



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:19 PM UTC

PDB ID : 6LIU / pdb_00006liu
Title : Crystal structure of apo Tyrosine decarboxylase
Authors : Yu, J.; Wang, H.; Yao, M.
Deposited on : 2019-12-13
Resolution : 2.80 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
Xtriage (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

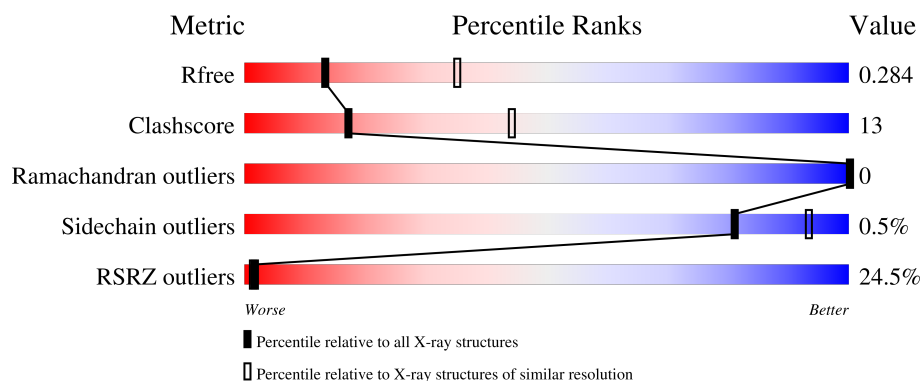
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	531	2% 73% 16% 10%
1	B	531	4% 75% 14% 10%
1	C	531	2% 78% 11% 11%
1	D	531	2% 76% 13% 11%
1	E	531	67% 47% 39% 14%

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Mol	Chain	Length	Quality of chain
1	F	531	52% 46% 33% 21%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22059 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 Tyrosine/DOPA decarboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3766	2420	632	690	24			
1	B	477	Total	C	N	O	S	0	0	0
			3766	2420	632	690	24			
1	C	474	Total	C	N	O	S	0	0	0
			3746	2409	629	684	24			
1	D	474	Total	C	N	O	S	0	0	0
			3746	2409	629	684	24			
1	E	459	Total	C	N	O	S	0	0	0
			3616	2323	606	663	24			
1	F	419	Total	C	N	O	S	0	0	0
			3295	2120	555	597	23			

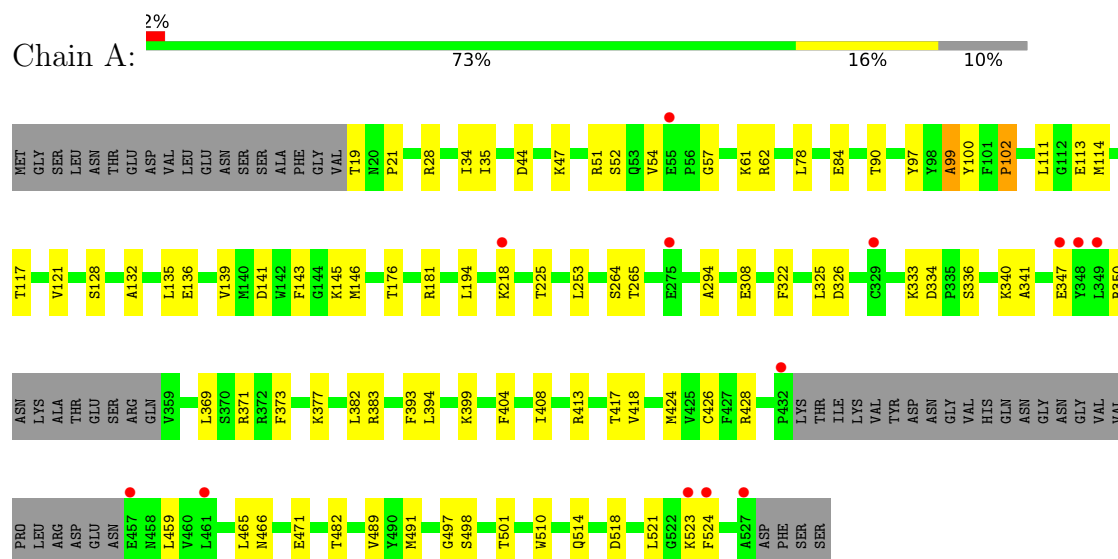
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	31	Total	O	0	0
			31	31		
2	B	28	Total	O	0	0
			28	28		
2	C	18	Total	O	0	0
			18	18		
2	D	31	Total	O	0	0
			31	31		
2	E	9	Total	O	0	0
			9	9		
2	F	7	Total	O	0	0
			7	7		

