Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 02:32 PM JST

PDB ID	:	6JAK
Title	:	OtsA apo structure
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Deposited on	:	2019-01-24
Resolution	:	2.41 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:

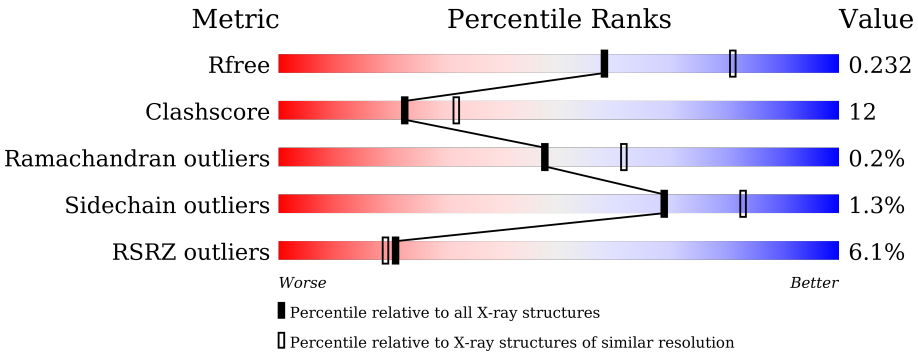
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.41 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	455	5%, 82%, 16%
1	B	455	7%, 76%, 19%
1	C	455	7%, 75%, 22%
1	D	455	5%, 75%, 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 14597 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 Trehalose-6-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3606	2319	626	654	7			
1	B	447	Total	C	N	O	S	0	0	0
			3583	2307	620	649	7			
1	C	447	Total	C	N	O	S	0	0	0
			3583	2307	620	649	7			
1	D	447	Total	C	N	O	S	0	0	0
			3583	2307	620	649	7			

- Molecule 2 is water.

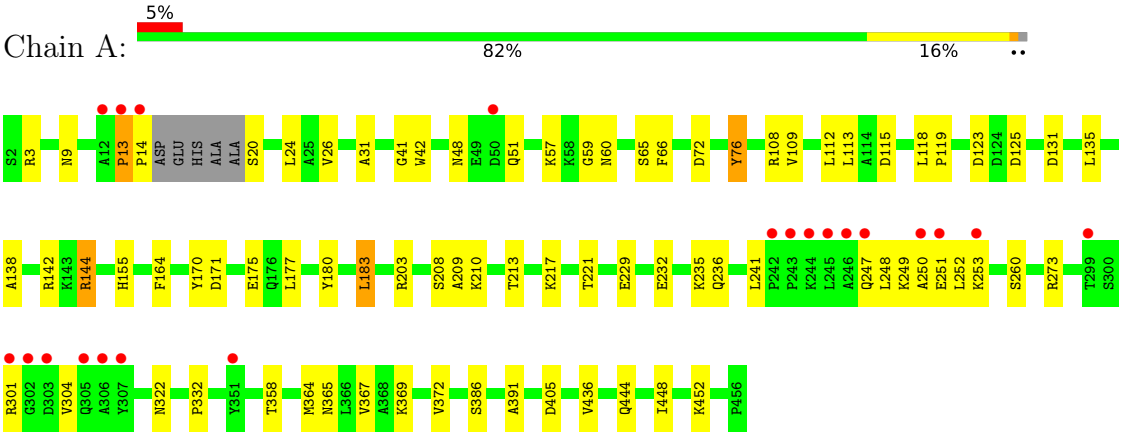
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	53	Total	O	0	0
			53	53		
2	C	44	Total	O	0	0
			44	44		
2	D	65	Total	O	0	0
			65	65		

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.

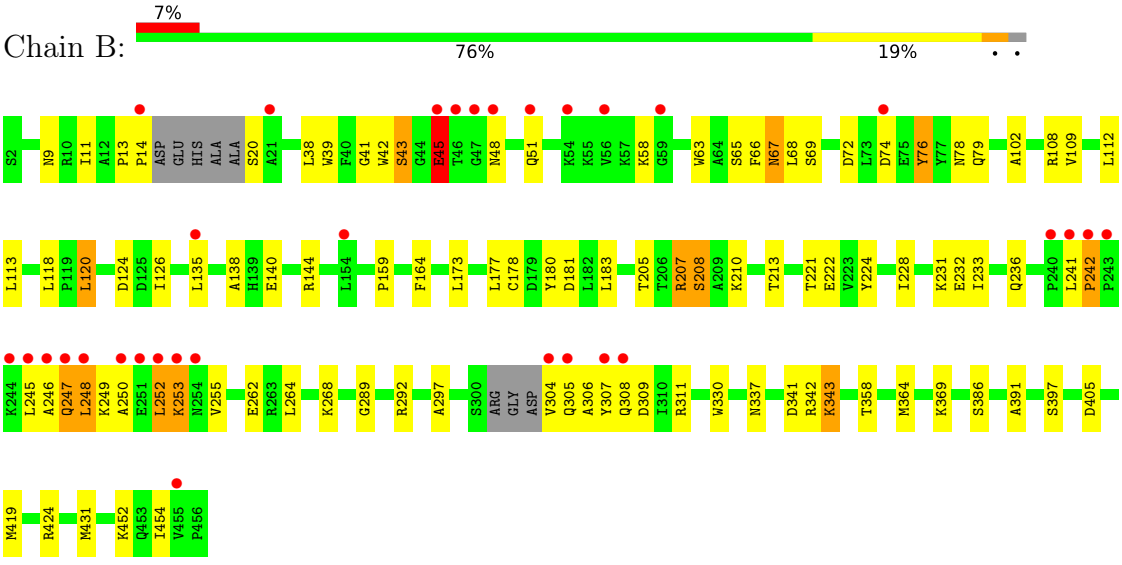
• Molecule 1: Trehalose-6-phosphate synthase

Chain A:



