



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:49 AM UTC

PDB ID : 4FFF / pdb_00004fff
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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

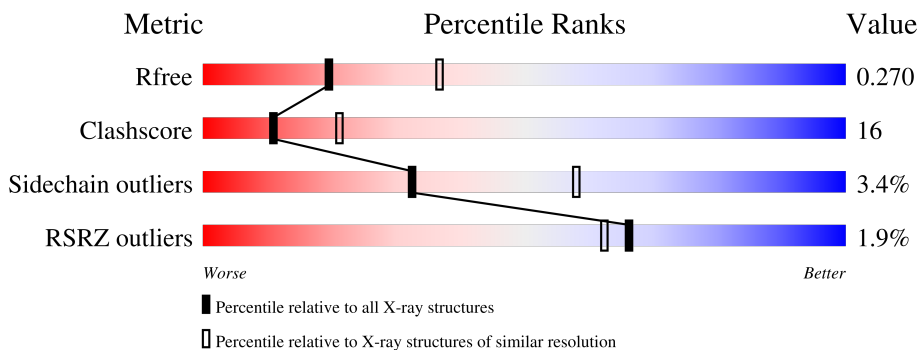
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 $\leq 5\%$. 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	490	 2% 68% 29% ..
1	B	490	 2% 70% 24% ..
1	C	490	 % 67% 29% ..
1	D	490	 2% 68% 27% ..

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
			Total	C	N	O	S			
1	A	479	3734	2372	644	710	8	0	0	0
1	B	479	3734	2372	644	710	8	0	0	0
1	C	479	3734	2372	644	710	8	0	0	0
1	D	479	3734	2372	644	710	8	0	0	0

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

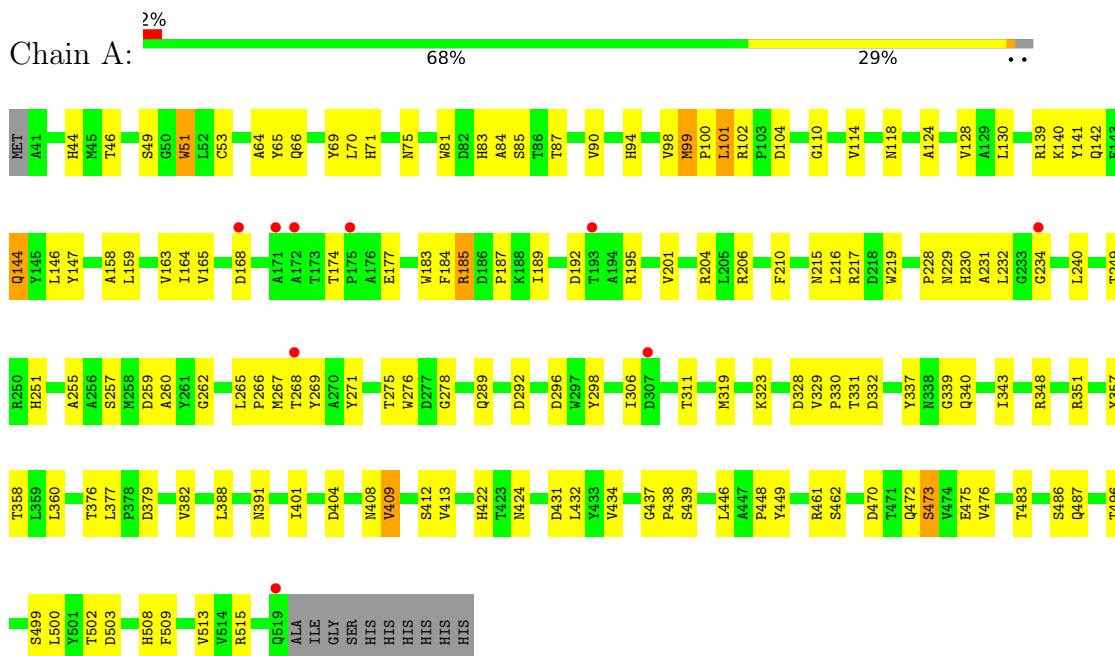
- Molecule 2 is water.