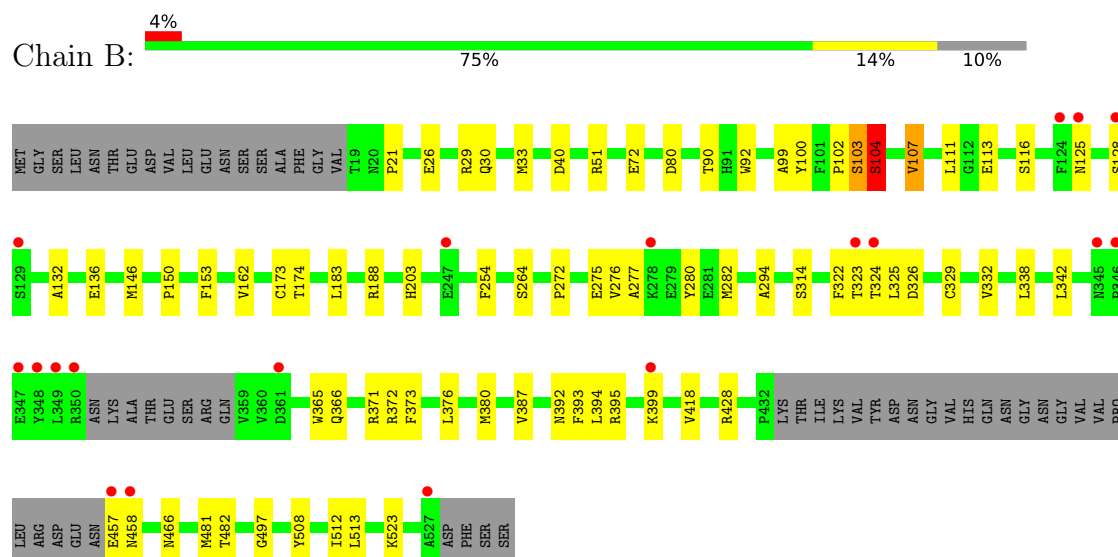
3 Residue-property plots [i](#)

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.

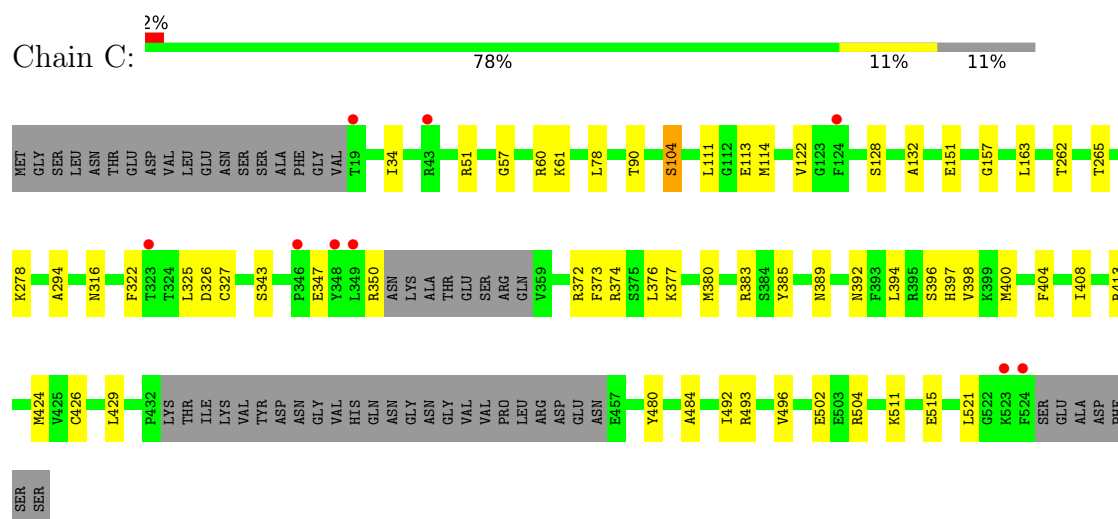
• Molecule 1: Tyrosine/DOPA decarboxylase 2



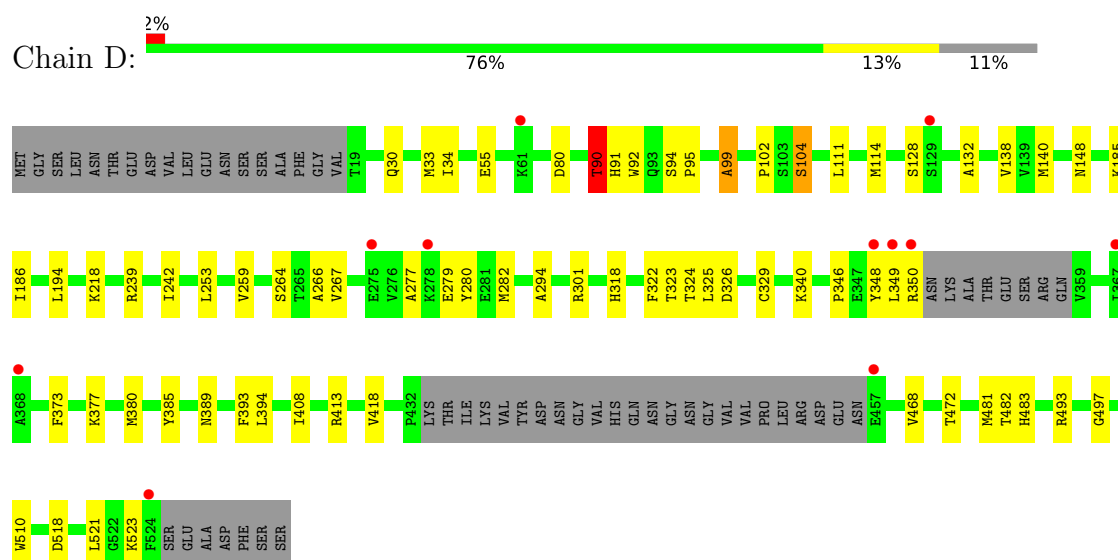
• Molecule 1: Tyrosine/DOPA decarboxylase 2



