEU:O	1:A:378:VAL:HA	2.20	0.41
1:B:201:PRO:HB2	1:B:202:THR:H	1.79	0.40
1:B:156:LEU:HD23	1:B:182:ARG:O	2.20	0.40
1:B:306:GLU:O	1:B:309:ASN:HB3	2.21	0.40
1:A:267:TYR:CD2	1:A:368:ILE:HG13	2.56	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	459/488 (94%)	399 (87%)	51 (11%)	9 (2%)	6 26
1	B	460/488 (94%)	400 (87%)	48 (10%)	12 (3%)	4 21
All	All	919/976 (94%)	799 (87%)	99 (11%)	21 (2%)	5 23

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	PRO
1	B	92	SER
1	B	94	GLN
1	A	344	ASN
1	B	48	PHE
1	B	207	PRO
1	B	279	VAL
1	B	335	SER
1	B	337	LEU
1	A	48	PHE
1	A	92	SER
1	A	276	ARG
1	B	82	PRO
1	B	95	PRO
1	A	96	GLU
1	A	116	SER
1	B	199	PRO
1	B	201	PRO
1	B	382	SER
1	A	176	ALA
1	A	68	SER

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	314/435 (72%)	265 (84%)	49 (16%)	2 9
1	B	318/435 (73%)	276 (87%)	42 (13%)	3 14
All	All	632/870 (73%)	541 (86%)	91 (14%)	2 11

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	THR
1	A	71	THR

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Mol	Chain	Res	Type
1	A	77	ILE
1	A	83	ASP
1	A	86	VAL
1	A	91	ILE
1	A	100	ASN
1	A	106	VAL
1	A	108	LYS
1	A	115	THR
1	A	128	VAL
1	A	135	LEU
1	A	138	SER
1	A	155	LEU
1	A	177	ASN
1	A	183	SER
1	A	195	ASP
1	A	207	PRO
1	A	261	ILE
1	A	278	ASP
1	A	279	VAL
1	A	296	VAL
1	A	315	ASN
1	A	330	ARG
1	A	336	ASN
1	A	339	MET
1	A	347	THR
1	A	362	THR
1	A	377	VAL
1	A	379	VAL
1	A	382	SER
1	A	383	ARG
1	A	387	VAL
1	A	389	THR
1	A	395	LEU
1	A	436	ARG
1	A	437	ILE
1	A	444	VAL
1	A	447	ASP
1	A	448	HIS
1	A	450	THR
1	A	452	THR
1	A	457	LEU
1	A	462	THR

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Mol	Chain	Res	Type
1	A	470	VAL
1	A	477	ILE
1	A	479	ILE
1	A	484	ILE
1	A	490	VAL
1	B	54	SER
1	B	57	THR
1	B	92	SER
1	B	128	VAL
1	B	129	ARG
1	B	142	ILE
1	B	143	GLU
1	B	145	LEU
1	B	177	ASN
1	B	181	ILE
1	B	195	ASP
1	B	200	VAL
1	B	239	ILE
1	B	251	THR
1	B	260	MET
1	B	268	ILE
1	B	296	VAL
1	B	315	ASN
1	B	330	ARG
1	B	341	ILE
1	B	379	VAL
1	B	381	ARG
1	B	383	ARG
1	B	388	LYS
1	B	394	LEU
1	B	395	LEU
1	B	396	VAL
1	B	430	VAL
1	B	444	VAL
1	B	446	LEU
1	B	448	HIS
1	B	450	THR
1	B	452	THR
1	B	457	LEU
1	B	462	THR
1	B	470	VAL
1	B	476	LYS

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Mol	Chain	Res	Type
1	B	477	ILE
1	B	479	ILE
1	B	484	ILE
1	B	485	LEU
1	B	488	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	162	ASN
1	A	177	ASN
1	A	244	ASN
1	A	259	HIS
1	A	320	ASN
1	A	336	ASN
1	A	370	HIS
1	A	448	HIS
1	A	475	HIS
1	A	487	ASN
1	B	110	ASN
1	B	159	ASN
1	B	186	GLN
1	B	235	GLN
1	B	258	ASN
1	B	259	HIS
1	B	359	GLN
1	B	370	HIS
1	B	448	HIS
1	B	487	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)

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

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^{th} 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	465/488 (95%)	-0.14	12 (2%) 57 38	38, 83, 112, 145	0
1	B	466/488 (95%)	-0.14	8 (1%) 69 50	38, 91, 115, 154	0
All	All	931/976 (95%)	-0.14	20 (2%) 63 44	38, 87, 114, 154	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	22	VAL	6.0
1	A	35	ALA	4.8
1	A	34	LEU	3.7
1	B	34	LEU	3.7
1	B	20	ASN	3.7
1	A	23	ALA	3.4
1	A	32	ASN	3.3
1	A	27	MET	2.9
1	A	31	LEU	2.9
1	B	374	ALA	2.7
1	A	26	GLN	2.6
1	A	30	ALA	2.6
1	B	190	PRO	2.4
1	B	314	THR	2.4
1	B	23	ALA	2.4
1	A	29	ASN	2.3
1	A	28	ARG	2.2
1	B	188	ARG	2.2
1	A	209	ASP	2.1
1	B	184	PHE	2.1

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 monosaccharides 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.