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

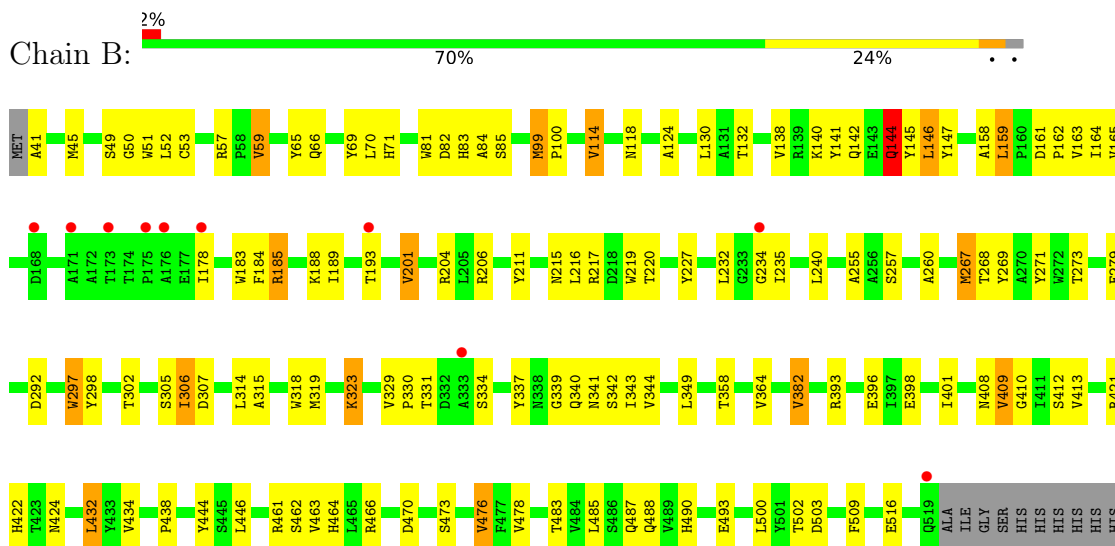
3 Residue-property plots

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.