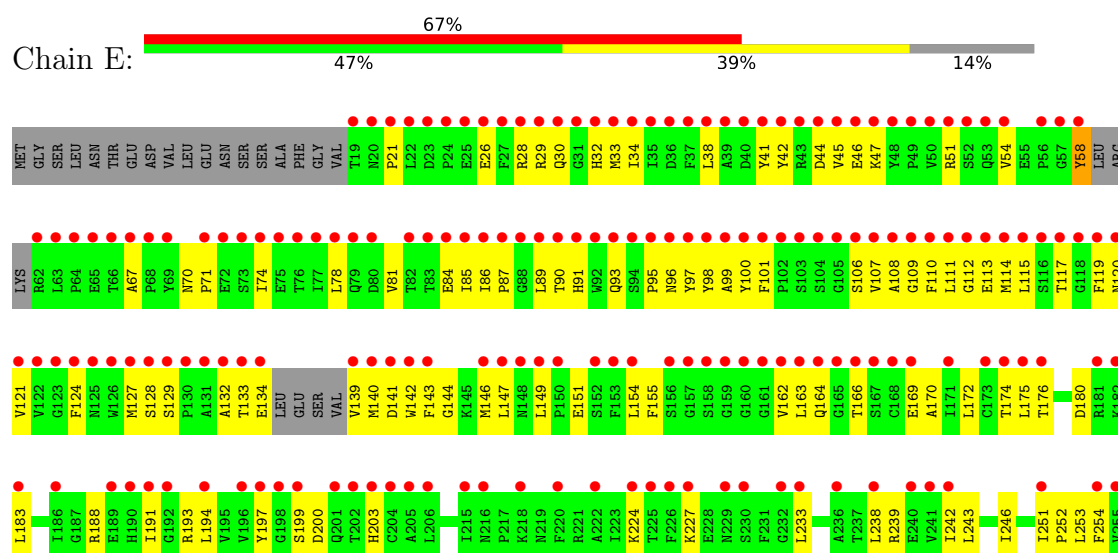
• Molecule 1: Tyrosine/DOPA decarboxylase 2

