Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 01:53 PM EST

PDB ID	:	4FFF
Title	:	Crystal Structure of Levan Fructotransferase from Arthrobacter ureafaciens
Authors	:	Park, J.; Rhee, S.
Deposited on	:	2012-06-01
Resolution	:	2.57 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:

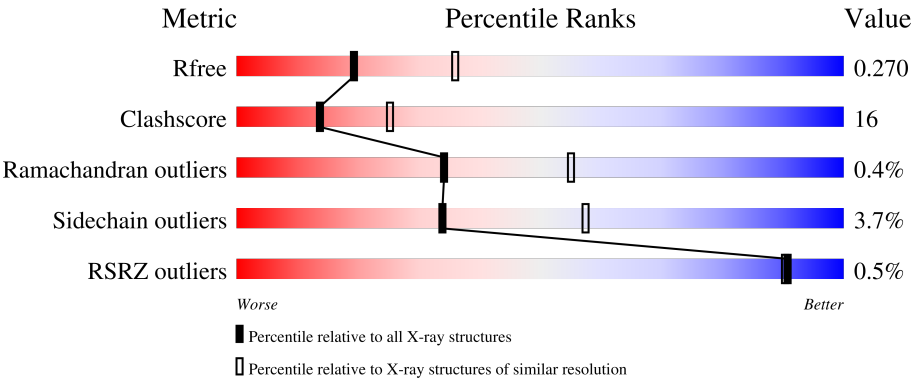
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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	490	% 71% 26%
1	B	490	% 72% 23%
1	C	490	69% 28%
1	D	490	70% 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15645 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 Levan fructotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3734	2372	644	710	8			
1	B	479	Total	C	N	O	S	0	0	0
			3734	2372	644	710	8			
1	C	479	Total	C	N	O	S	0	0	0
			3734	2372	644	710	8			
1	D	479	Total	C	N	O	S	0	0	0
			3734	2372	644	710	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	expression tag	UNP Q9KJD0
A	115	ASP	GLY	conflict	UNP Q9KJD0
A	522	GLY	-	expression tag	UNP Q9KJD0
A	523	SER	-	expression tag	UNP Q9KJD0
A	524	HIS	-	expression tag	UNP Q9KJD0
A	525	HIS	-	expression tag	UNP Q9KJD0
A	526	HIS	-	expression tag	UNP Q9KJD0
A	527	HIS	-	expression tag	UNP Q9KJD0
A	528	HIS	-	expression tag	UNP Q9KJD0
A	529	HIS	-	expression tag	UNP Q9KJD0
B	40	MET	-	expression tag	UNP Q9KJD0
B	115	ASP	GLY	conflict	UNP Q9KJD0
B	522	GLY	-	expression tag	UNP Q9KJD0
B	523	SER	-	expression tag	UNP Q9KJD0
B	524	HIS	-	expression tag	UNP Q9KJD0
B	525	HIS	-	expression tag	UNP Q9KJD0
B	526	HIS	-	expression tag	UNP Q9KJD0
B	527	HIS	-	expression tag	UNP Q9KJD0
B	528	HIS	-	expression tag	UNP Q9KJD0
B	529	HIS	-	expression tag	UNP Q9KJD0
C	40	MET	-	expression tag	UNP Q9KJD0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	115	ASP	GLY	conflict	UNP Q9KJD0
C	522	GLY	-	expression tag	UNP Q9KJD0
C	523	SER	-	expression tag	UNP Q9KJD0
C	524	HIS	-	expression tag	UNP Q9KJD0
C	525	HIS	-	expression tag	UNP Q9KJD0
C	526	HIS	-	expression tag	UNP Q9KJD0
C	527	HIS	-	expression tag	UNP Q9KJD0
C	528	HIS	-	expression tag	UNP Q9KJD0
C	529	HIS	-	expression tag	UNP Q9KJD0
D	40	MET	-	expression tag	UNP Q9KJD0
D	115	ASP	GLY	conflict	UNP Q9KJD0
D	522	GLY	-	expression tag	UNP Q9KJD0
D	523	SER	-	expression tag	UNP Q9KJD0
D	524	HIS	-	expression tag	UNP Q9KJD0
D	525	HIS	-	expression tag	UNP Q9KJD0
D	526	HIS	-	expression tag	UNP Q9KJD0
D	527	HIS	-	expression tag	UNP Q9KJD0
D	528	HIS	-	expression tag	UNP Q9KJD0
D	529	HIS	-	expression tag	UNP Q9KJD0

- Molecule 2 is water.

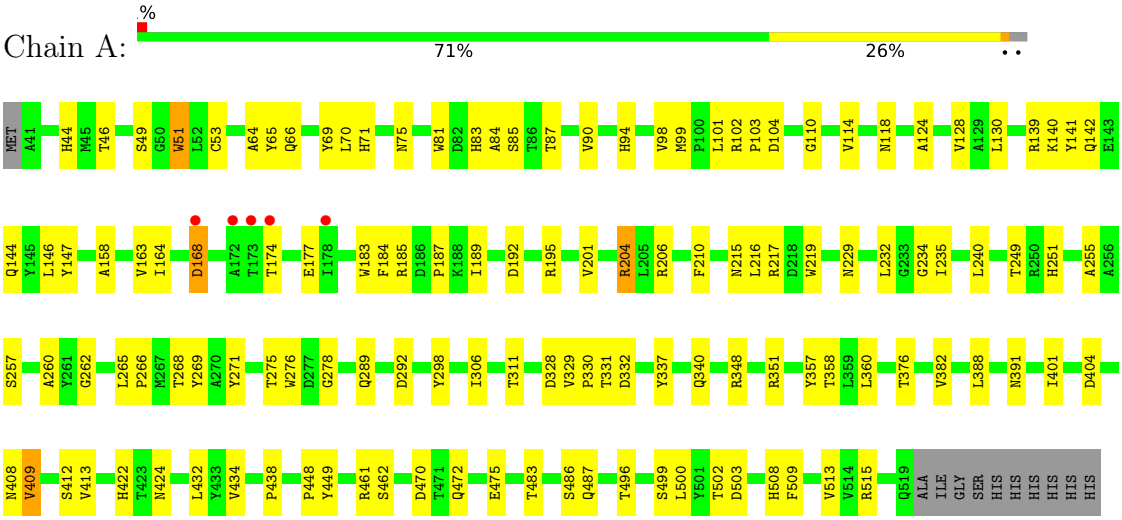
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	189	Total	O	0	0
			189	189		
2	B	153	Total	O	0	0
			153	153		
2	C	199	Total	O	0	0
			199	199		
2	D	168	Total	O	0	0
			168	168		

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.