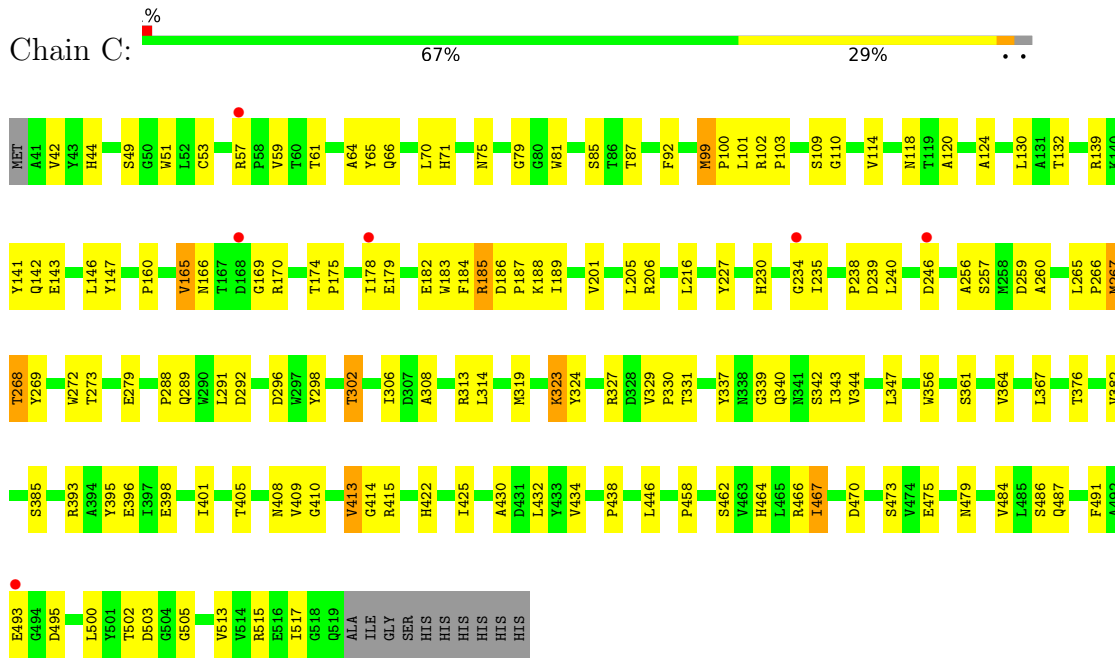
- Molecule 1: Levan fructotransferase



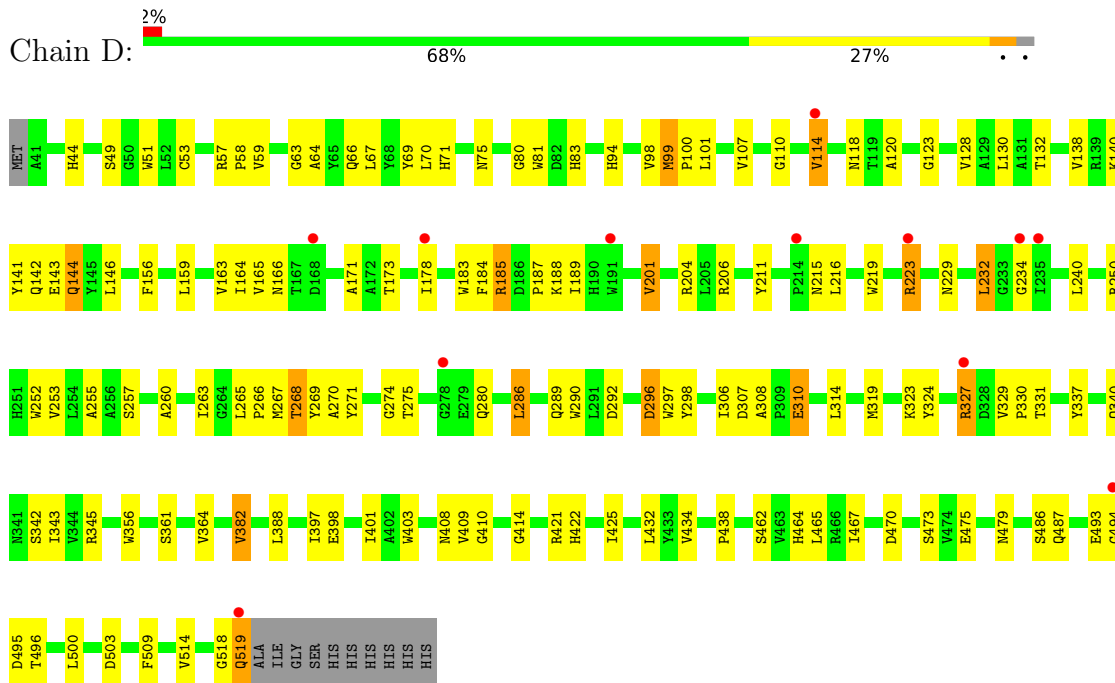
- Molecule 1: Levan fructotransferase



- Molecule 1: Levan fructotransferase



• Molecule 1: Levan fructotransferase



4 Data and refinement statistics

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 50.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	91.0 (50.00-2.57) 97.9 (50.00-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.96 (at 2.58Å)	Xtrriage
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	Xtrriage
Anisotropy	0.955	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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	0.41	0/3858	0.95	21/5305 (0.4%)
1	B	0.41	0/3858	0.94	17/5305 (0.3%)
1	C	0.44	0/3858	0.96	22/5305 (0.4%)
1	D	0.41	0/3858	0.95	17/5305 (0.3%)
All	All	0.42	0/15432	0.95	77/21220 (0.4%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	99	MET	CA-C-N	10.88	130.98	119.89
1	C	99	MET	C-N-CA	10.88	130.98	119.89
1	B	99	MET	CA-C-N	8.72	128.76	119.78
1	B	99	MET	C-N-CA	8.72	128.76	119.78
1	D	185	ARG	N-CA-C	8.33	119.63	108.38
1	A	99	MET	CA-C-N	7.88	128.35	119.92
1	A	99	MET	C-N-CA	7.88	128.35	119.92
1	D	99	MET	CA-C-N	7.72	128.18	119.92
1	D	99	MET	C-N-CA	7.72	128.18	119.92
1	D	432	LEU	N-CA-C	-7.45	92.71	107.69
1	C	343	ILE	N-CA-C	-7.20	100.22	109.80
1	A	185	ARG	N-CA-C	7.17	119.37	109.18
1	B	488	GLN	N-CA-C	-6.90	98.44	109.76
1	B	100	PRO	N-CA-C	6.90	122.18	111.21
1	A	100	PRO	N-CA-C	6.89	122.03	111.34
1	D	343	ILE	N-CA-C	-6.88	100.65	109.80
1	C	185	ARG	N-CA-C	6.75	118.06	108.74
1	A	165	VAL	N-CA-C	6.70	119.05	108.87
1	A	476	VAL	N-CA-C	6.65	117.46	107.75
1	A	339	GLY	N-CA-C	6.61	120.37	111.72
1	C	432	LEU	N-CA-C	-6.52	94.58	107.69
1	C	339	GLY	N-CA-C	6.44	120.16	111.72
1	B	267	MET	N-CA-C	-6.40	102.15	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	SER	N-CA-C	6.39	119.18	110.55
1	B	432	LEU	N-CA-C	-6.38	95.05	107.62
1	B	410	GLY	N-CA-C	6.37	119.78	110.80
1	A	432	LEU	N-CA-C	-6.37	95.08	107.62