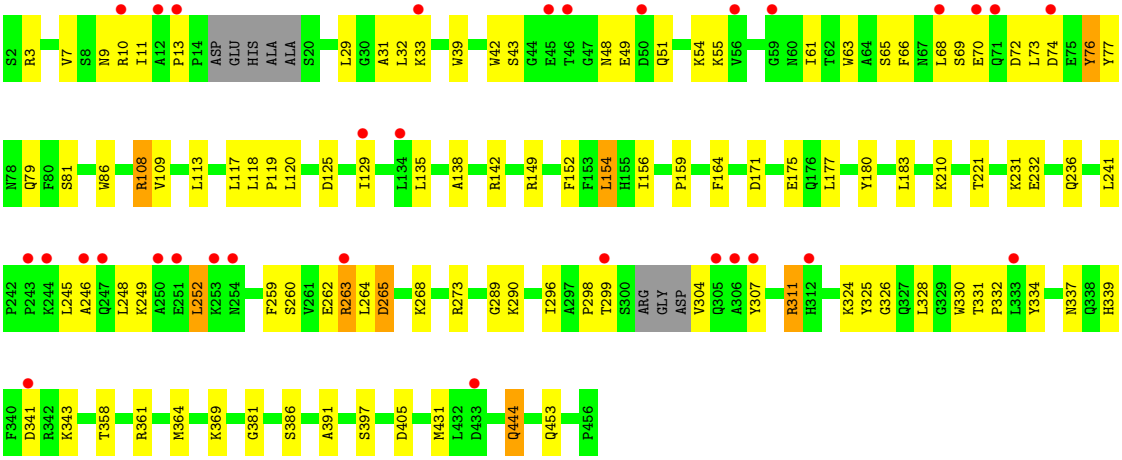
• Molecule 1: Trehalose-6-phosphate synthase

Chain B:



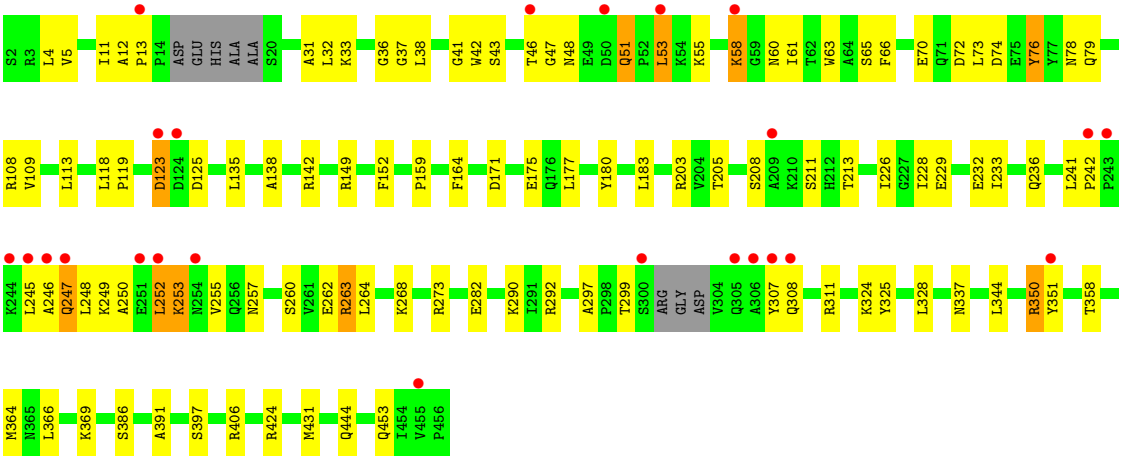
• Molecule 1: Trehalose-6-phosphate synthase

Chain C:



• Molecule 1: Trehalose-6-phosphate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.47Å 119.66Å 99.43Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	29.69 – 2.41 29.69 – 2.41	Depositor EDS
% Data completeness (in resolution range)	95.3 (29.69-2.41) 95.3 (29.69-2.41)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.180 , 0.231 0.180 , 0.232	Depositor DCC
R_{free} test set	3733 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14597	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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	0.60	0/3697	0.76	5/5026 (0.1%)
1	B	0.71	7/3673 (0.2%)	0.84	10/4993 (0.2%)
1	C	0.67	6/3673 (0.2%)	0.83	11/4993 (0.2%)
1	D	0.65	4/3673 (0.1%)	0.87	18/4993 (0.4%)
All	All	0.66	17/14716 (0.1%)	0.82	44/20005 (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	B	0	1
1	D	0	1
All	All	0	2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	ARG	CZ-NH1	-11.27	1.18	1.33
1	B	207	ARG	CZ-NH1	10.87	1.47	1.33
1	D	13	PRO	N-CA	-8.40	1.32	1.47
1	B	45	GLU	CB-CG	-8.07	1.36	1.52
1	B	67	ASN	CG-ND2	-7.63	1.13	1.32
1	D	263	ARG	CZ-NH1	7.37	1.42	1.33
1	C	263	ARG	CZ-NH2	-7.07	1.23	1.33
1	C	263	ARG	NE-CZ	-6.71	1.24	1.33
1	B	207	ARG	CG-CD	-6.65	1.35	1.51
1	B	242	PRO	N-CA	-6.49	1.36	1.47
1	C	70	GLU	CB-CG	-6.28	1.40	1.52
1	C	311	ARG	CZ-NH2	-6.09	1.25	1.33
1	B	45	GLU	CD-OE1	-5.52	1.19	1.25
1	D	263	ARG	CZ-NH2	5.32	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	265	ASP	CB-CG	-5.32	1.40	1.51
1	D	12	ALA	CA-CB	5.22	1.63	1.52
1	B	253	LYS	CD-CE	-5.06	1.38	1.51