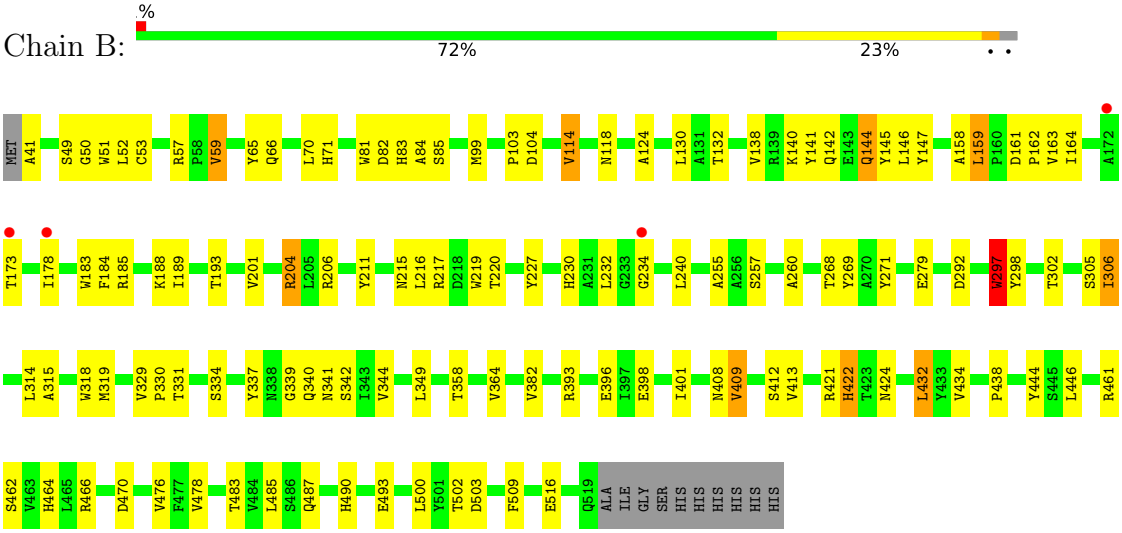
• Molecule 1: Levan fructotransferase

Chain A:



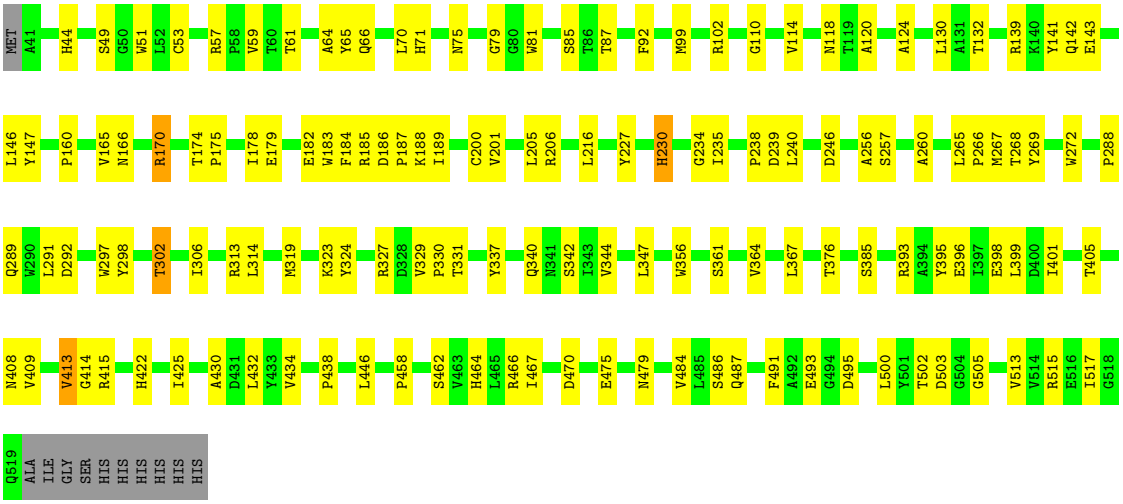
• Molecule 1: Levan fructotransferase

Chain B:



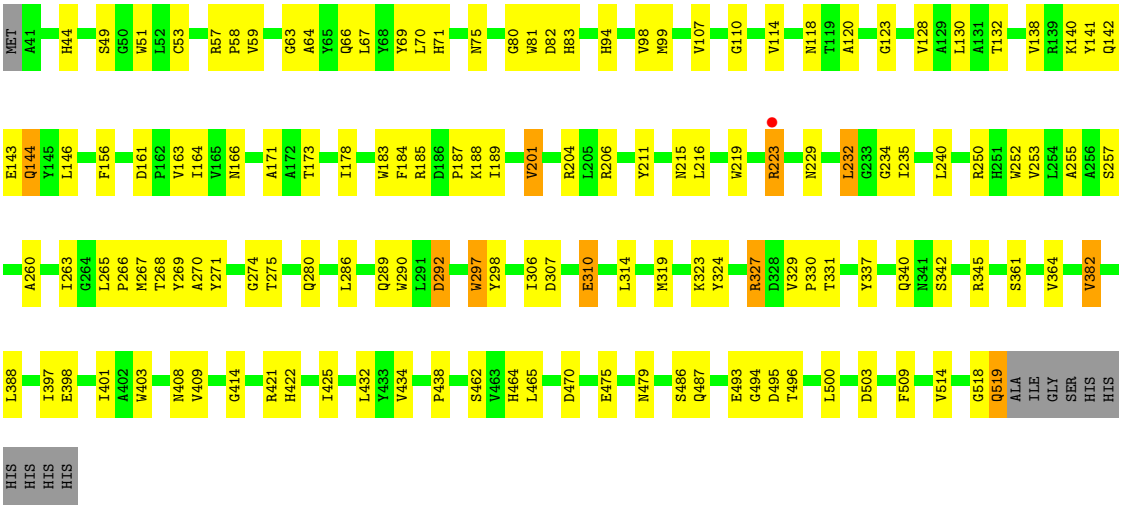
• Molecule 1: Levan fructotransferase

Chain C:



• Molecule 1: Levan fructotransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.96Å 166.62Å 261.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.57 48.91 – 2.57	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.57) 97.8 (48.91-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.96 (at 2.58Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.256 0.227 , 0.270	Depositor DCC
R_{free} test set	11507 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.955	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15645	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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	0.37	0/3858	0.65	1/5305 (0.0%)
1	B	0.36	0/3858	0.64	1/5305 (0.0%)
1	C	0.39	0/3858	0.66	1/5305 (0.0%)
1	D	0.36	0/3858	0.64	1/5305 (0.0%)
All	All	0.37	0/15432	0.65	4/21220 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	432	LEU	N-CA-C	-6.77	92.71	111.00
1	C	432	LEU	N-CA-C	-6.08	94.58	111.00
1	B	432	LEU	N-CA-C	-5.91	95.05	111.00
1	A	432	LEU	N-CA-C	-5.90	95.08	111.00

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	3734	0	3484	105	0
1	B	3734	0	3484	99	0
1	C	3734	0	3484	132	0
1	D	3734	0	3484	123	0
2	A	189	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	153	0	0	4	0
2	C	199	0	0	6	0
2	D	168	0	0	3	0
All	All	15645	0	13936	458	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 16.