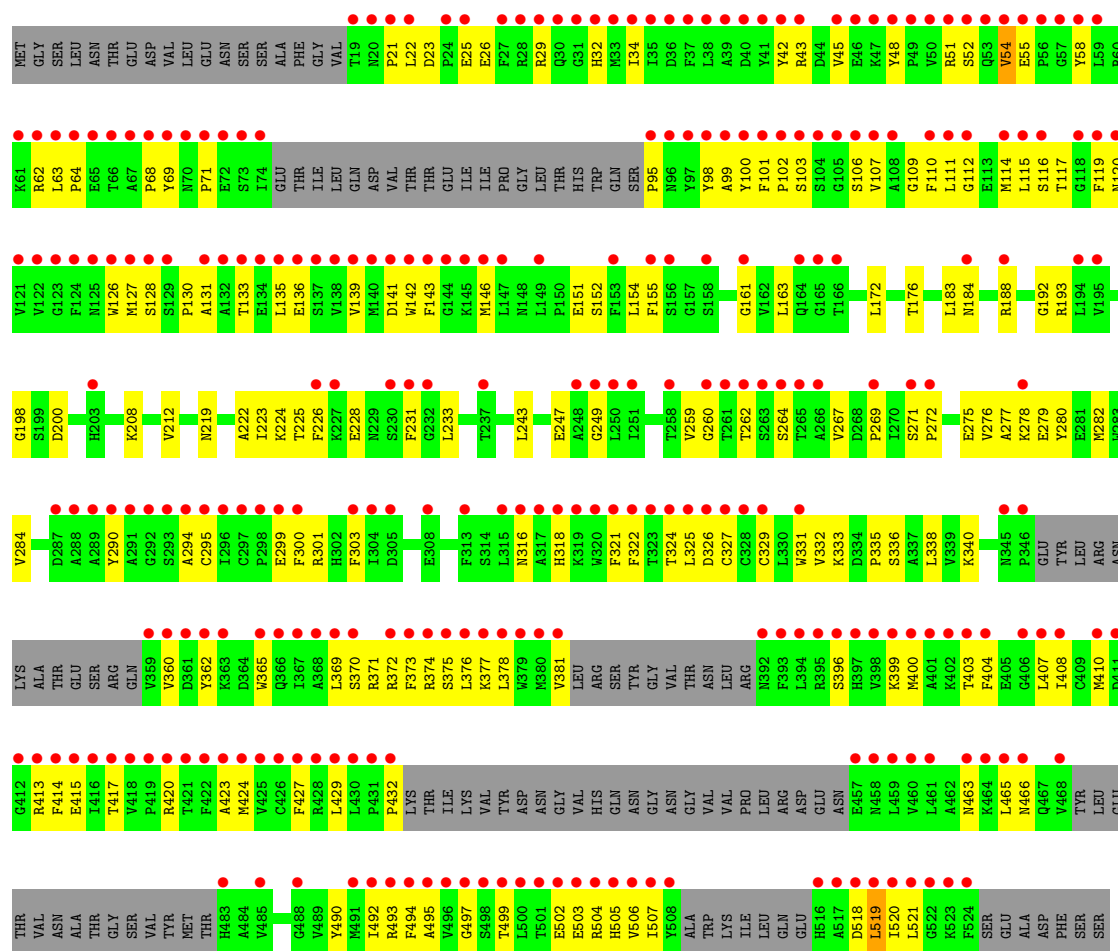


• Molecule 1: Tyrosine/DOPA decarboxylase 2



• Molecule 1: Tyrosine/DOPA decarboxylase 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	118.04Å 180.86Å 217.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.13 – 2.80 48.13 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.13-2.80) 94.0 (48.13-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.241 , 0.280 0.247 , 0.284	Depositor DCC
R_{free} test set	5754 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	47.9	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22059	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.17 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4684e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.38	4/3859 (0.1%)	0.37	0/5241
1	B	0.33	2/3859 (0.1%)	0.40	2/5241 (0.0%)
1	C	0.29	0/3839	0.37	0/5214
1	D	0.39	3/3839 (0.1%)	0.43	4/5214 (0.1%)
1	E	0.27	0/3705	0.53	1/5033 (0.0%)
1	F	0.24	0/3374	0.49	0/4570
All	All	0.32	9/22475 (0.0%)	0.43	7/30513 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	TYR	C-O	-7.12	1.17	1.24
1	A	102	PRO	C-O	-6.05	1.16	1.23
1	A	97	TYR	C-O	-5.80	1.17	1.24
1	D	94	SER	CA-C	-5.64	1.46	1.53
1	B	100	TYR	C-O	-5.58	1.19	1.24
1	B	107	VAL	C-O	-5.35	1.18	1.24
1	D	99	ALA	C-O	-5.30	1.16	1.23
1	D	95	PRO	C-O	-5.29	1.17	1.24
1	A	99	ALA	C-O	-5.01	1.17	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	90	THR	N-CA-C	-6.54	97.85	108.52
1	D	94	SER	CA-C-N	5.67	125.29	119.56
1	D	94	SER	C-N-CA	5.67	125.29	119.56
1	B	104	SER	N-CA-C	5.59	118.66	109.76
1	E	515	GLU	N-CA-C	-5.44	105.00	111.69
1	B	103	SER	N-CA-C	-5.09	98.56	107.73
1	D	91	HIS	N-CA-C	5.01	117.44	108.17

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	3766	0	3724	62	0
1	B	3766	0	3724	61	0
1	C	3746	0	3708	48	0
1	D	3746	0	3708	56	0
1	E	3616	0	3563	207	0
1	F	3295	0	3257	177	0
2	A	31	0	0	4	0
2	B	28	0	0	0	0
2	C	18	0	0	1	0
2	D	31	0	0	2	0
2	E	9	0	0	8	0
2	F	7	0	0	1	0
All	All	22059	0	21684	551	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 13.