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	252	LEU	CB-CG-CD2	-11.39	91.63	111.00
1	A	183	LEU	CB-CG-CD2	-10.58	93.02	111.00
1	D	263	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	D	58	LYS	CD-CE-NZ	10.02	134.74	111.70
1	D	53	LEU	CB-CG-CD2	-9.43	94.98	111.00
1	D	58	LYS	CG-CD-CE	-8.82	85.42	111.90
1	C	252	LEU	CB-CG-CD1	8.58	125.59	111.00
1	B	207	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	C	252	LEU	CA-CB-CG	8.30	134.38	115.30
1	C	154	LEU	CA-CB-CG	8.05	133.81	115.30
1	D	73	LEU	CA-CB-CG	-7.99	96.91	115.30
1	B	248	LEU	CA-CB-CG	7.80	133.23	115.30
1	D	73	LEU	CB-CG-CD2	-7.56	98.15	111.00
1	D	252	LEU	CA-CB-CG	7.05	131.52	115.30
1	A	304	VAL	CG1-CB-CG2	7.05	122.18	110.90
1	C	252	LEU	CB-CG-CD2	-6.98	99.13	111.00
1	D	252	LEU	CB-CG-CD1	6.93	122.78	111.00
1	C	263	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	290	LYS	CG-CD-CE	6.81	132.33	111.90
1	D	248	LEU	CA-CB-CG	6.78	130.88	115.30
1	D	53	LEU	CA-CB-CG	6.69	130.68	115.30
1	C	108	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	D	13	PRO	CA-N-CD	6.36	120.60	111.70
1	B	207	ARG	NH1-CZ-NH2	6.09	126.09	119.40
1	B	242	PRO	N-CA-CB	-6.07	95.93	102.60
1	B	207	ARG	CB-CA-C	-5.85	98.70	110.40
1	D	350	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	D	13	PRO	CA-CB-CG	5.67	115.57	104.80
1	B	452	LYS	CA-CB-CG	5.38	125.24	113.40
1	A	112	LEU	CA-CB-CG	5.32	127.52	115.30
1	D	424	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	70	GLU	CB-CA-C	-5.29	99.82	110.40
1	B	252	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	C	68	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	53	LEU	CB-CG-CD1	5.17	119.79	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	144	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	241	LEU	CA-CB-CG	5.16	127.17	115.30
1	C	248	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	B	68	LEU	N-CA-CB	-5.10	100.19	110.40
1	D	13	PRO	N-CA-CB	-5.10	96.99	102.60
1	D	252	LEU	C-N-CA	-5.09	108.98	121.70
1	B	207	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	154	LEU	CB-CG-CD1	5.03	119.55	111.00
1	B	183	LEU	CB-CG-CD2	5.02	119.53	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	247	GLN	Peptide
1	D	247	GLN	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	3606	0	3580	49	1
1	B	3583	0	3559	92	0
1	C	3583	0	3559	96	0
1	D	3583	0	3559	100	1
2	A	80	0	0	4	0
2	B	53	0	0	5	0
2	C	44	0	0	6	0
2	D	65	0	0	4	0
All	All	14597	0	14257	333	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 12.