All (458) 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:268:THR:HG23	1:A:269:TYR:H	1.24	0.99
1:C:409:VAL:HG23	1:C:502:THR:HG22	1.51	0.93
1:D:319:MET:HE2	1:D:342:SER:HA	1.51	0.93
1:C:57:ARG:HD2	1:C:188:LYS:HE3	1.52	0.90
1:C:425:ILE:HD13	1:C:467:ILE:HD13	1.54	0.90
1:D:327:ARG:HB3	1:D:327:ARG:NH1	1.90	0.85
1:D:327:ARG:HB3	1:D:327:ARG:HH11	1.37	0.85
1:B:268:THR:HG21	1:B:292:ASP:HB3	1.58	0.85
1:A:434:VAL:HB	1:A:487:GLN:HE22	1.39	0.85
1:A:268:THR:HG21	1:A:292:ASP:O	1.77	0.85
1:B:268:THR:HG22	1:B:269:TYR:N	1.93	0.83
1:A:331:THR:HG23	1:A:337:TYR:O	1.79	0.82
1:A:130:LEU:HG	1:A:189:ILE:HD11	1.62	0.82
1:B:331:THR:HG23	1:B:337:TYR:O	1.79	0.81
1:A:142:GLN:NE2	1:A:184:PHE:H	1.79	0.81
1:C:302:THR:HG22	1:C:313:ARG:HH21	1.46	0.80
1:D:268:THR:HG22	1:D:269:TYR:N	1.96	0.80
1:D:250:ARG:HH12	1:D:310:GLU:HG3	1.46	0.79
1:D:324:TYR:O	1:D:327:ARG:HD2	1.82	0.79
1:B:268:THR:HG22	1:B:269:TYR:H	1.47	0.79
1:C:268:THR:HG23	1:C:269:TYR:H	1.47	0.79
1:A:268:THR:HG23	1:A:269:TYR:N	1.96	0.78
1:A:329:VAL:HG13	1:A:330:PRO:HD2	1.64	0.78
1:A:66:GLN:HE22	1:A:85:SER:HB3	1.48	0.77
1:D:434:VAL:CG1	1:D:487:GLN:HE22	1.97	0.77
1:C:331:THR:HG21	2:C:659:HOH:O	1.84	0.76
1:C:57:ARG:HH11	1:C:188:LYS:NZ	1.82	0.76
1:C:302:THR:CG2	1:C:313:ARG:HE	1.98	0.76
1:B:142:GLN:HE22	1:B:185:ARG:HH11	1.34	0.76
1:C:302:THR:HG21	1:C:313:ARG:HE	1.47	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:VAL:HG13	1:D:330:PRO:HD2	1.66	0.76
1:D:142:GLN:NE2	1:D:184:PHE:H	1.85	0.75
1:D:268:THR:HG22	1:D:269:TYR:H	1.51	0.75
1:A:174:THR:OG1	1:A:177:GLU:HG3	1.87	0.74
1:C:268:THR:HG21	1:C:292:ASP:O	1.88	0.73
1:C:130:LEU:HG	1:C:189:ILE:HD11	1.69	0.73
1:C:329:VAL:HG13	1:C:330:PRO:HD2	1.72	0.72
1:C:142:GLN:NE2	1:C:184:PHE:H	1.88	0.72
1:B:118:ASN:HB2	1:B:124:ALA:HA	1.71	0.72
1:B:146:LEU:HD13	1:B:147:TYR:N	2.05	0.72
1:B:329:VAL:HG13	1:B:330:PRO:HD2	1.72	0.71
1:A:434:VAL:HB	1:A:487:GLN:NE2	2.06	0.71
1:C:59:VAL:HG12	1:C:66:GLN:HB2	1.73	0.71
1:D:268:THR:HG21	1:D:292:ASP:HB3	1.71	0.71
1:C:268:THR:HG23	1:C:269:TYR:N	2.06	0.71
1:B:485:LEU:HB3	1:B:487:GLN:HE22	1.55	0.71
1:C:464:HIS:H	1:C:479:ASN:ND2	1.88	0.71
1:B:145:TYR:CZ	1:B:162:PRO:HG3	2.27	0.70
1:A:434:VAL:CB	1:A:487:GLN:HE22	2.05	0.69
1:A:206:ARG:HH11	1:A:234:GLY:HA3	1.57	0.69
1:D:464:HIS:H	1:D:479:ASN:ND2	1.91	0.68
1:C:266:PRO:HB2	1:C:268:THR:HG22	1.76	0.68
1:A:174:THR:HG23	1:A:177:GLU:OE2	1.93	0.68
1:C:434:VAL:HB	1:C:487:GLN:HE22	1.58	0.68
1:A:53:CYS:HB3	1:A:70:LEU:HB2	1.77	0.67
1:D:250:ARG:NH1	1:D:310:GLU:HG3	2.09	0.67
1:D:66:GLN:NE2	1:D:83:HIS:NE2	2.42	0.67
1:D:57:ARG:HD2	1:D:188:LYS:HE2	1.76	0.67
1:D:434:VAL:HG11	1:D:487:GLN:HE22	1.59	0.66
1:C:414:GLY:O	1:C:495:ASP:HB3	1.96	0.66
1:D:267:MET:HE1	1:D:323:LYS:HG2	1.78	0.65
1:D:401:ILE:HG21	1:D:409:VAL:HG11	1.78	0.65
1:D:268:THR:HG23	1:D:297:TRP:HB3	1.77	0.65
1:D:388:LEU:HD21	1:D:500:LEU:HG	1.79	0.65
1:A:201:VAL:CG2	1:A:240:LEU:HD22	2.26	0.65
1:A:66:GLN:NE2	1:A:85:SER:HB3	2.11	0.65
1:D:268:THR:HG23	1:D:297:TRP:O	1.95	0.65
1:D:329:VAL:CG1	1:D:331:THR:HG22	2.27	0.65
1:D:434:VAL:CB	1:D:487:GLN:HE22	2.10	0.65
1:A:142:GLN:HE21	1:A:184:PHE:H	1.43	0.64
1:A:128:VAL:HG11	1:A:216:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:VAL:HG12	1:D:331:THR:HG22	1.79	0.64
1:B:142:GLN:NE2	1:B:184:PHE:H	1.96	0.64
1:C:405:THR:HG23	1:C:505:GLY:HA3	1.79	0.64
1:D:206:ARG:HH11	1:D:234:GLY:HA3	1.63	0.64
1:B:408:ASN:HB3	1:B:503:ASP:HB2	1.79	0.64
1:C:143:GLU:HG2	1:C:166:ASN:H	1.63	0.63
1:C:515:ARG:HG3	1:C:515:ARG:HH11	1.62	0.63
1:D:252:TRP:HB2	1:D:274:GLY:O	1.99	0.63
1:A:404:ASP:HB3	2:A:733:HOH:O	1.97	0.63
1:C:344:VAL:O	1:C:364:VAL:HG13	1.98	0.63
1:D:422:HIS:O	1:D:438:PRO:HG2	1.98	0.63
1:C:376:THR:HG22	1:C:513:VAL:HG22	1.81	0.62
1:D:44:HIS:HD2	1:D:470:ASP:OD2	1.82	0.62
1:D:401:ILE:HG21	1:D:409:VAL:CG1	2.28	0.62
1:C:329:VAL:CG1	1:C:331:THR:HG22	2.30	0.62
1:B:66:GLN:HE22	1:B:85:SER:HB3	1.65	0.62
1:D:141:TYR:O	1:D:143:GLU:HG3	2.00	0.62
1:D:331:THR:HG23	1:D:337:TYR:O	1.99	0.62
1:A:69:TYR:OH	1:A:94:HIS:HD2	1.83	0.62
1:C:49:SER:O	1:C:71:HIS:HE1	1.82	0.62
1:D:53:CYS:HB3	1:D:70:LEU:HB2	1.81	0.61
1:C:329:VAL:CG1	1:C:330:PRO:HD2	2.30	0.61
1:C:146:LEU:HD23	1:C:147:TYR:N	2.14	0.61
1:A:44:HIS:HD2	1:A:470:ASP:OD2	1.83	0.61
1:C:319:MET:HE2	1:C:342:SER:HA	1.81	0.61
1:A:192:ASP:OD2	1:A:195:ARG:HG3	2.00	0.61
1:A:412:SER:OG	1:A:424:ASN:ND2	2.34	0.61
1:C:329:VAL:HG12	1:C:331:THR:HG22	1.83	0.61
1:A:260:ALA:CB	1:A:265:LEU:HB2	2.31	0.60
1:C:422:HIS:O	1:C:438:PRO:HB2	2.01	0.60
1:A:329:VAL:CG1	1:A:330:PRO:HD2	2.31	0.60
1:C:81:TRP:HB2	1:C:99:MET:HB2	1.82	0.60
1:C:393:ARG:HH22	1:C:491:PHE:HB3	1.66	0.60
1:B:65:TYR:OH	1:B:306:ILE:HG12	2.02	0.60
1:A:81:TRP:HB2	1:A:99:MET:HB2	1.83	0.60
1:C:53:CYS:HB3	1:C:70:LEU:HB2	1.83	0.60
1:C:267:MET:HE3	1:C:323:LYS:HE2	1.84	0.60
1:B:183:TRP:O	1:B:204:ARG:HD2	2.00	0.59
1:C:160:PRO:HG2	2:C:714:HOH:O	2.02	0.59
1:D:329:VAL:CG1	1:D:330:PRO:HD2	2.31	0.59
1:B:330:PRO:HG3	1:B:444:TYR:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ALA:HA	1:D:215:ASN:HB2	1.85	0.59
1:B:398:GLU:HG2	1:B:464:HIS:CE1	2.38	0.59
1:B:470:ASP:HB3	2:B:735:HOH:O	2.03	0.59