All (551) 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:F:100:TYR:HA	1:F:493:ARG:HH22	1.14	1.10
1:E:113:GLU:CD	1:F:117:THR:HG21	1.77	1.09
1:F:100:TYR:HA	1:F:493:ARG:NH2	1.73	1.03
1:E:473:VAL:HG12	1:E:516:HIS:ND1	1.73	1.02
1:E:113:GLU:OE2	1:F:117:THR:HG21	1.59	1.00
1:F:111:LEU:O	1:F:115:LEU:HD23	1.62	0.99
1:F:63:LEU:HA	2:F:601:HOH:O	1.61	0.99
1:E:44:ASP:HB2	1:E:47:LYS:HD3	1.47	0.96
1:F:100:TYR:CA	1:F:493:ARG:HH22	1.78	0.95
1:E:113:GLU:OE1	1:F:117:THR:HG21	1.68	0.94
1:A:117:THR:HG23	1:B:324:THR:HG21	1.54	0.89
1:F:316:ASN:HD22	1:F:318:HIS:HE1	1.22	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:MET:SD	1:F:410:MET:O	2.35	0.84
1:E:424:MET:SD	1:E:493:ARG:NH1	2.51	0.83
1:F:278:LYS:HZ3	1:F:284:VAL:CG2	1.92	0.83
1:E:203:HIS:HE1	1:F:369:LEU:HD11	1.44	0.82
1:E:111:LEU:HD22	1:F:34:ILE:HG13	1.63	0.80
1:E:26:GLU:HG2	1:E:29:ARG:HD3	1.62	0.79
1:F:278:LYS:NZ	1:F:284:VAL:HG23	1.99	0.78
1:E:81:VAL:HA	1:E:85:ILE:HD13	1.64	0.78
1:D:483:HIS:HD2	2:D:621:HOH:O	1.67	0.78
1:E:107:VAL:HA	1:E:110:PHE:HB3	1.67	0.77
1:F:100:TYR:CA	1:F:493:ARG:NH2	2.40	0.77
1:E:54:VAL:HG11	1:E:58:TYR:CD2	2.19	0.77
1:F:278:LYS:NZ	1:F:284:VAL:CG2	2.48	0.77
1:D:277:ALA:HA	1:D:282:MET:HE3	1.67	0.76
1:F:102:PRO:HG3	1:F:497:GLY:HA3	1.64	0.76
1:F:519:LEU:HD12	1:F:519:LEU:C	2.12	0.74
1:F:136:GLU:OE2	1:F:371:ARG:NH2	2.21	0.74
1:E:389:ASN:OD1	1:F:71:PRO:HB3	1.87	0.74
1:C:114:MET:HG2	1:D:114:MET:HE2	1.70	0.73
1:E:113:GLU:OE2	1:F:117:THR:CG2	2.37	0.73
1:E:120:ASN:HA	2:E:604:HOH:O	1.89	0.72
1:A:99:ALA:HB1	1:A:482:THR:HG23	1.71	0.72
1:B:277:ALA:HA	1:B:282:MET:HE3	1.70	0.72
1:E:457:GLU:CG	2:E:603:HOH:O	2.37	0.71
1:A:264:SER:HB2	1:A:418:VAL:HG21	1.70	0.71
1:E:378:LEU:O	1:E:382:LEU:HD12	1.91	0.71
1:F:111:LEU:O	1:F:115:LEU:CD2	2.38	0.71
1:E:382:LEU:O	1:E:386:GLY:N	2.24	0.71
1:D:264:SER:HB2	1:D:418:VAL:HG21	1.73	0.69
1:E:51:ARG:HA	1:E:90:THR:HG23	1.73	0.69
1:F:278:LYS:HZ3	1:F:284:VAL:HG21	1.56	0.69
1:E:398:VAL:HG22	1:E:423:ALA:HB2	1.75	0.69
1:E:397:HIS:CG	1:E:497:GLY:HA2	2.27	0.69
1:A:143:PHE:HA	1:A:146:MET:HE3	1.74	0.68
1:F:100:TYR:N	1:F:493:ARG:HH22	1.92	0.68
1:A:113:GLU:HG2	1:A:377:LYS:HD3	1.74	0.67
1:C:128:SER:O	1:D:90:THR:HB	1.94	0.67
1:D:99:ALA:HB1	1:D:482:THR:HG23	1.77	0.67
1:E:457:GLU:HB2	2:E:603:HOH:O	1.95	0.67
1:F:280:TYR:HB2	1:F:282:MET:HE2	1.77	0.67
1:F:116:SER:HB2	1:F:376:LEU:HD12	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:GLU:OE1	1:F:117:THR:CG2	2.43	0.66
1:E:457:GLU:HG2	2:E:603:HOH:O	1.94	0.66
1:C:343:SER:HB3	1:C:350:ARG:HD3	1.77	0.65
1:E:114:MET:HG3	1:E:117:THR:HG21	1.78	0.65
1:E:67:ALA:HB2	1:F:142:TRP:HB3	1.78	0.65
1:B:102:PRO:HG2	1:B:497:GLY:HA3	1.78	0.65
1:F:399:LYS:HD3	1:F:399:LYS:H	1.61	0.65
1:C:429:LEU:HD11	1:C:521:LEU:HD11	1.78	0.65
1:E:289:ALA:HA	1:E:316:ASN:H	1.61	0.65
1:F:408:ILE:HG23	1:F:414:PHE:HB3	1.77	0.65
1:A:21:PRO:O	1:B:107:VAL:HG23	1.97	0.65
1:E:140:MET:HE3	1:E:140:MET:HA	1.79	0.64
1:F:396:SER:O	1:F:400:MET:HG2	1.97	0.64
1:E:127:MET:HE1	1:F:51:ARG:NH2	2.12	0.64
1:F:415:GLU:HG2	1:F:417:THR:HG23	1.78	0.64
1:B:523:LYS:HE2	1:D:218:LYS:HE2	1.79	0.64
1:F:372:ARG:HE	1:F:372:ARG:HA	1.63	0.64
1:F:427:PHE:CZ	1:F:492:ILE:HG23	2.33	0.64
1:F:429:LEU:HD22	1:F:465:LEU:HD21	1.78	0.63
1:A:35:ILE:HD11	1:A:114:MET:HE1	1.80	0.63
1:A:336:SER:O	1:A:340:LYS:HG3	1.98	0.63
1:C:113:GLU:OE2	1:C:372:ARG:NH2	2.31	0.63