All (333) 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:305:GLN:NE2	1:B:308:GLN:HE21	1.33	1.27
1:B:249:LYS:O	1:B:253:LYS:NZ	1.68	1.24
1:C:263:ARG:HH21	1:C:298:PRO:HG2	1.07	1.16
1:B:305:GLN:CD	1:B:308:GLN:NE2	1.98	1.15
1:D:252:LEU:HD22	1:D:255:VAL:CG1	1.77	1.14
1:D:252:LEU:HB2	1:D:255:VAL:HG12	1.29	1.14
1:D:252:LEU:CD2	1:D:255:VAL:HG11	1.79	1.11
1:B:305:GLN:CD	1:B:308:GLN:HE21	1.57	1.07
1:C:263:ARG:NH2	1:C:298:PRO:O	1.88	1.04
1:C:10:ARG:HH21	1:C:42:TRP:HZ3	1.02	0.98
1:C:263:ARG:HH21	1:C:298:PRO:CG	1.77	0.98
1:B:305:GLN:OE1	1:B:308:GLN:NE2	1.97	0.97
1:B:264:LEU:HD21	1:B:297:ALA:HB1	1.45	0.96
1:D:252:LEU:HD22	1:D:255:VAL:HG11	0.98	0.95
1:A:72:ASP:OD1	1:A:108:ARG:NH1	2.01	0.94
1:B:419:MET:SD	2:B:551:HOH:O	2.25	0.94
1:C:72:ASP:OD1	1:C:108:ARG:NH1	1.99	0.94
1:B:304:VAL:HG12	1:B:306:ALA:H	1.34	0.92
1:D:444:GLN:NE2	2:D:502:HOH:O	1.99	0.92
1:B:305:GLN:NE2	1:B:308:GLN:NE2	2.15	0.92
1:D:252:LEU:HB2	1:D:255:VAL:CG1	2.01	0.90
1:D:247:GLN:OE1	1:D:250:ALA:N	2.07	0.88
1:A:405:ASP:OD1	2:A:501:HOH:O	1.93	0.86
1:D:125:ASP:O	2:D:501:HOH:O	1.94	0.84
1:B:45:GLU:OE2	1:B:67:ASN:ND2	2.10	0.84
1:D:253:LYS:HA	1:D:253:LYS:HE2	1.58	0.84
1:D:48:ASN:O	1:D:51:GLN:NE2	2.10	0.83
1:A:364:MET:HE1	1:A:391:ALA:HA	1.61	0.82
1:D:249:LYS:HG3	1:D:351:TYR:CZ	2.14	0.82
1:B:205:THR:HG1	1:B:213:THR:HG1	1.22	0.82
1:B:419:MET:HE2	1:B:424:ARG:HG2	1.60	0.82
1:D:46:THR:HG21	1:D:70:GLU:HG3	1.61	0.82
1:D:308:GLN:OE1	1:D:311:ARG:NH1	2.13	0.82
1:B:72:ASP:OD1	1:B:108:ARG:NH1	2.12	0.81
1:B:247:GLN:HB2	1:B:250:ALA:HB3	1.64	0.80
1:C:311:ARG:NH2	1:C:337:ASN:HD22	1.79	0.80
1:C:10:ARG:NH2	1:C:42:TRP:HZ3	1.80	0.80
1:D:72:ASP:OD1	1:D:108:ARG:NH1	2.15	0.79
1:C:263:ARG:NH2	1:C:298:PRO:C	2.36	0.79
1:C:263:ARG:NH2	1:C:298:PRO:HG2	1.93	0.79
1:D:252:LEU:HD21	1:D:292:ARG:NH2	1.97	0.78
1:D:33:LYS:HG2	1:D:61:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ARG:NH2	1:A:125:ASP:OD2	2.17	0.75
1:A:229:GLU:HG2	1:A:232:GLU:HB2	1.68	0.75
1:B:307:TYR:OH	2:B:501:HOH:O	2.05	0.74
1:D:46:THR:HG21	1:D:70:GLU:CG	2.16	0.74
1:C:263:ARG:HH22	1:C:298:PRO:C	1.90	0.74
1:C:311:ARG:HH21	1:C:337:ASN:HD22	1.33	0.73
1:B:178:CYS:O	2:B:502:HOH:O	2.07	0.72
1:D:252:LEU:CB	1:D:255:VAL:HG12	2.13	0.72
1:D:252:LEU:HD21	1:D:292:ARG:CZ	2.21	0.71
1:B:241:LEU:HD12	1:B:241:LEU:H	1.55	0.70
1:B:364:MET:HE1	1:B:391:ALA:HA	1.73	0.70
1:D:46:THR:CG2	1:D:70:GLU:HG3	2.21	0.70
1:D:11:ILE:HD11	1:D:65:SER:HB2	1.73	0.70
1:D:242:PRO:O	1:D:246:ALA:N	2.24	0.70
1:D:241:LEU:HB2	1:D:246:ALA:HA	1.72	0.70
1:B:241:LEU:HB2	1:B:246:ALA:HA	1.74	0.69
1:A:13:PRO:HG2	1:A:14:PRO:HD3	1.74	0.69
1:B:69:SER:OG	1:B:72:ASP:OD2	2.06	0.68
1:C:42:TRP:HB2	1:C:66:PHE:CE1	2.29	0.68
1:D:53:LEU:CD2	1:D:66:PHE:HB3	2.23	0.68
1:B:135:LEU:HD22	1:B:177:LEU:HD21	1.74	0.68
1:A:131:ASP:OD2	2:A:502:HOH:O	2.12	0.68
1:B:51:GLN:CD	1:B:51:GLN:H	1.96	0.68
1:C:11:ILE:HD11	1:C:65:SER:HB3	1.74	0.68
1:C:304:VAL:N	2:C:506:HOH:O	2.27	0.67
1:B:9:ASN:O	1:B:42:TRP:HB3	1.94	0.67
1:B:250:ALA:HA	1:B:253:LYS:CE	2.24	0.67
1:B:311:ARG:HH21	1:B:337:ASN:HD21	1.43	0.67
1:B:419:MET:HE2	1:B:424:ARG:CG	2.25	0.67
1:D:253:LYS:HE3	1:D:351:TYR:OH	1.95	0.67
1:C:381:GLY:O	2:C:502:HOH:O	2.12	0.66
1:A:208:SER:OG	1:A:209:ALA:N	2.29	0.65
1:B:13:PRO:HG2	1:B:14:PRO:HD3	1.77	0.65
1:C:154:LEU:HD13	1:C:156:ILE:O	1.96	0.65
1:C:405:ASP:OD1	2:C:503:HOH:O	2.15	0.65
1:C:74:ASP:OD2	1:C:79:GLN:NE2	2.29	0.65
1:B:140:GLU:O	1:B:144:ARG:HD3	1.97	0.65
1:C:241:LEU:HB2	1:C:246:ALA:HB2	1.79	0.64
1:C:328:LEU:HD12	1:D:245:LEU:HD22	1.79	0.64
1:C:364:MET:HE1	1:C:391:ALA:HA	1.78	0.64
1:B:305:GLN:HE22	1:B:308:GLN:HE21	1.42	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:THR:HA	1:D:307:TYR:OH	1.98	0.64