1:D:223:ARG:HG3	1:D:223:ARG:HH11	1.68	0.59
1:C:319:MET:CE	1:C:340:GLN:HE21	2.15	0.58
1:A:168:ASP:HB3	2:A:703:HOH:O	2.02	0.58
1:C:132:THR:HG21	1:C:185:ARG:HB3	1.85	0.58
1:B:53:CYS:HB3	1:B:70:LEU:HB2	1.85	0.58
1:C:57:ARG:NH1	1:C:188:LYS:NZ	2.51	0.58
1:D:434:VAL:HB	1:D:487:GLN:HE22	1.68	0.58
1:C:331:THR:HG23	1:C:337:TYR:O	2.04	0.58
1:D:58:PRO:HG3	1:D:67:LEU:HD13	1.86	0.58
1:A:229:ASN:O	1:A:232:LEU:HB2	2.02	0.58
1:A:275:THR:HG22	1:A:276:TRP:N	2.18	0.58
1:D:184:PHE:HD1	1:D:204:ARG:HD3	1.67	0.58
1:D:470:ASP:HB3	2:D:617:HOH:O	2.03	0.57
1:A:140:LYS:HG3	1:A:141:TYR:CD1	2.39	0.57
1:C:302:THR:HG22	1:C:313:ARG:NH2	2.17	0.57
1:B:118:ASN:HB2	1:B:124:ALA:CA	2.34	0.57
1:C:257:SER:HA	1:C:268:THR:O	2.03	0.57
1:C:302:THR:CG2	1:C:313:ARG:NE	2.67	0.57
1:D:260:ALA:HB1	1:D:265:LEU:HB2	1.86	0.57
1:C:464:HIS:H	1:C:479:ASN:HD21	1.51	0.57
1:D:216:LEU:HA	1:D:219:TRP:CZ2	2.40	0.57
1:C:430:ALA:HB2	1:C:458:PRO:HG3	1.86	0.57
1:D:44:HIS:HE1	1:D:475:GLU:OE1	1.88	0.56
1:A:201:VAL:HG22	1:A:210:PHE:CE2	2.39	0.56
1:C:142:GLN:HE21	1:C:184:PHE:H	1.53	0.56
1:D:128:VAL:HG11	1:D:216:LEU:HD13	1.87	0.56
1:A:260:ALA:HB1	1:A:265:LEU:HB2	1.87	0.56
1:C:139:ARG:HD3	2:C:722:HOH:O	2.04	0.56
1:A:201:VAL:HG23	1:A:240:LEU:HD22	1.87	0.56
1:A:329:VAL:O	1:A:332:ASP:HB2	2.05	0.56
1:A:142:GLN:HE22	1:A:185:ARG:HH11	1.51	0.56
1:C:141:TYR:O	1:C:143:GLU:HG3	2.05	0.56
1:D:110:GLY:HA3	1:D:130:LEU:O	2.05	0.56
1:B:393:ARG:NH1	1:B:493:GLU:HA	2.21	0.56
1:A:348:ARG:CZ	1:A:360:LEU:HD12	2.36	0.56
1:D:49:SER:O	1:D:71:HIS:HE1	1.88	0.56
1:A:515:ARG:HD3	2:A:756:HOH:O	2.05	0.55
1:A:408:ASN:HB3	1:A:503:ASP:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ARG:HD3	2:C:763:HOH:O	2.06	0.55
1:B:268:THR:HG23	1:B:297:TRP:O	2.07	0.55
1:A:101:LEU:O	1:A:102:ARG:HG3	2.07	0.55
1:C:408:ASN:HB3	1:C:503:ASP:HB2	1.89	0.55
1:D:268:THR:HG21	1:D:292:ASP:CB	2.37	0.55
1:D:408:ASN:HB3	1:D:503:ASP:HB2	1.88	0.55
1:A:101:LEU:C	1:A:102:ARG:HG3	2.28	0.55
1:A:409:VAL:HG23	1:A:502:THR:HG22	1.88	0.55
1:C:257:SER:HB3	1:C:298:TYR:CE2	2.42	0.54
1:A:146:LEU:HD23	1:A:147:TYR:N	2.22	0.54
1:B:52:LEU:HD12	1:B:53:CYS:H	1.73	0.54
1:C:260:ALA:CB	1:C:265:LEU:HB2	2.37	0.54
1:C:319:MET:CE	1:C:342:SER:HA	2.38	0.54
1:B:163:VAL:HG13	1:B:164:ILE:HG13	1.89	0.54
1:C:142:GLN:HE22	1:C:185:ARG:HH11	1.55	0.54
1:D:260:ALA:CB	1:D:265:LEU:HB2	2.37	0.54
1:B:66:GLN:NE2	1:B:83:HIS:NE2	2.56	0.54
1:B:81:TRP:HB2	1:B:99:MET:HB2	1.90	0.54
1:B:268:THR:HG23	1:B:297:TRP:HB3	1.88	0.54
1:C:118:ASN:HB2	1:C:124:ALA:CA	2.37	0.54
1:C:143:GLU:CD	1:C:170:ARG:HH22	2.11	0.54
1:D:257:SER:HA	1:D:268:THR:O	2.07	0.54
1:B:66:GLN:NE2	1:B:85:SER:HB3	2.23	0.54
1:C:59:VAL:HG13	1:C:61:THR:HG23	1.90	0.54
1:B:201:VAL:HG21	1:B:240:LEU:HB2	1.89	0.54
1:B:41:ALA:HB2	1:B:340:GLN:HE21	1.72	0.53
1:B:329:VAL:CG1	1:B:330:PRO:HD2	2.38	0.53
1:B:206:ARG:HA	1:B:234:GLY:HA2	1.90	0.53
1:D:81:TRP:HB2	1:D:99:MET:HB2	1.89	0.53
1:C:120:ALA:HB2	1:C:216:LEU:HD12	1.90	0.53
1:C:319:MET:HE3	1:C:340:GLN:HE21	1.74	0.53
1:A:163:VAL:HG21	1:A:217:ARG:HA	1.91	0.53
1:C:425:ILE:CD1	1:C:467:ILE:HD13	2.35	0.53
1:D:414:GLY:O	1:D:495:ASP:HB3	2.09	0.53
1:C:230:HIS:HE1	2:C:750:HOH:O	1.90	0.52
1:D:324:TYR:HB2	1:D:327:ARG:CZ	2.40	0.52
1:A:139:ARG:NH1	2:A:740:HOH:O	2.41	0.52
1:C:239:ASP:OD1	1:C:302:THR:HB	2.09	0.52
1:A:329:VAL:HG12	1:A:331:THR:HG22	1.92	0.52
1:B:329:VAL:HG12	1:B:331:THR:H	1.75	0.52
1:B:52:LEU:HB3	1:B:339:GLY:HA3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:ASN:HB2	1:C:124:ALA:N	2.26	0.51
1:D:146:LEU:HD23	1:D:146:LEU:C	2.31	0.51
1:A:49:SER:O	1:A:71:HIS:HE1	1.93	0.51
1:C:434:VAL:CB	1:C:487:GLN:HE22	2.21	0.51
1:C:515:ARG:HG3	1:C:515:ARG:NH1	2.23	0.51
1:D:138:VAL:HG12	1:D:140:LYS:HG2	1.91	0.51
1:A:163:VAL:CG2	1:A:217:ARG:HA	2.40	0.51
1:A:276:TRP:NE1	1:A:278:GLY:HA2	2.25	0.51
1:B:142:GLN:HE21	1:B:184:PHE:H	1.57	0.51
1:C:367:LEU:HD11	1:C:517:ILE:HD13	1.91	0.51
1:C:174:THR:HB	1:C:175:PRO:HD2	1.93	0.51
1:D:267:MET:HE1	1:D:323:LYS:CG	2.41	0.51
1:D:434:VAL:CG1	1:D:487:GLN:NE2	2.69	0.51
1:C:44:HIS:HE1	1:C:475:GLU:OE1	1.92	0.51
1:C:143:GLU:OE2	1:C:165:VAL:HG13	2.10	0.51
1:C:395:TYR:OH	1:C:413:VAL:HG22	2.10	0.51
1:B:215:ASN:O	1:B:216:LEU:HB2	2.10	0.51
1:C:57:ARG:CD	1:C:188:LYS:HE3	2.34	0.51
1:D:324:TYR:O	1:D:327:ARG:NH1	2.44	0.51
1:B:59:VAL:HG12	1:B:66:GLN:HB2	1.92	0.51
1:C:44:HIS:HD2	1:C:470:ASP:OD2	1.94	0.51
1:B:57:ARG:HD2	1:B:188:LYS:HE2	1.92	0.50
1:C:393:ARG:HH22	1:C:491:PHE:CB	2.23	0.50
1:C:260:ALA:HB1	1:C:265:LEU:HB2	1.93	0.50
1:B:476:VAL:HG22	1:B:485:LEU:HB2	1.92	0.50
1:D:204:ARG:O	1:D:234:GLY:O	2.29	0.50
1:B:478:VAL:HB	1:B:483:THR:OG1	2.11	0.50
1:C:393:ARG:NH2	1:C:491:PHE:HB3	2.27	0.50
1:A:268:THR:CG2	1:A:269:TYR:H	2.03	0.50
1:C:57:ARG:HH11	1:C:188:LYS:HZ1	1.56	0.50
1:D:329:VAL:HG13	1:D:330:PRO:CD	2.40	0.50
1:B:257:SER:HB3	1:B:298:TYR:CE2	2.47	0.49
1:D:69:TYR:OH	1:D:94:HIS:HD2	1.95	0.49
1:D:518:GLY:O	1:D:519:GLN:HB3	2.11	0.49
1:B:401:ILE:O	1:B:462:SER:HA	2.12	0.49
1:C:141:TYR:CE1	1:C:170:ARG:HD3	2.47	0.49
1:C:409:VAL:CG2	1:C:502:THR:HG22	2.34	0.49
1:C:118:ASN:HB2	1:C:124:ALA:HA	1.92	0.49
1:C:132:THR:HG1	1:C:187:PRO:HD3	1.77	0.49