1:F:325:LEU:HD12	1:F:325:LEU:H	1.63	0.63
1:E:408:ILE:HG23	1:E:414:PHE:HB3	1.81	0.63
1:A:399:LYS:NZ	2:A:602:HOH:O	2.32	0.63
1:E:325:LEU:HD22	1:F:372:ARG:HD2	1.81	0.62
1:E:115:LEU:HD12	1:E:380:MET:HE1	1.81	0.62
1:E:301:ARG:HD3	1:E:304:ILE:HG13	1.79	0.62
1:E:476:THR:HG21	1:E:516:HIS:HE1	1.65	0.62
1:D:280:TYR:HB2	1:D:282:MET:HE2	1.80	0.62
1:E:383:ARG:HD3	1:F:68:PRO:HG3	1.81	0.62
1:D:408:ILE:HD13	1:D:510:TRP:CZ3	2.33	0.62
1:A:136:GLU:OE1	1:A:371:ARG:NH2	2.30	0.62
1:D:408:ILE:HD13	1:D:510:TRP:HZ3	1.64	0.61
1:E:96:ASN:HB3	1:E:479:VAL:HG12	1.81	0.61
1:E:141:ASP:OD2	1:E:155:PHE:HB2	2.00	0.61
1:D:346:PRO:HB2	1:D:348:TYR:CE1	2.36	0.61
1:B:104:SER:HG	1:B:322:PHE:H	1.48	0.61
1:E:100:TYR:O	1:E:493:ARG:NH2	2.33	0.61
1:B:264:SER:HB2	1:B:418:VAL:HG21	1.82	0.61
1:E:38:LEU:HD11	1:F:115:LEU:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:ARG:HH22	1:F:64:PRO:HG2	1.66	0.61
1:C:347:GLU:HA	1:C:350:ARG:HG2	1.83	0.61
1:B:280:TYR:HB2	1:B:282:MET:HE2	1.83	0.60
1:E:290:TYR:HB2	1:E:319:LYS:HG2	1.83	0.60
1:E:289:ALA:HA	1:E:315:LEU:HA	1.84	0.60
1:F:278:LYS:HZ3	1:F:284:VAL:HG23	1.59	0.60
1:C:325:LEU:HG	1:C:326:ASP:HB3	1.83	0.60
1:E:134:GLU:C	2:E:605:HOH:O	2.44	0.60
1:E:117:THR:HB	1:F:110:PHE:CE2	2.36	0.60
1:A:413:ARG:NH1	1:A:518:ASP:OD1	2.35	0.60
1:B:523:LYS:HE2	1:D:218:LYS:CE	2.31	0.60
1:E:143:PHE:HA	1:E:146:MET:HE3	1.83	0.60
1:A:181:ARG:NH2	1:A:334:ASP:OD2	2.34	0.60
1:E:30:GLN:HB3	1:F:111:LEU:HD11	1.82	0.60
1:E:113:GLU:O	1:E:117:THR:HG23	2.01	0.60
1:E:151:GLU:HA	1:E:154:LEU:HB2	1.83	0.60
1:E:106:SER:HB3	1:E:109:GLY:H	1.66	0.60
1:E:502:GLU:HG3	1:E:503:GLU:H	1.65	0.60
1:B:104:SER:OG	1:B:322:PHE:N	2.32	0.59
1:F:112:GLY:HA2	1:F:115:LEU:HD21	1.84	0.59
1:E:97:TYR:CZ	1:E:99:ALA:HB3	2.38	0.59
1:E:51:ARG:CZ	1:E:474:ASN:HB3	2.31	0.59
1:E:30:GLN:HA	1:E:33:MET:HE3	1.84	0.59
1:E:28:ARG:HG2	1:E:32:HIS:CE1	2.38	0.59
1:F:277:ALA:HA	1:F:282:MET:HE3	1.85	0.58
1:B:102:PRO:CG	1:B:497:GLY:HA3	2.34	0.58
1:E:89:LEU:HD23	1:E:91:HIS:ND1	2.19	0.58
1:F:23:ASP:OD1	1:F:25:GLU:HG2	2.04	0.58
1:F:326:ASP:OD1	1:F:326:ASP:N	2.36	0.58
1:A:57:GLY:O	1:A:61:LYS:HD2	2.04	0.58
1:E:111:LEU:C	1:E:114:MET:H	2.11	0.58
1:F:420:ARG:HD3	1:F:420:ARG:N	2.19	0.58
1:F:324:THR:HG23	1:F:377:LYS:HD3	1.87	0.57
1:C:122:VAL:HB	1:D:92:TRP:CZ2	2.40	0.57
1:E:406:GLY:O	1:E:410:MET:HG2	2.04	0.57
1:E:84:GLU:HB2	1:E:85:ILE:HD12	1.86	0.57
1:E:111:LEU:HD23	1:E:114:MET:HE3	1.87	0.57
1:F:155:PHE:HE2	1:F:161:GLY:H	1.51	0.57
1:F:404:PHE:HA	1:F:407:LEU:HD12	1.87	0.56
1:A:19:THR:N	2:A:603:HOH:O	2.36	0.56
1:E:95:PRO:O	1:E:501:THR:OG1	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:ARG:HD3	1:F:420:ARG:H	1.69	0.56
1:F:278:LYS:NZ	1:F:284:VAL:HG21	2.19	0.56
1:A:417:THR:HG21	1:A:491:MET:HG2	1.87	0.56
1:E:30:GLN:HG3	1:E:33:MET:HE3	1.87	0.56
1:B:150:PRO:HD2	1:B:153:PHE:HD2	1.70	0.56
1:E:34:ILE:HG13	1:F:111:LEU:HD22	1.88	0.56
1:F:424:MET:HA	1:F:494:PHE:O	2.06	0.56
1:B:26:GLU:OE2	1:B:29:ARG:NH2	2.30	0.55
1:D:239:ARG:NH2	1:D:279:GLU:OE1	2.37	0.55
1:E:321:PHE:HE1	1:E:394:LEU:HD11	1.72	0.55
1:F:135:LEU:O	1:F:139:VAL:HG23	2.05	0.55
1:F:372:ARG:NH2	1:F:373:PHE:HB2	2.21	0.55
1:A:176:THR:HG22	1:A:341:ALA:HB1	1.87	0.55
1:D:413:ARG:HD2	1:D:521:LEU:HD12	1.87	0.55
1:F:316:ASN:HD22	1:F:318:HIS:CE1	2.14	0.55
1:A:34:ILE:HG13	1:B:111:LEU:HD22	1.88	0.55