1:D:31:ALA:HB2	1:D:444:GLN:HG3	1.80	0.63
1:A:135:LEU:HD22	1:A:177:LEU:HD21	1.79	0.63
1:A:364:MET:HE2	1:A:369:LYS:NZ	2.13	0.63
1:D:208:SER:HB2	1:D:211:SER:HB3	1.80	0.63
1:B:43:SER:HB3	1:B:45:GLU:OE2	1.99	0.63
1:B:252:LEU:HD22	1:B:255:VAL:HG21	1.81	0.63
1:B:364:MET:CE	1:B:391:ALA:HA	2.28	0.62
1:A:249:LYS:HA	1:A:252:LEU:HG	1.80	0.62
1:C:262:GLU:CG	1:C:268:LYS:HD2	2.31	0.61
1:C:361:ARG:NH1	2:C:501:HOH:O	2.07	0.61
1:C:263:ARG:NH1	1:C:307:TYR:HE1	1.99	0.61
1:B:245:LEU:HA	1:B:248:LEU:CD2	2.30	0.61
1:B:242:PRO:O	1:B:246:ALA:N	2.33	0.61
1:C:54:LYS:HD2	1:C:54:LYS:N	2.16	0.61
1:D:252:LEU:HD13	1:D:255:VAL:CG1	2.30	0.61
1:B:210:LYS:NZ	1:B:222:GLU:OE1	2.28	0.61
1:C:263:ARG:CZ	1:C:298:PRO:O	2.49	0.61
1:D:282:GLU:OE1	1:D:325:TYR:OH	2.07	0.60
1:D:364:MET:HE1	1:D:391:ALA:HA	1.81	0.60
1:C:29:LEU:HB3	1:C:33:LYS:HE3	1.84	0.60
1:C:77:TYR:HA	1:C:81:SER:OG	2.02	0.60
1:A:364:MET:CE	1:A:391:ALA:HA	2.32	0.60
1:D:42:TRP:HB2	1:D:66:PHE:CE1	2.36	0.60
1:C:358:THR:HA	1:C:386:SER:HB2	1.83	0.59
1:B:311:ARG:HH21	1:B:337:ASN:ND2	2.01	0.59
1:C:9:ASN:HD22	1:C:10:ARG:NH1	2.01	0.59
1:B:210:LYS:HB3	1:B:221:THR:O	2.03	0.59
1:C:210:LYS:HB3	1:C:221:THR:O	2.03	0.59
1:B:308:GLN:N	1:B:308:GLN:OE1	2.36	0.59
1:D:228:ILE:HD12	1:D:233:ILE:HD13	1.86	0.58
1:B:311:ARG:NH2	1:B:337:ASN:HD21	2.01	0.58
1:C:263:ARG:NH2	1:C:298:PRO:CG	2.57	0.58
1:D:262:GLU:OE2	1:D:268:LYS:HD2	2.04	0.58
1:C:311:ARG:HD2	1:C:337:ASN:ND2	2.19	0.58
1:C:364:MET:CE	1:C:391:ALA:HA	2.34	0.57
1:A:138:ALA:HB2	1:A:180:TYR:CE1	2.40	0.57
1:C:263:ARG:NH1	1:C:298:PRO:O	2.38	0.57
1:C:311:ARG:NH2	1:C:337:ASN:ND2	2.49	0.56
1:D:43:SER:HB3	1:D:65:SER:OG	2.05	0.56
1:D:358:THR:HA	1:D:386:SER:HB2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:SER:OG	1:C:431:MET:HG3	2.05	0.56
1:B:247:GLN:HB2	1:B:250:ALA:CB	2.33	0.56
1:A:57:LYS:NZ	1:A:59:GLY:O	2.28	0.56
1:C:299:THR:HG23	1:C:307:TYR:OH	2.06	0.55
1:B:250:ALA:HA	1:B:253:LYS:HE2	1.87	0.55
1:D:74:ASP:OD1	1:D:79:GLN:NE2	2.39	0.55
1:D:241:LEU:H	1:D:241:LEU:HD12	1.71	0.55
1:A:210:LYS:HB3	1:A:221:THR:O	2.07	0.55
1:C:29:LEU:O	1:C:33:LYS:HG3	2.07	0.55
1:C:117:LEU:HD12	1:C:120:LEU:HD12	1.87	0.55
1:B:252:LEU:HD11	1:B:292:ARG:HH12	1.72	0.55
1:D:252:LEU:CG	1:D:255:VAL:CG1	2.85	0.55
1:A:171:ASP:O	1:A:175:GLU:HG3	2.06	0.55
1:A:232:GLU:O	1:A:236:GLN:HG3	2.06	0.55
1:B:250:ALA:HA	1:B:253:LYS:NZ	2.22	0.54
1:B:262:GLU:CG	1:B:268:LYS:HD2	2.38	0.54
1:D:255:VAL:HG23	1:D:290:LYS:C	2.28	0.54
1:C:311:ARG:NH2	1:C:337:ASN:HB2	2.22	0.54
1:D:31:ALA:HB2	1:D:444:GLN:CG	2.37	0.54
1:D:138:ALA:HB2	1:D:180:TYR:CE1	2.42	0.54
1:D:205:THR:OG1	1:D:213:THR:OG1	2.26	0.54
1:D:252:LEU:CD2	1:D:255:VAL:CG1	2.59	0.54
1:D:232:GLU:O	1:D:236:GLN:HG3	2.07	0.53
1:C:328:LEU:HD12	1:D:245:LEU:CD2	2.38	0.53
1:A:60:ASN:ND2	2:A:517:HOH:O	2.40	0.53
1:C:32:LEU:HB3	1:C:61:ILE:HD13	1.90	0.53
1:C:324:LYS:HD3	1:C:325:TYR:CE2	2.44	0.53
1:B:138:ALA:HB2	1:B:180:TYR:CE1	2.44	0.52
1:C:249:LYS:HD3	1:C:252:LEU:HD12	1.90	0.52
1:D:252:LEU:CB	1:D:255:VAL:CG1	2.80	0.52
1:D:364:MET:HE2	1:D:369:LYS:NZ	2.25	0.52
1:C:311:ARG:NH2	1:C:337:ASN:CB	2.73	0.52
1:B:364:MET:HE2	1:B:369:LYS:NZ	2.25	0.52
1:D:135:LEU:HD22	1:D:177:LEU:HD21	1.92	0.52
1:B:305:GLN:OE1	1:B:305:GLN:O	2.28	0.52
1:D:53:LEU:HD21	1:D:66:PHE:HB3	1.92	0.52
1:D:241:LEU:CB	1:D:246:ALA:HA	2.39	0.52
1:A:31:ALA:HB1	1:A:448:ILE:HD11	1.92	0.52
1:D:253:LYS:CE	1:D:351:TYR:OH	2.57	0.52
1:D:311:ARG:HH21	1:D:337:ASN:HD21	1.56	0.52
1:D:247:GLN:NE2	1:D:249:LYS:HB3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASP:O	1:D:76:TYR:HB3	2.11	0.51