1:D:58:PRO:HG3	1:D:67:LEU:CD1	2.42	0.49
1:D:163:VAL:HG23	1:D:164:ILE:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLN:HE22	1:B:185:ARG:NH1	2.07	0.49
1:C:396:GLU:OE1	1:C:466:ARG:NH2	2.45	0.49
1:D:257:SER:HB3	1:D:298:TYR:CE2	2.47	0.49
1:B:461:ARG:HH21	1:D:171:ALA:HB2	1.78	0.49
1:C:401:ILE:O	1:C:462:SER:HA	2.13	0.48
1:D:206:ARG:HD3	1:D:234:GLY:HA2	1.95	0.48
1:D:215:ASN:O	1:D:216:LEU:HB2	2.13	0.48
1:A:401:ILE:O	1:A:462:SER:HA	2.13	0.48
1:C:486:SER:O	1:C:487:GLN:HG3	2.13	0.48
1:D:434:VAL:HB	1:D:487:GLN:NE2	2.27	0.48
1:A:140:LYS:HE3	1:A:141:TYR:HE1	1.77	0.48
1:C:206:ARG:HD3	1:C:234:GLY:HA2	1.95	0.48
1:D:118:ASN:HD21	1:D:123:GLY:HA2	1.77	0.48
1:B:382:VAL:HG22	1:B:509:PHE:CE2	2.49	0.48
1:D:142:GLN:HE21	1:D:184:PHE:H	1.59	0.48
1:D:401:ILE:O	1:D:462:SER:HA	2.14	0.48
1:B:138:VAL:HB	1:B:141:TYR:CD2	2.48	0.48
1:B:255:ALA:HB2	1:B:271:TYR:HB3	1.95	0.48
1:B:331:THR:HA	1:B:334:SER:OG	2.13	0.48
1:C:268:THR:CG2	1:C:269:TYR:N	2.73	0.48
1:A:266:PRO:HB2	1:A:268:THR:HG22	1.96	0.48
1:A:306:ILE:HD13	2:A:770:HOH:O	2.14	0.48
1:B:138:VAL:HG12	1:B:140:LYS:HG2	1.94	0.48
1:A:46:THR:HG22	1:A:340:GLN:HB3	1.96	0.48
1:A:183:TRP:HA	1:A:185:ARG:NH1	2.29	0.48
1:A:206:ARG:HA	1:A:234:GLY:HA2	1.96	0.48
1:A:483:THR:HA	2:A:690:HOH:O	2.13	0.48
1:D:403:TRP:CZ3	1:D:462:SER:HA	2.49	0.48
1:B:132:THR:OG1	1:B:144:GLN:NE2	2.37	0.48
1:D:434:VAL:HG11	1:D:487:GLN:NE2	2.28	0.48
1:A:114:VAL:HG23	1:A:114:VAL:O	2.14	0.47
1:B:59:VAL:HG22	1:B:114:VAL:HG12	1.96	0.47
1:B:487:GLN:HG2	2:B:659:HOH:O	2.13	0.47
1:D:138:VAL:CG1	1:D:140:LYS:HG2	2.44	0.47
1:B:382:VAL:HG22	1:B:509:PHE:HE2	1.78	0.47
1:C:268:THR:CG2	1:C:269:TYR:H	2.14	0.47
1:A:206:ARG:NH1	1:A:234:GLY:HA3	2.25	0.47
1:C:272:TRP:CE2	1:C:288:PRO:HB3	2.49	0.47
1:B:232:LEU:HA	1:B:260:ALA:HB2	1.97	0.47
1:B:422:HIS:O	1:B:438:PRO:HB2	2.15	0.47
1:C:64:ALA:HB2	1:C:87:THR:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:PRO:HA	1:D:201:VAL:O	2.15	0.47
1:D:493:GLU:HA	2:D:627:HOH:O	2.14	0.47
1:A:249:THR:CG2	1:A:251:HIS:NE2	2.78	0.47
1:B:49:SER:O	1:B:71:HIS:HE1	1.98	0.47
1:D:206:ARG:HH11	1:D:234:GLY:CA	2.28	0.47
1:A:260:ALA:HB3	1:A:265:LEU:HB2	1.97	0.47
1:A:275:THR:HG22	1:A:276:TRP:H	1.79	0.47
1:C:267:MET:HE1	1:C:323:LYS:HG2	1.96	0.47
1:D:44:HIS:CE1	1:D:475:GLU:OE1	2.67	0.47
1:D:398:GLU:HA	1:D:465:LEU:O	2.14	0.47
1:D:319:MET:HE1	1:D:340:GLN:OE1	2.15	0.47
1:B:401:ILE:HG21	1:B:409:VAL:CG1	2.45	0.46
1:B:401:ILE:HG21	1:B:409:VAL:HG13	1.96	0.46
1:C:329:VAL:CG1	1:C:330:PRO:CD	2.92	0.46
1:A:66:GLN:NE2	1:A:83:HIS:NE2	2.63	0.46
1:B:83:HIS:CD2	1:B:84:ALA:N	2.83	0.46
1:C:183:TRP:CE3	1:C:205:LEU:HD13	2.50	0.46
1:C:110:GLY:HA3	1:C:130:LEU:O	2.16	0.46
1:A:340:GLN:NE2	1:A:472:GLN:HB2	2.30	0.46
1:B:500:LEU:HD13	1:B:509:PHE:CG	2.51	0.46
1:C:206:ARG:NH1	1:C:234:GLY:H	2.14	0.46
1:C:235:ILE:HG23	1:C:256:ALA:CB	2.46	0.46
1:D:171:ALA:O	1:D:173:THR:HG23	2.15	0.46
1:B:130:LEU:HG	1:B:189:ILE:HD11	1.98	0.46
1:C:385:SER:HA	1:C:500:LEU:O	2.16	0.46
1:D:329:VAL:CG1	1:D:330:PRO:CD	2.94	0.46
1:D:184:PHE:CD1	1:D:204:ARG:HD3	2.48	0.45
1:C:324:TYR:O	1:C:327:ARG:HG2	2.16	0.45
1:D:130:LEU:HD13	1:D:189:ILE:HD11	1.99	0.45
1:D:183:TRP:O	1:D:204:ARG:HD2	2.16	0.45
1:B:344:VAL:HG12	1:B:364:VAL:HG13	1.97	0.45
1:D:143:GLU:HG2	1:D:166:ASN:H	1.81	0.45
1:D:178:ILE:HD11	2:D:757:HOH:O	2.16	0.45
1:D:494:GLY:O	1:D:496:THR:N	2.49	0.45
1:B:421:ARG:O	1:B:422:HIS:HB3	2.17	0.45
1:B:132:THR:HG21	1:B:185:ARG:HB3	1.97	0.45
1:B:446:LEU:HD21	1:B:490:HIS:CD2	2.51	0.45
1:C:206:ARG:NH1	1:C:234:GLY:N	2.64	0.45
1:C:206:ARG:HA	1:C:227:TYR:OH	2.17	0.45
1:D:229:ASN:O	1:D:232:LEU:HB2	2.17	0.45
1:A:329:VAL:CG1	1:A:331:THR:HG22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:NH1	1:C:188:LYS:HZ1	2.12	0.45
1:C:415:ARG:HA	1:C:422:HIS:HB3	1.99	0.45
1:D:464:HIS:H	1:D:479:ASN:HD21	1.63	0.45
1:A:110:GLY:HA3	1:A:130:LEU:O	2.17	0.45
1:D:252:TRP:HB2	1:D:275:THR:HA	1.99	0.45
1:A:64:ALA:HB2	1:A:87:THR:HG22	1.99	0.45
1:A:83:HIS:CD2	1:A:84:ALA:N	2.85	0.45
1:A:139:ARG:HD2	2:A:740:HOH:O	2.17	0.45
1:A:268:THR:CG2	1:A:269:TYR:N	2.68	0.45
1:B:268:THR:CG2	1:B:269:TYR:H	2.14	0.45
1:B:147:TYR:CE1	1:B:158:ALA:HB2	2.51	0.45
1:A:44:HIS:CE1	1:A:475:GLU:OE1	2.71	0.44
1:A:163:VAL:CG2	1:A:217:ARG:O	2.65	0.44
1:A:486:SER:O	1:A:487:GLN:HG3	2.17	0.44
1:A:201:VAL:HG21	1:A:240:LEU:HB2	1.99	0.44
1:B:138:VAL:CG1	1:B:140:LYS:HG2	2.46	0.44
1:B:211:TYR:HA	1:B:220:THR:O	2.18	0.44
1:C:188:LYS:HG2	1:C:239:ASP:HA	2.00	0.44
1:C:266:PRO:CB	1:C:268:THR:HG22	2.43	0.44
1:A:508:HIS:HD2	2:A:785:HOH:O	2.00	0.44
1:B:201:VAL:HG22	1:B:240:LEU:HD22	2.00	0.44
1:D:329:VAL:HG12	1:D:331:THR:H	1.81	0.44
1:A:140:LYS:HE3	1:A:141:TYR:CE1	2.52	0.44
1:B:163:VAL:CG2	1:B:217:ARG:HA	2.47	0.44
1:C:361:SER:HB2	1:C:484:VAL:HG21	2.00	0.44
1:A:118:ASN:HB2	1:A:124:ALA:HA	1.99	0.44
1:A:376:THR:HG22	1:A:513:VAL:HG22	1.99	0.44
1:B:305:SER:HB3	1:B:314:LEU:HD13	1.99	0.44
1:A:422:HIS:O	1:A:438:PRO:HB2	2.17	0.44
1:B:319:MET:HG3	1:B:342:SER:HA	2.00	0.44
1:B:349:LEU:HD12	1:B:358:THR:O	2.17	0.44
1:D:255:ALA:HB2	1:D:271:TYR:HB3	1.99	0.44
1:D:268:THR:CG2	1:D:297:TRP:HB3	2.46	0.44
1:A:140:LYS:HG3	1:A:141:TYR:HD1	1.83	0.44