1:F:115:LEU:HD23	1:F:115:LEU:H	1.71	0.55
1:F:336:SER:O	1:F:340:LYS:HG3	2.07	0.55
1:D:102:PRO:HG2	1:D:497:GLY:HA3	1.89	0.55
1:A:90:THR:HB	1:B:128:SER:O	2.07	0.54
1:E:114:MET:HA	1:E:117:THR:HG23	1.89	0.54
1:C:90:THR:HB	1:D:128:SER:O	2.08	0.54
1:F:184:ASN:HA	1:F:188:ARG:NH1	2.21	0.54
1:A:413:ARG:HD2	1:A:521:LEU:HD12	1.89	0.54
1:E:197:TYR:CD1	1:E:282:MET:HE1	2.41	0.54
1:B:457:GLU:HG3	1:B:458:ASN:H	1.72	0.54
1:C:111:LEU:HD11	1:D:30:GLN:HB3	1.87	0.54
1:E:373:PHE:CD1	1:E:376:LEU:HG	2.43	0.54
1:F:295:CYS:HB3	1:F:301:ARG:HG3	1.90	0.54
1:E:191:ILE:HG13	1:E:194:LEU:HD12	1.88	0.54
1:E:172:LEU:O	1:E:176:THR:HG22	2.08	0.54
1:E:315:LEU:HG	1:E:331:TRP:HH2	1.72	0.54
1:F:192:GLY:O	1:F:219:ASN:ND2	2.40	0.54
1:C:404:PHE:CE2	1:C:408:ILE:HD11	2.43	0.53
1:E:90:THR:HB	1:F:128:SER:O	2.08	0.53
1:E:163:LEU:HD22	1:E:327:CYS:SG	2.49	0.53
1:F:372:ARG:CZ	1:F:373:PHE:HB2	2.38	0.53
1:F:427:PHE:CE1	1:F:492:ILE:HG23	2.43	0.53
1:E:470:LEU:HD22	1:E:492:ILE:HD12	1.91	0.53
1:B:146:MET:HE3	1:B:387:VAL:HG22	1.91	0.53
1:F:43:ARG:HG3	1:F:43:ARG:HH11	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:LEU:HD23	1:F:370:SER:H	1.74	0.53
1:E:46:GLU:OE2	1:E:504:ARG:NH2	2.42	0.53
1:E:89:LEU:HD23	1:E:91:HIS:HD1	1.73	0.53
1:C:265:THR:HB	1:C:424:MET:HE2	1.91	0.53
1:A:194:LEU:HD13	1:A:253:LEU:HD22	1.91	0.53
1:E:470:LEU:HD13	1:E:492:ILE:HG23	1.91	0.53
1:E:470:LEU:HB2	1:E:492:ILE:HD12	1.90	0.52
1:E:383:ARG:CZ	1:F:68:PRO:HD3	2.38	0.52
1:E:429:LEU:HD13	1:E:430:LEU:N	2.25	0.52
1:B:428:ARG:HB2	1:B:466:ASN:ND2	2.25	0.52
1:C:294:ALA:HA	1:C:394:LEU:HD13	1.91	0.52
1:D:104:SER:HB3	1:D:322:PHE:H	1.74	0.52
1:D:294:ALA:HA	1:D:394:LEU:HD13	1.90	0.52
1:E:58:TYR:CD1	1:E:58:TYR:C	2.85	0.52
1:E:41:TYR:HA	1:E:44:ASP:OD1	2.10	0.52
1:C:34:ILE:HG13	1:D:111:LEU:HD22	1.92	0.52
1:C:111:LEU:HD22	1:D:34:ILE:HG13	1.91	0.52
1:D:185:LYS:HG3	1:D:186:ILE:HG23	1.92	0.52
1:E:162:VAL:HG23	1:E:374:ARG:HH22	1.75	0.52
1:B:272:PRO:HA	1:B:275:GLU:HG2	1.91	0.52
1:E:233:LEU:HD21	1:E:238:LEU:HB2	1.91	0.52
1:F:95:PRO:N	1:F:505:HIS:HE2	2.07	0.52
1:A:459:LEU:HD11	1:A:489:VAL:HG22	1.91	0.51
1:E:139:VAL:O	1:E:142:TRP:HB2	2.11	0.51
1:E:297:CYS:HB3	1:E:391:ARG:NH1	2.25	0.51
1:F:143:PHE:HA	1:F:146:MET:HE3	1.91	0.51
1:E:100:TYR:CE1	1:E:482:THR:HG21	2.46	0.51
1:E:238:LEU:O	1:E:242:ILE:HG13	2.10	0.51
1:F:152:SER:HB2	1:F:333:LYS:HE2	1.93	0.51
1:A:128:SER:O	1:B:90:THR:HB	2.10	0.51
1:B:30:GLN:HA	1:B:33:MET:HE3	1.91	0.51
1:B:136:GLU:OE1	1:B:371:ARG:NH2	2.44	0.51
1:E:408:ILE:HG12	1:E:510:TRP:CH2	2.45	0.51
1:B:366:GLN:OE1	1:B:371:ARG:NH1	2.41	0.51
1:C:392:ASN:O	1:C:396:SER:OG	2.27	0.51
1:E:391:ARG:NH2	1:E:391:ARG:HB3	2.25	0.51
1:F:424:MET:HG3	1:F:495:ALA:HB2	1.92	0.51
1:B:332:VAL:HG11	1:B:338:LEU:HD11	1.92	0.51
1:E:472:THR:O	1:E:476:THR:HG23	2.11	0.51
1:F:504:ARG:HA	1:F:507:ILE:HD12	1.93	0.51
1:A:136:GLU:CD	1:A:371:ARG:HH22	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:THR:HG22	1:E:360:VAL:HG13	1.91	0.51
1:F:267:VAL:HG21	1:F:303:PHE:CD1	2.44	0.51
1:D:242:ILE:HD13	1:D:282:MET:HE1	1.92	0.51
1:E:193:ARG:NH1	1:E:251:ILE:HD11	2.25	0.51
1:A:424:MET:HE3	1:A:426:CYS:SG	2.51	0.51
1:B:173:CYS:SG	1:B:366:GLN:HA	2.51	0.51
1:E:476:THR:HG21	1:E:516:HIS:CE1	2.46	0.51
1:F:58:TYR:O	1:F:62:ARG:HG3	2.11	0.51
1:F:321:PHE:HA	1:F:322:PHE:CD2	2.46	0.50
1:E:415:GLU:HB2	1:E:430:LEU:HD11	1.93	0.50