1:A:364:MET:HE2	1:A:369:LYS:HZ3	1.75	0.51
1:B:241:LEU:HD13	1:B:246:ALA:HA	1.92	0.51
1:C:31:ALA:HB2	1:C:444:GLN:HG3	1.92	0.51
1:B:11:ILE:HD11	1:B:65:SER:HB3	1.92	0.51
1:C:11:ILE:HG22	1:C:39:TRP:NE1	2.26	0.51
1:C:263:ARG:NH2	1:C:298:PRO:CA	2.74	0.51
1:C:31:ALA:HB2	1:C:444:GLN:CG	2.42	0.50
1:D:118:LEU:HB3	1:D:119:PRO:HD3	1.93	0.50
1:D:397:SER:OG	1:D:431:MET:HG3	2.10	0.50
1:A:20:SER:HB3	1:A:26:VAL:HG22	1.92	0.50
1:A:109:VAL:O	1:A:113:LEU:HG	2.11	0.50
1:D:324:LYS:HD3	1:D:325:TYR:CE2	2.46	0.50
1:D:364:MET:CE	1:D:391:ALA:HA	2.41	0.50
1:C:364:MET:HE2	1:C:369:LYS:NZ	2.27	0.50
1:C:54:LYS:HD2	1:C:54:LYS:H	1.76	0.49
1:C:73:LEU:HD12	1:C:77:TYR:HB3	1.94	0.49
1:C:289:GLY:HA2	1:C:330:TRP:CG	2.47	0.49
1:B:252:LEU:HD11	1:B:292:ARG:NH1	2.26	0.49
1:D:252:LEU:CD2	1:D:292:ARG:NH2	2.72	0.49
1:A:138:ALA:O	1:A:142:ARG:HG2	2.11	0.49
1:C:135:LEU:HD22	1:C:177:LEU:HD21	1.95	0.49
1:C:231:LYS:HG3	1:C:232:GLU:N	2.28	0.49
1:C:72:ASP:O	1:C:76:TYR:HB3	2.13	0.49
1:C:138:ALA:HB2	1:C:180:TYR:CE1	2.48	0.49
1:C:138:ALA:O	1:C:142:ARG:HG2	2.13	0.49
1:D:249:LYS:HG3	1:D:351:TYR:OH	2.11	0.49
1:B:74:ASP:OD1	1:B:79:GLN:NE2	2.46	0.49
1:C:245:LEU:HD23	1:D:328:LEU:HD12	1.93	0.49
1:D:299:THR:HG23	1:D:337:ASN:OD1	2.12	0.49
1:A:48:ASN:HB3	1:A:51:GLN:HG2	1.94	0.49
1:C:152:PHE:HB3	1:C:183:LEU:HD23	1.95	0.49
1:C:299:THR:H	1:C:339:HIS:CD2	2.31	0.49
1:C:326:GLY:HA2	1:C:332:PRO:HD3	1.93	0.48
1:D:5:VAL:HG13	1:D:38:LEU:HD12	1.93	0.48
1:A:260:SER:OG	1:A:273:ARG:NH1	2.46	0.48
1:B:72:ASP:HB3	1:B:109:VAL:CG2	2.43	0.48
1:D:171:ASP:O	1:D:175:GLU:HG3	2.13	0.48
1:D:252:LEU:CG	1:D:255:VAL:HG12	2.43	0.48
1:C:149:ARG:NH1	1:C:453:GLN:O	2.36	0.48
1:B:289:GLY:HA2	1:B:330:TRP:CG	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:SER:OG	1:C:65:SER:HB2	2.14	0.48
1:B:43:SER:OG	1:B:65:SER:HB2	2.14	0.48
1:A:9:ASN:O	1:A:42:TRP:HB3	2.13	0.48
1:C:117:LEU:O	1:C:117:LEU:HG	2.14	0.48
1:C:311:ARG:HH22	1:C:337:ASN:HB2	1.79	0.47
1:C:444:GLN:NE2	2:C:515:HOH:O	2.48	0.47
1:C:262:GLU:HG3	1:C:268:LYS:HD2	1.96	0.47
1:A:66:PHE:CZ	1:A:113:LEU:HD22	2.50	0.47
1:A:444:GLN:O	1:A:448:ILE:HD12	2.15	0.47
1:C:55:LYS:HA	1:C:63:TRP:O	2.15	0.47
1:B:11:ILE:HG23	1:B:41:GLY:HA3	1.96	0.47
1:B:228:ILE:HD12	1:B:233:ILE:HD12	1.95	0.47
1:C:263:ARG:HH12	1:C:307:TYR:HE1	1.62	0.47
1:D:260:SER:OG	1:D:273:ARG:NH1	2.48	0.47
1:B:72:ASP:O	1:B:76:TYR:HB3	2.14	0.47
1:B:51:GLN:CD	1:B:51:GLN:N	2.68	0.47
1:B:358:THR:HA	1:B:386:SER:HB2	1.97	0.46
1:D:109:VAL:O	1:D:113:LEU:HG	2.15	0.46
1:C:10:ARG:NH2	1:C:77:TYR:CE2	2.70	0.46
1:B:181:ASP:HB3	1:B:454:ILE:HG21	1.96	0.46
1:B:245:LEU:HA	1:B:248:LEU:HD23	1.97	0.46
1:B:231:LYS:HA	1:B:231:LYS:HD3	1.72	0.46
1:B:343:LYS:HD2	1:B:343:LYS:C	2.36	0.46
1:D:11:ILE:HG23	1:D:41:GLY:HA3	1.98	0.46
1:D:55:LYS:HA	1:D:63:TRP:O	2.15	0.46
1:D:226:ILE:HG23	1:D:366:LEU:HD21	1.98	0.46
1:A:118:LEU:HB3	1:A:119:PRO:HD3	1.97	0.46
1:C:431:MET:HE1	2:C:531:HOH:O	2.16	0.46
1:D:46:THR:HG22	1:D:47:GLY:N	2.31	0.46
1:C:262:GLU:HG2	1:C:268:LYS:HD2	1.98	0.46
1:B:48:ASN:HB2	1:B:51:GLN:NE2	2.31	0.45
1:A:41:GLY:O	1:A:65:SER:HA	2.16	0.45
1:D:33:LYS:NZ	1:D:60:ASN:HB2	2.31	0.45
1:D:4:LEU:O	1:D:37:GLY:HA3	2.16	0.45
1:C:66:PHE:CZ	1:C:113:LEU:HD22	2.51	0.45
1:D:123:ASP:OD1	1:D:123:ASP:N	2.49	0.45
1:B:79:GLN:OE1	1:B:102:ALA:HB2	2.17	0.45
1:B:264:LEU:HD21	1:B:297:ALA:CB	2.32	0.45
1:B:308:GLN:OE1	1:B:309:ASP:N	2.46	0.45
1:B:74:ASP:O	1:B:79:GLN:N	2.49	0.45
1:B:232:GLU:O	1:B:236:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:GLN:OE1	1:D:249:LYS:N	2.50	0.45
1:A:448:ILE:HG22	1:A:452:LYS:HE2	1.99	0.44
1:C:249:LYS:NZ	1:C:252:LEU:O	2.35	0.44
1:A:72:ASP:O	1:A:76:TYR:HB3	2.16	0.44