1:B:330:PRO:HG3	1:B:444:TYR:CE2	2.53	0.44
1:C:515:ARG:NH1	2:C:720:HOH:O	2.50	0.44
1:D:382:VAL:HG13	1:D:509:PHE:CD2	2.52	0.44
1:A:44:HIS:HE1	1:A:475:GLU:OE1	2.01	0.44
1:C:44:HIS:CE1	1:C:475:GLU:OE1	2.70	0.44
1:A:257:SER:HA	1:A:268:THR:O	2.18	0.43
1:B:302:THR:HG22	1:B:315:ALA:HB2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLU:HG2	1:C:166:ASN:N	2.32	0.43
1:C:319:MET:HE1	1:C:340:GLN:HE21	1.83	0.43
1:A:500:LEU:HD13	1:A:509:PHE:CG	2.53	0.43
1:C:434:VAL:HB	1:C:487:GLN:NE2	2.28	0.43
1:D:63:GLY:O	1:D:64:ALA:HB2	2.18	0.43
1:A:183:TRP:O	1:A:204:ARG:HD2	2.18	0.43
1:B:217:ARG:NH1	2:B:695:HOH:O	2.52	0.43
1:C:143:GLU:CD	1:C:170:ARG:NH2	2.72	0.43
1:D:144:GLN:NE2	1:D:144:GLN:CA	2.81	0.43
1:C:201:VAL:CG2	1:C:240:LEU:HD22	2.49	0.43
1:B:184:PHE:HD1	1:B:204:ARG:HD3	1.83	0.43
1:C:179:GLU:HG2	1:C:205:LEU:HD22	2.00	0.43
1:D:345:ARG:HD3	1:D:361:SER:HB3	2.00	0.43
1:A:65:TYR:OH	1:A:306:ILE:HG12	2.19	0.43
1:B:145:TYR:CE2	1:B:162:PRO:HG3	2.54	0.43
1:B:158:ALA:HB1	2:B:632:HOH:O	2.19	0.43
1:B:412:SER:OG	1:B:424:ASN:ND2	2.52	0.43
1:C:146:LEU:HD23	1:C:146:LEU:C	2.38	0.43
1:A:391:ASN:HA	1:A:496:THR:O	2.18	0.43
1:C:329:VAL:HG13	1:C:330:PRO:CD	2.43	0.43
1:D:206:ARG:HA	1:D:234:GLY:HA2	2.01	0.43
1:A:255:ALA:HB2	1:A:271:TYR:HB3	2.01	0.42
1:B:144:GLN:O	1:B:163:VAL:HG12	2.19	0.42
1:D:66:GLN:NE2	1:D:66:GLN:HA	2.33	0.42
1:D:114:VAL:O	1:D:114:VAL:CG2	2.67	0.42
1:A:262:GLY:HA3	2:A:789:HOH:O	2.19	0.42
1:B:341:ASN:HD22	1:B:341:ASN:HA	1.64	0.42
1:D:51:TRP:HB2	1:D:75:ASN:HA	2.00	0.42
1:A:146:LEU:HD23	1:A:146:LEU:C	2.40	0.42
1:B:206:ARG:HD3	1:B:234:GLY:HA2	2.01	0.42
1:C:186:ASP:HB2	1:C:238:PRO:HD2	2.01	0.42
1:C:130:LEU:CG	1:C:189:ILE:HD11	2.46	0.42
1:C:178:ILE:HG13	1:C:179:GLU:N	2.34	0.42
1:D:130:LEU:HB2	1:D:189:ILE:HD11	2.02	0.42
1:D:306:ILE:HG13	1:D:307:ASP:N	2.35	0.42
1:D:486:SER:C	1:D:487:GLN:HG3	2.40	0.42
1:D:142:GLN:HE22	1:D:185:ARG:HH11	1.67	0.42
1:D:232:LEU:HD12	1:D:263:ILE:HD11	2.00	0.42
1:A:69:TYR:OH	1:A:94:HIS:CD2	2.70	0.42
1:A:144:GLN:NE2	1:A:187:PRO:HD3	2.35	0.42
1:A:351:ARG:HA	1:A:357:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:VAL:HG12	1:C:331:THR:H	1.85	0.42
1:D:425:ILE:N	1:D:425:ILE:HD12	2.34	0.42
1:A:164:ILE:HD11	1:A:219:TRP:CG	2.55	0.42
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.87	0.42
1:C:85:SER:O	1:C:92:PHE:HA	2.19	0.42
1:B:329:VAL:HG13	1:B:330:PRO:CD	2.48	0.41
1:B:432:LEU:HD22	1:B:432:LEU:HA	1.92	0.41
1:C:51:TRP:HB2	1:C:75:ASN:HA	2.01	0.41
1:C:132:THR:HA	1:C:143:GLU:O	2.20	0.41
1:C:291:LEU:HD23	1:C:291:LEU:HA	1.89	0.41
1:A:139:ARG:HG2	1:A:139:ARG:HH11	1.85	0.41
1:A:249:THR:HG22	1:A:251:HIS:NE2	2.36	0.41
1:B:211:TYR:HB3	1:B:219:TRP:HB3	2.01	0.41
1:D:421:ARG:O	1:D:422:HIS:HB3	2.20	0.41
1:B:161:ASP:HA	1:B:162:PRO:HD3	1.88	0.41
1:D:144:GLN:HG2	1:D:164:ILE:HB	2.02	0.41
1:A:340:GLN:HE22	1:A:472:GLN:HB2	1.86	0.41
1:B:50:GLY:HA3	1:B:71:HIS:HE1	1.85	0.41
1:C:65:TYR:OH	1:C:306:ILE:HG12	2.21	0.41
1:D:240:LEU:HA	1:D:253:VAL:O	2.21	0.41
1:A:51:TRP:HB2	1:A:75:ASN:HA	2.03	0.41
1:B:183:TRP:HA	1:B:185:ARG:NH1	2.36	0.41
1:B:409:VAL:HG22	1:B:502:THR:HG22	2.02	0.41
1:C:71:HIS:O	1:C:79:GLY:HA3	2.20	0.41
1:D:80:GLY:HA2	1:D:107:VAL:HB	2.03	0.41
1:B:144:GLN:HG2	1:B:164:ILE:HB	2.01	0.41
1:B:434:VAL:HG11	1:B:487:GLN:OE1	2.20	0.41
1:D:255:ALA:HB2	1:D:271:TYR:CB	2.51	0.41
1:A:289:GLN:HE22	1:A:358:THR:CB	2.34	0.41
1:A:412:SER:HB2	1:A:499:SER:OG	2.21	0.41
1:A:448:PRO:HD2	1:A:449:TYR:CE1	2.56	0.41
1:B:59:VAL:HG22	1:B:114:VAL:CG1	2.50	0.41
1:C:175:PRO:HA	1:C:178:ILE:HG12	2.03	0.41
1:C:289:GLN:NE2	1:C:356:TRP:HZ3	2.18	0.41
1:C:344:VAL:HG12	1:C:364:VAL:CG1	2.51	0.41
1:A:147:TYR:CE1	1:A:158:ALA:HB2	2.56	0.41
1:C:57:ARG:HH11	1:C:188:LYS:CE	2.33	0.41
1:C:66:GLN:HA	1:C:66:GLN:NE2	2.36	0.41
1:C:139:ARG:HG2	1:C:182:GLU:HG2	2.03	0.41
1:D:223:ARG:HB3	1:D:280:GLN:HB3	2.03	0.41
1:A:257:SER:HB3	1:A:298:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ARG:HD3	1:A:461:ARG:HA	1.93	0.40
1:B:227:TYR:CD1	1:B:227:TYR:N	2.89	0.40
1:C:188:LYS:HA	1:C:188:LYS:HD2	1.98	0.40
1:B:396:GLU:OE2	1:B:466:ARG:NE	2.48	0.40
1:C:302:THR:CG2	1:C:313:ARG:HH21	2.26	0.40
1:D:519:GLN:HB3	1:D:519:GLN:HE21	1.63	0.40
1:A:215:ASN:O	1:A:216:LEU:HB2	2.22	0.40
1:B:318:TRP:HA	1:B:341:ASN:HD22	1.85	0.40
1:C:398:GLU:HG2	1:C:466:ARG:HG3	2.03	0.40
1:D:98:VAL:HG22	1:D:156:PHE:CD1	2.57	0.40
1:D:132:THR:HG21	1:D:185:ARG:HB3	2.02	0.40
1:D:211:TYR:HB3	1:D:219:TRP:HB3	2.03	0.40
1:D:266:PRO:HB2	1:D:290:TRP:CE3	2.56	0.40
1:D:397:ILE:HD12	1:D:514:VAL:HG22	2.03	0.40
1:D:286:LEU:HD23	1:D:286:LEU:HA	1.79	0.40
1:B:344:VAL:HG12	1:B:364:VAL:CG1	2.52	0.40
1:D:268:THR:CG2	1:D:269:TYR:H	2.17	0.40
1:D:270:ALA:HA	1:D:289:GLN:O	2.21	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	477/490 (97%)	447 (94%)	28 (6%)	2 (0%)	34	55
1	B	477/490 (97%)	450 (94%)	23 (5%)	4 (1%)	19	37
1	C	477/490 (97%)	448 (94%)	29 (6%)	0	100	100
1	D	477/490 (97%)	440 (92%)	36 (8%)	1 (0%)	47	69
All	All	1908/1960 (97%)	1785 (94%)	116 (6%)	7 (0%)	34	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	B	173	THR
1	B	297	TRP
1	A	103	PRO
1	B	103	PRO
1	B	422	HIS
1	D	235	ILE