1	A	473	SER	N-CA-C	6.36	118.21	108.42
1	A	101	LEU	N-CA-C	-6.25	102.28	110.53
1	D	100	PRO	N-CA-C	6.23	121.00	111.34
1	C	473	SER	N-CA-C	6.21	117.67	108.60
1	A	159	LEU	CA-C-N	6.14	127.52	119.84
1	A	159	LEU	C-N-CA	6.14	127.52	119.84
1	A	231	ALA	N-CA-C	-6.12	105.80	113.20
1	B	144	GLN	N-CA-C	6.11	118.65	108.20
1	B	307	ASP	N-CA-C	6.04	118.83	111.82
1	A	144	GLN	N-CA-C	6.01	118.52	108.96
1	D	308	ALA	CA-C-N	5.99	126.15	119.32
1	D	308	ALA	C-N-CA	5.99	126.15	119.32
1	B	473	SER	N-CA-C	5.96	117.31	108.60
1	B	165	VAL	N-CA-C	5.92	117.25	109.21
1	C	296	ASP	N-CA-C	5.91	118.93	107.71
1	D	286	LEU	N-CA-C	5.87	118.62	111.82
1	C	169	GLY	N-CA-C	5.76	119.64	112.73
1	B	235	ILE	N-CA-C	5.73	116.05	107.51
1	B	463	VAL	CB-CA-C	-5.72	103.84	111.80
1	D	268	THR	N-CA-C	5.65	116.65	108.34
1	C	100	PRO	N-CA-C	5.62	120.04	111.11
1	D	473	SER	N-CA-C	5.59	117.34	108.79
1	B	323	LYS	N-CA-C	-5.56	106.45	113.18
1	D	159	LEU	CA-C-N	5.56	126.79	119.84
1	D	159	LEU	C-N-CA	5.56	126.79	119.84
1	D	296	ASP	N-CA-C	5.49	118.14	107.71
1	A	343	ILE	N-CA-C	-5.48	102.52	109.80
1	A	431	ASP	N-CA-C	5.48	118.33	109.40
1	D	410	GLY	N-CA-C	5.47	118.52	110.80
1	C	42	VAL	N-CA-C	5.38	116.15	110.72
1	C	165	VAL	N-CA-C	5.36	116.50	109.21
1	A	379	ASP	N-CA-C	-5.33	103.44	110.43
1	A	228	PRO	N-CA-C	5.21	120.77	113.53
1	B	343	ILE	N-CA-C	-5.19	102.39	109.55
1	A	296	ASP	N-CA-C	5.17	118.66	107.49
1	C	101	LEU	N-CA-C	-5.17	102.83	110.48
1	C	268	THR	N-CA-C	5.16	115.93	108.34
1	B	185	ARG	N-CA-C	5.16	116.14	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	467	ILE	N-CA-C	5.15	115.27	107.75
1	C	410	GLY	N-CA-C	5.12	118.02	110.80
1	A	377	LEU	CA-C-N	5.12	125.12	119.90
1	A	377	LEU	C-N-CA	5.12	125.12	119.90
1	B	273	THR	N-CA-C	-5.07	102.97	110.48
1	D	165	VAL	N-CA-C	5.07	116.10	109.21
1	C	308	ALA	CA-C-N	5.05	125.08	119.32
1	C	308	ALA	C-N-CA	5.05	125.08	119.32
1	C	273	THR	N-CA-C	-5.04	103.06	110.52
1	C	323	LYS	N-CA-C	-5.02	106.66	112.89
1	C	267	MET	N-CA-C	-5.01	100.13	110.80
1	D	467	ILE	N-CA-C	5.00	115.06	107.80