1:C:3:ARG:HB3	1:C:125:ASP:OD1	2.17	0.44
1:C:331:THR:HG23	1:C:334:TYR:CE1	2.52	0.44
1:C:118:LEU:HB3	1:C:119:PRO:HD3	2.00	0.44
1:D:350:ARG:HH11	1:D:350:ARG:HD2	1.63	0.44
1:D:364:MET:HE2	1:D:369:LYS:HZ3	1.83	0.44
1:A:247:GLN:HG3	1:A:248:LEU:HD13	2.00	0.44
1:D:58:LYS:HB2	1:D:63:TRP:CZ3	2.53	0.44
1:A:138:ALA:HB2	1:A:180:TYR:CD1	2.53	0.44
1:B:38:LEU:HD21	1:B:120:LEU:HD22	2.00	0.44
1:C:232:GLU:O	1:C:236:GLN:HG3	2.18	0.44
1:C:7:VAL:HB	1:C:129:ILE:HD13	2.00	0.44
1:C:54:LYS:NZ	1:C:66:PHE:HA	2.32	0.44
1:D:229:GLU:CD	1:D:232:GLU:HG3	2.37	0.44
1:A:213:THR:HA	1:A:217:LYS:O	2.18	0.44
1:D:58:LYS:HB2	1:D:63:TRP:HZ3	1.83	0.44
1:A:248:LEU:HD12	1:A:251:GLU:HB2	1.98	0.44
1:B:419:MET:CE	1:B:424:ARG:HA	2.48	0.43
1:C:109:VAL:O	1:C:113:LEU:HG	2.18	0.43
1:D:48:ASN:HB3	1:D:51:GLN:NE2	2.33	0.43
1:A:250:ALA:HA	1:A:253:LYS:HE2	2.00	0.43
1:D:46:THR:HG21	1:D:70:GLU:HG2	1.97	0.43
1:D:242:PRO:HG3	1:D:344:LEU:HD13	1.99	0.43
1:A:180:TYR:HB2	1:A:183:LEU:HD11	2.00	0.43
1:B:58:LYS:HB3	1:B:63:TRP:CZ3	2.53	0.43
1:B:405:ASP:OD1	2:B:503:HOH:O	2.21	0.43
1:D:53:LEU:HD23	1:D:66:PHE:HB3	1.97	0.43
1:A:365:ASN:OD1	1:A:367:VAL:HB	2.19	0.43
1:C:48:ASN:HB3	1:C:51:GLN:CD	2.39	0.43
1:B:135:LEU:HD12	1:B:173:LEU:HD22	2.01	0.43
1:B:222:GLU:HB3	1:B:224:TYR:CE1	2.54	0.43
1:C:49:GLU:OE1	1:C:69:SER:HB3	2.18	0.43
1:B:66:PHE:CZ	1:B:113:LEU:HD22	2.53	0.43
1:C:260:SER:OG	1:C:273:ARG:NH1	2.52	0.43
1:D:138:ALA:O	1:D:142:ARG:HG2	2.19	0.43
1:A:252:LEU:O	1:A:252:LEU:HD12	2.19	0.42
1:A:436:VAL:O	2:A:503:HOH:O	2.22	0.42
1:D:32:LEU:O	1:D:36:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ASN:OD1	1:A:332:PRO:HD2	2.20	0.42
1:B:13:PRO:CG	1:B:14:PRO:HD3	2.47	0.42
1:B:58:LYS:HB3	1:B:63:TRP:HZ3	1.85	0.42
1:C:263:ARG:NH1	1:C:307:TYR:CE1	2.83	0.42
1:A:13:PRO:CG	1:A:14:PRO:HD3	2.44	0.42
1:B:126:ILE:HG13	1:B:126:ILE:O	2.20	0.42
1:D:252:LEU:CD1	1:D:255:VAL:CG1	2.97	0.42
1:D:135:LEU:CD2	1:D:177:LEU:HD21	2.50	0.42
1:B:159:PRO:HG2	1:B:164:PHE:HB2	2.01	0.42
1:C:341:ASP:OD1	1:C:343:LYS:HG2	2.19	0.42
1:D:149:ARG:NH1	1:D:453:GLN:O	2.51	0.42
1:B:74:ASP:HA	1:B:78:ASN:HB2	2.02	0.42
1:B:11:ILE:HG22	1:B:39:TRP:CD1	2.55	0.41
1:D:264:LEU:HD21	1:D:297:ALA:HB1	2.02	0.41
1:A:31:ALA:HB1	1:A:448:ILE:CD1	2.49	0.41
1:A:358:THR:HA	1:A:386:SER:HB2	2.02	0.41
1:B:228:ILE:HD12	1:B:233:ILE:CD1	2.50	0.41
1:B:341:ASP:OD2	1:B:342:ARG:N	2.53	0.41
1:D:262:GLU:CD	1:D:273:ARG:HH22	2.23	0.41
1:B:51:GLN:H	1:B:51:GLN:NE2	2.17	0.41
1:D:74:ASP:HA	1:D:78:ASN:HB2	2.03	0.41
1:D:152:PHE:HB3	1:D:183:LEU:HD23	2.01	0.41
1:C:86:TRP:CH2	1:C:265:ASP:OD1	2.73	0.41
1:C:249:LYS:HD3	1:C:249:LYS:HA	1.85	0.41
1:D:257:ASN:ND2	2:D:504:HOH:O	2.09	0.41
1:B:118:LEU:HA	1:B:118:LEU:HD12	1.85	0.41
1:C:259:PHE:HZ	1:C:296:ILE:HD12	1.86	0.41
1:A:24:LEU:HD13	1:A:155:HIS:HE1	1.85	0.41
1:B:112:LEU:HD23	1:B:113:LEU:HD23	2.02	0.41
1:A:164:PHE:CE2	1:A:170:TYR:HB2	2.56	0.41
1:A:203:ARG:HD3	1:A:203:ARG:HA	1.89	0.41
1:C:11:ILE:HG22	1:C:39:TRP:CE2	2.56	0.41
1:C:245:LEU:CD2	1:D:328:LEU:HD12	2.51	0.41
1:D:51:GLN:HE21	1:D:51:GLN:HB2	1.75	0.41
1:B:20:SER:OG	2:B:504:HOH:O	2.22	0.41
1:C:159:PRO:HG2	1:C:164:PHE:HB2	2.04	0.41
1:B:207:ARG:C	1:B:208:SER:O	2.54	0.40
1:C:264:LEU:HD23	1:C:264:LEU:HA	1.79	0.40
1:B:252:LEU:CD1	1:B:292:ARG:NH1	2.84	0.40
1:B:397:SER:OG	1:B:431:MET:HG3	2.21	0.40
1:C:171:ASP:O	1:C:175:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PRO:HG2	1:D:164:PHE:HB2	2.03	0.40
1:A:115:ASP:OD1	1:A:144:ARG:NE	2.48	0.40
1:B:109:VAL:O	1:B:113:LEU:HG	2.21	0.40
1:D:406:ARG:HB3	2:D:523:HOH:O	2.21	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:253:LYS:NZ	1:D:253:LYS:O[1_655]	2.12	0.08