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	381/390 (98%)	369 (97%)	12 (3%)	40	64
1	B	381/390 (98%)	364 (96%)	17 (4%)	27	50
1	C	381/390 (98%)	368 (97%)	13 (3%)	37	60
1	D	381/390 (98%)	366 (96%)	15 (4%)	32	56
All	All	1524/1560 (98%)	1467 (96%)	57 (4%)	34	57

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TRP
1	A	90	VAL
1	A	98	VAL
1	A	104	ASP
1	A	168	ASP
1	A	204	ARG
1	A	311	THR
1	A	328	ASP
1	A	382	VAL
1	A	388	LEU
1	A	409	VAL
1	A	413	VAL
1	B	51	TRP
1	B	59	VAL
1	B	82	ASP

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Mol	Chain	Res	Type
1	B	104	ASP
1	B	114	VAL
1	B	144	GLN
1	B	159	LEU
1	B	178	ILE
1	B	193	THR
1	B	204	ARG
1	B	230	HIS
1	B	279	GLU
1	B	297	TRP
1	B	306	ILE
1	B	409	VAL
1	B	413	VAL
1	B	516	GLU
1	C	114	VAL
1	C	170	ARG
1	C	200	CYS
1	C	230	HIS
1	C	246	ASP
1	C	297	TRP
1	C	302	THR
1	C	314	LEU
1	C	347	LEU
1	C	399	LEU
1	C	413	VAL
1	C	446	LEU
1	C	493	GLU
1	D	59	VAL
1	D	82	ASP
1	D	144	GLN
1	D	161	ASP
1	D	201	VAL
1	D	223	ARG
1	D	232	LEU
1	D	292	ASP
1	D	297	TRP
1	D	310	GLU
1	D	314	LEU
1	D	327	ARG
1	D	364	VAL
1	D	382	VAL
1	D	519	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	66	GLN
1	A	71	HIS
1	A	94	HIS
1	A	133	GLN
1	A	142	GLN
1	A	144	GLN
1	A	180	ASN
1	A	190	HIS
1	A	280	GLN
1	A	289	GLN
1	A	341	ASN
1	A	408	ASN
1	A	424	ASN
1	A	479	ASN
1	A	487	GLN
1	A	508	HIS
1	A	519	GLN
1	B	66	GLN
1	B	71	HIS
1	B	74	GLN
1	B	76	ASN
1	B	133	GLN
1	B	142	GLN
1	B	144	GLN
1	B	180	ASN
1	B	230	HIS
1	B	280	GLN
1	B	289	GLN
1	B	341	ASN
1	B	408	ASN
1	B	424	ASN
1	B	479	ASN
1	B	487	GLN
1	B	488	GLN
1	C	44	HIS
1	C	66	GLN
1	C	71	HIS
1	C	94	HIS
1	C	133	GLN
1	C	142	GLN