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	113	0
1	B	3734	0	3484	105	0
1	C	3734	0	3484	131	0
1	D	3734	0	3484	127	0
2	A	189	0	0	9	0
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	475	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 (475) 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:319:MET:HE2	1:C:342:SER:HA	1.46	0.96
1:D:319:MET:HE2	1:D:342:SER:HA	1.46	0.95
1:C:409:VAL:HG23	1:C:502:THR:HG22	1.51	0.93
1:C:319:MET:HE3	1:C:340:GLN:HE21	1.34	0.90
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	0.82
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:D:267:MET:HE1	1:D:323:LYS:HG2	1.65	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:302:THR:CG2	1:C:313:ARG:HE	1.98	0.76
1:C:57:ARG:HH11	1:C:188:LYS:NZ	1.82	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
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:B:267:MET:HE1	1:B:323:LYS:HE2	1.68	0.75
1:D:268:THR:HG22	1:D:269:TYR:H	1.51	0.75
1:C:57:ARG:HH11	1:C:188:LYS:HZ1	1.33	0.74
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:D:267:MET:HE1	1:D:323:LYS:CG	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:267:MET:HE1	1:C:323:LYS:HG2	1.71	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:C:57:ARG:NH1	1:C:188:LYS:HZ1	1.89	0.70
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:A:319:MET:HE1	1:A:473:SER:CB	2.25	0.66
1:C:414:GLY:O	1:C:495:ASP:HB3	1.96	0.66
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:319:MET:HE3	1:B:340:GLN:OE1	2.00	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:B:267:MET:HE1	1:B:323:LYS:CE	2.30	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: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:A:101:LEU:C	1:A:102:ARG:HG3	2.28	0.59
1:B:330:PRO:HG3	1:B:444:TYR:CD2	2.37	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ARG:HG3	1:D:223:ARG:HH11	1.68	0.59
1:C:143:GLU:CD	1:C:170:ARG:HH22	2.11	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: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: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:A:275:THR:HG22	1:A:276:TRP:N	2.18	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:C:57:ARG:NH1	1:C:188:LYS:NZ	2.51	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:D:146:LEU:HD23	1:D:146:LEU:C	2.31	0.55
1:A:408:ASN:HB3	1:A:503:ASP:HB2	1.88	0.55
1:C:102:ARG:HD3	2:C:763:HOH:O	2.06	0.55
1:C:319:MET:CE	1:C:340:GLN:HE21	2.15	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:267:MET:HE1	1:C:323:LYS:CG	2.37	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: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: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
1:C:118:ASN:HB2	1:C:124:ALA:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:D:518:GLY:O	1:D:519:GLN:HB3	2.11	0.49
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:C:146:LEU:HD23	1:C:146:LEU:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:259:ASP:OD1	1:A:267:MET:HE3	2.13	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: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:B:59:VAL:HG22	1:B:114:VAL:HG12	1.96	0.47
1:C:143:GLU:CD	1:C:170:ARG:NH2	2.72	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:A:267:MET:HE1	1:A:323:LYS:CE	2.45	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:A:146:LEU:HD23	1:A:146:LEU:C	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:206:ARG:HH11	1:D:234:GLY:CA	2.28	0.47
1:D:486:SER:C	1:D:487:GLN:HG3	2.40	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: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:A:114:VAL:O	1:A:114:VAL:HG23	2.14	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:319:MET:HE1	1:A:473:SER:HB2	1.97	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:TRP:H	1:D:356:TRP:CD1	2.34	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
1:C:143:GLU:HG2	1:C:166:ASN:N	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:142:GLN:HE21	1:D:184:PHE:C	2.27	0.43
1:B:217:ARG:NH1	2:B:695:HOH:O	2.52	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: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:C:259:ASP:OD2	1:C:267:MET:HE3	2.19	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:331:THR:HA	1:B:334:SER:HG	1.83	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: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:A:144:GLN:CD	1:A:144:GLN:N	2.78	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: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
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:A:230:HIS:C	1:A:232:LEU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:319:MET:HE3	1:D:340:GLN:OE1	2.21	0.41
1:A:340:GLN:HE22	1:A:472:GLN:HB2	1.86	0.41
1:A:486:SER:C	1:A:487:GLN:HG3	2.45	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:45:MET:HE1	1:B:69:TYR:CD2	2.56	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:437:GLY:C	1:A:439:SER:H	2.29	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:102:ARG:O	1:C:103:PRO:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ARG:HB3	1:D:280:GLN:HB3	2.03	0.41
1:D:267:MET:HE1	1:D:323:LYS:HG3	1.99	0.41
1:A:257:SER:HB3	1:A:298:TYR:CE2	2.56	0.40
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:141:TYR:O	1:B:142:GLN:C	2.62	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
1:D:296:ASP:HB3	1:D:319:MET:C	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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%)	370 (97%)	11 (3%)	37	63
1	B	381/390 (98%)	363 (95%)	18 (5%)	23	46
1	C	381/390 (98%)	371 (97%)	10 (3%)	40	66
1	D	381/390 (98%)	368 (97%)	13 (3%)	32	58
All	All	1524/1560 (98%)	1472 (97%)	52 (3%)	32	58