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	446/455 (98%)	434 (97%)	11 (2%)	1 (0%)	47	61
1	B	441/455 (97%)	426 (97%)	14 (3%)	1 (0%)	47	61
1	C	441/455 (97%)	425 (96%)	15 (3%)	1 (0%)	47	61
1	D	441/455 (97%)	427 (97%)	14 (3%)	0	100	100
All	All	1769/1820 (97%)	1712 (97%)	54 (3%)	3 (0%)	47	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	208	SER
1	C	13	PRO
1	A	13	PRO

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	380/383 (99%)	375 (99%)	5 (1%)	69	83
1	B	378/383 (99%)	372 (98%)	6 (2%)	62	78
1	C	378/383 (99%)	376 (100%)	2 (0%)	88	95
1	D	378/383 (99%)	372 (98%)	6 (2%)	62	78
All	All	1514/1532 (99%)	1495 (99%)	19 (1%)	69	83

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	TYR
1	A	123	ASP
1	A	235	LYS
1	A	301	ARG
1	A	372	VAL
1	B	43	SER
1	B	45	GLU
1	B	76	TYR
1	B	120	LEU
1	B	124	ASP
1	B	343	LYS
1	C	76	TYR
1	C	444	GLN
1	D	51	GLN
1	D	76	TYR
1	D	123	ASP
1	D	203	ARG
1	D	253	LYS
1	D	263	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	GLN
1	B	51	GLN
1	B	305	GLN
1	B	337	ASN
1	C	67	ASN
1	C	189	ASN
1	C	254	ASN
1	C	308	GLN
1	C	327	GLN
1	C	337	ASN
1	D	327	GLN
1	D	337	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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^{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	450/455 (98%)	-0.04	21 (4%)	31	29	33, 46, 91, 134	0
1	B	447/455 (98%)	0.11	32 (7%)	15	13	36, 52, 107, 134	0
1	C	447/455 (98%)	0.16	32 (7%)	15	13	37, 51, 95, 132	0
1	D	447/455 (98%)	0.08	24 (5%)	25	23	35, 50, 90, 130	0
All	All	1791/1820 (98%)	0.08	109 (6%)	21	19	33, 50, 98, 134	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	247	GLN	7.7
1	C	243	PRO	7.1
1	A	246	ALA	7.1
1	D	252	LEU	6.4
1	D	251	GLU	6.4
1	D	243	PRO	6.3
1	C	251	GLU	6.3
1	D	13	PRO	6.0
1	B	245	LEU	5.7
1	A	302	GLY	5.5
1	C	250	ALA	5.4
1	D	246	ALA	5.3
1	A	301	ARG	5.1
1	A	303	ASP	5.1
1	A	247	GLN	5.0
1	D	244	LYS	5.0
1	B	46	THR	4.9
1	A	306	ALA	4.9
1	B	47	GLY	4.8
1	C	246	ALA	4.5
1	B	251	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	455	VAL	4.5
1	A	245	LEU	4.4
1	C	305	GLN	4.3
1	A	251	GLU	4.2
1	C	13	PRO	4.1
1	B	246	ALA	4.0
1	B	250	ALA	4.0
1	A	244	LYS	4.0
1	D	306	ALA	3.9
1	C	299	THR	3.9
1	D	245	LEU	3.9
1	B	242	PRO	3.9
1	B	14	PRO	3.8
1	A	13	PRO	3.8
1	B	45	GLU	3.7
1	D	455	VAL	3.6
1	B	74	ASP	3.5
1	A	14	PRO	3.5
1	C	307	TYR	3.4
1	B	243	PRO	3.4
1	C	306	ALA	3.4
1	D	307	TYR	3.4
1	B	48	ASN	3.3
1	D	305	GLN	3.3
1	C	244	LYS	3.3
1	B	305	GLN	3.2
1	C	46	THR	3.2
1	A	243	PRO	3.2
1	A	50	ASP	3.2
1	A	242	PRO	3.2
1	A	250	ALA	3.2
1	B	304	VAL	3.1
1	B	307	TYR	3.1
1	C	74	ASP	3.1
1	C	45	GLU	3.1
1	D	209	ALA	3.1
1	D	124	ASP	3.0
1	A	305	GLN	2.9
1	D	247	GLN	2.9
1	A	253	LYS	2.9
1	B	253	LYS	2.9
1	A	307	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	71	GLN	2.8
1	B	21	ALA	2.8
1	C	254	ASN	2.8
1	C	253	LYS	2.7
1	D	46	THR	2.7
1	B	248	LEU	2.7
1	B	244	LYS	2.7
1	D	351	TYR	2.7
1	C	56	VAL	2.6
1	C	10	ARG	2.6
1	C	68	LEU	2.6
1	B	254	ASN	2.6
1	D	308	GLN	2.6
1	D	50	ASP	2.6
1	C	333	LEU	2.5
1	D	242	PRO	2.5
1	B	135	LEU	2.5
1	C	70	GLU	2.5
1	A	351	TYR	2.4
1	A	12	ALA	2.4
1	D	254	ASN	2.4
1	B	241	LEU	2.4
1	A	299	THR	2.4
1	B	54	LYS	2.3
1	D	300	SER	2.3
1	C	33	LYS	2.3
1	B	308	GLN	2.3
1	C	134	LEU	2.3
1	B	56	VAL	2.2
1	C	129	ILE	2.2
1	C	12	ALA	2.2
1	B	154	LEU	2.2
1	B	252	LEU	2.2
1	B	247	GLN	2.1
1	D	53	LEU	2.1
1	C	433	ASP	2.1
1	C	50	ASP	2.1
1	B	240	PRO	2.1
1	B	59	GLY	2.1
1	C	59	GLY	2.1
1	C	263	ARG	2.1
1	D	58	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	51	GLN	2.0
1	C	341	ASP	2.0
1	D	123	ASP	2.0
1	C	312	HIS	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 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.