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Mol	Chain	Res	Type
1	C	144	GLN
1	C	230	HIS
1	C	289	GLN
1	C	340	GLN
1	C	341	ASN
1	C	424	ASN
1	C	479	ASN
1	C	487	GLN
1	C	508	HIS
1	C	519	GLN
1	D	44	HIS
1	D	66	GLN
1	D	71	HIS
1	D	94	HIS
1	D	118	ASN
1	D	133	GLN
1	D	142	GLN
1	D	144	GLN
1	D	180	ASN
1	D	289	GLN
1	D	341	ASN
1	D	408	ASN
1	D	424	ASN
1	D	479	ASN
1	D	482	HIS
1	D	487	GLN
1	D	519	GLN

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 (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	479/490 (97%)	-0.10	5 (1%) 82 81	12, 24, 39, 55	0
1	B	479/490 (97%)	-0.09	4 (0%) 86 85	11, 27, 44, 59	0
1	C	479/490 (97%)	-0.13	0 100 100	12, 24, 36, 47	0
1	D	479/490 (97%)	-0.08	1 (0%) 95 95	13, 26, 39, 53	0
All	All	1916/1960 (97%)	-0.10	10 (0%) 91 90	11, 25, 39, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	173	THR	3.3
1	A	172	ALA	3.0
1	A	178	ILE	2.8
1	D	223	ARG	2.6
1	A	174	THR	2.5
1	B	172	ALA	2.5
1	B	178	ILE	2.4
1	B	234	GLY	2.1
1	A	168	ASP	2.1
1	A	173	THR	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.