All (52) 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	311	THR
1	A	328	ASP
1	A	382	VAL
1	A	388	LEU
1	A	409	VAL
1	A	413	VAL
1	A	446	LEU
1	B	51	TRP
1	B	59	VAL
1	B	82	ASP
1	B	114	VAL
1	B	144	GLN
1	B	146	LEU
1	B	159	LEU
1	B	178	ILE
1	B	193	THR
1	B	201	VAL
1	B	279	GLU
1	B	297	TRP
1	B	306	ILE
1	B	382	VAL
1	B	409	VAL
1	B	413	VAL
1	B	476	VAL
1	B	516	GLU
1	C	114	VAL
1	C	246	ASP
1	C	279	GLU
1	C	302	THR

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Mol	Chain	Res	Type
1	C	314	LEU
1	C	347	LEU
1	C	382	VAL
1	C	413	VAL
1	C	446	LEU
1	C	493	GLU
1	D	59	VAL
1	D	101	LEU
1	D	114	VAL
1	D	144	GLN
1	D	201	VAL
1	D	223	ARG
1	D	232	LEU
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 (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	62	HIS
1	A	66	GLN
1	A	71	HIS
1	A	76	ASN
1	A	94	HIS
1	A	142	GLN
1	A	144	GLN
1	A	180	ASN
1	A	280	GLN
1	A	289	GLN
1	A	341	ASN
1	A	422	HIS
1	A	424	ASN
1	A	479	ASN
1	A	487	GLN
1	A	519	GLN
1	B	66	GLN
1	B	71	HIS

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Mol	Chain	Res	Type
1	B	74	GLN
1	B	76	ASN
1	B	142	GLN
1	B	144	GLN
1	B	280	GLN
1	B	289	GLN
1	B	341	ASN
1	B	391	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	62	HIS
1	C	66	GLN
1	C	71	HIS
1	C	94	HIS
1	C	133	GLN
1	C	142	GLN
1	C	144	GLN
1	C	180	ASN
1	C	230	HIS
1	C	289	GLN
1	C	340	GLN
1	C	341	ASN
1	C	408	ASN
1	C	424	ASN
1	C	479	ASN
1	C	487	GLN
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	282	HIS
1	D	289	GLN

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Mol	Chain	Res	Type
1	D	341	ASN
1	D	391	ASN
1	D	408	ASN
1	D	424	ASN
1	D	479	ASN
1	D	482	HIS
1	D	487	GLN
1	D	508	HIS
1	D	519	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 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	479/490 (97%)	-0.04	9 (1%) 66 62	12, 24, 39, 55	0
1	B	479/490 (97%)	0.08	10 (2%) 63 59	11, 27, 44, 59	0
1	C	479/490 (97%)	-0.04	6 (1%) 75 72	12, 24, 36, 47	0
1	D	479/490 (97%)	0.17	12 (2%) 58 54	13, 26, 39, 53	0
All	All	1916/1960 (97%)	0.04	37 (1%) 66 62	11, 25, 39, 59	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	GLY	4.3
1	C	234	GLY	3.7
1	D	234	GLY	3.6
1	A	171	ALA	3.4
1	B	519	GLN	3.3
1	B	168	ASP	3.2
1	A	234	GLY	3.1
1	A	519	GLN	3.1
1	A	168	ASP	3.1
1	C	178	ILE	3.0
1	D	178	ILE	2.9
1	D	327	ARG	2.9
1	D	494	GLY	2.7
1	B	176	ALA	2.7
1	D	223	ARG	2.7
1	D	114	VAL	2.7
1	C	57	ARG	2.7
1	C	493	GLU	2.6
1	B	171	ALA	2.5
1	B	173	THR	2.5
1	B	193	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	175	PRO	2.3
1	C	246	ASP	2.3
1	B	333	ALA	2.3
1	C	168	ASP	2.2
1	D	519	GLN	2.2
1	A	268	THR	2.2
1	A	172	ALA	2.1
1	D	278	GLY	2.1
1	B	178	ILE	2.1
1	D	168	ASP	2.1
1	A	193	THR	2.1
1	D	191	TRP	2.0
1	D	235	ILE	2.0
1	A	307	ASP	2.0
1	B	175	PRO	2.0
1	D	214	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.