1:F:54:VAL:HG11	1:F:58:TYR:CG	2.46	0.50
1:B:113:GLU:OE2	1:B:372:ARG:NH2	2.44	0.50
1:E:133:THR:O	1:E:362:TYR:HE2	1.93	0.50
1:B:174:THR:HG22	1:B:254:PHE:CE1	2.47	0.50
1:E:108:ALA:HB3	1:E:385:TYR:HE1	1.75	0.50
1:A:225:THR:HA	2:A:607:HOH:O	2.10	0.50
1:F:48:TYR:HE2	1:F:52:SER:HA	1.76	0.50
1:E:326:ASP:OD1	1:E:326:ASP:N	2.43	0.50
1:E:332:VAL:HG22	1:E:334:ASP:H	1.77	0.50
1:E:498:SER:HB3	1:E:501:THR:OG1	2.12	0.50
1:E:183:LEU:HD11	1:E:191:ILE:HB	1.94	0.50
1:A:333:LYS:CD	2:A:605:HOH:O	2.59	0.50
1:D:102:PRO:CG	1:D:497:GLY:HA3	2.42	0.50
1:E:264:SER:O	1:E:264:SER:OG	2.25	0.50
1:F:294:ALA:HB1	1:F:300:PHE:CD2	2.47	0.50
1:B:481:MET:HE1	1:B:513:LEU:HD21	1.94	0.50
1:E:111:LEU:CD2	1:E:114:MET:HE3	2.42	0.50
1:E:166:THR:HB	1:E:169:GLU:H	1.77	0.50
1:E:42:TYR:CE2	1:F:22:LEU:HD21	2.47	0.49
1:E:381:VAL:O	1:E:385:TYR:HB2	2.12	0.49
1:F:200:ASP:OD2	1:F:224:LYS:HD2	2.12	0.49
1:F:316:ASN:HB3	1:F:318:HIS:CE1	2.46	0.49
1:A:135:LEU:O	1:A:139:VAL:HG22	2.11	0.49
1:D:346:PRO:HB2	1:D:348:TYR:HE1	1.75	0.49
1:E:393:PHE:HA	1:E:396:SER:HB3	1.93	0.49
1:D:413:ARG:NH1	1:D:518:ASP:OD1	2.45	0.49
1:E:252:PRO:HB2	1:E:282:MET:SD	2.51	0.49
1:E:400:MET:SD	1:E:502:GLU:HA	2.51	0.49
1:E:481:MET:HE1	1:E:513:LEU:HD21	1.93	0.49
1:F:260:GLY:H	1:F:267:VAL:HG12	1.77	0.49
1:F:378:LEU:O	1:F:381:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:MET:HE1	1:A:382:LEU:HD22	1.94	0.49
1:A:393:PHE:CZ	1:B:21:PRO:HG3	2.47	0.49
1:E:180:ASP:CG	1:E:188:ARG:HH22	2.21	0.49
1:E:41:TYR:O	1:E:45:VAL:HG13	2.13	0.49
1:E:387:VAL:N	1:F:68:PRO:O	2.45	0.49
1:F:99:ALA:C	1:F:493:ARG:NH2	2.71	0.49
1:D:346:PRO:HD2	1:D:349:LEU:HD12	1.94	0.49
1:E:321:PHE:CE1	1:E:394:LEU:HD11	2.47	0.49
1:F:101:PHE:CE2	1:F:262:THR:HA	2.48	0.49
1:D:325:LEU:HG	1:D:326:ASP:HB3	1.95	0.49
1:F:98:TYR:HB3	1:F:494:PHE:HA	1.94	0.49
1:B:183:LEU:HB3	1:B:188:ARG:HD3	1.95	0.48
1:E:127:MET:HE1	1:F:51:ARG:CZ	2.43	0.48
1:E:277:ALA:HB1	1:E:282:MET:HB2	1.94	0.48
1:B:107:VAL:O	1:B:111:LEU:HG	2.12	0.48
1:D:148:ASN:HB3	1:D:301:ARG:HE	1.78	0.48
1:E:101:PHE:CE2	1:E:262:THR:HA	2.49	0.48
1:F:223:ILE:HB	1:F:233:LEU:HD11	1.94	0.48
1:C:502:GLU:OE1	1:C:504:ARG:NH1	2.39	0.48
1:E:112:GLY:HA3	1:E:377:LYS:HA	1.93	0.48
1:E:233:LEU:O	1:E:269:PRO:HD2	2.13	0.48
1:E:325:LEU:CD2	1:F:372:ARG:HD2	2.44	0.48
1:A:62:ARG:HD2	1:A:84:GLU:OE1	2.14	0.48
1:E:385:TYR:HB3	1:E:389:ASN:HB3	1.95	0.48
1:A:322:PHE:CZ	1:A:393:PHE:HB3	2.49	0.48
1:E:114:MET:HA	1:E:117:THR:CG2	2.43	0.48
1:F:420:ARG:H	1:F:420:ARG:CD	2.27	0.48
1:F:503:GLU:O	1:F:506:VAL:HB	2.14	0.48
1:B:125:ASN:H	1:B:128:SER:HB2	1.78	0.48
1:D:259:VAL:HG13	1:D:267:VAL:HG13	1.96	0.48
1:E:366:GLN:NE2	1:E:368:ALA:HB3	2.29	0.48
1:F:372:ARG:HG3	1:F:373:PHE:H	1.77	0.48
1:A:428:ARG:HB2	1:A:466:ASN:ND2	2.28	0.48
1:E:30:GLN:HG2	1:E:74:ILE:HG21	1.96	0.48
1:F:372:ARG:NE	1:F:373:PHE:H	2.12	0.48
1:A:102:PRO:CG	1:A:497:GLY:HA3	2.44	0.48
1:F:103:SER:O	1:F:103:SER:OG	2.26	0.48
1:F:327:CYS:SG	1:F:374:ARG:HB3	2.54	0.48
1:B:51:ARG:HA	1:B:90:THR:HG23	1.96	0.48
1:E:380:MET:HE3	1:E:380:MET:HB2	1.75	0.48
1:F:243:LEU:O	1:F:247:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:ILE:HD13	1:C:78:LEU:HD21	1.95	0.47
1:D:322:PHE:CZ	1:D:393:PHE:HB3	2.48	0.47
1:E:457:GLU:CB	2:E:603:HOH:O	2.54	0.47
1:F:141:ASP:OD2	1:F:155:PHE:HB2	2.14	0.47
1:E:499:THR:OG1	1:E:500:LEU:N	2.45	0.47
1:D:325:LEU:HA	1:D:326:ASP:HA	1.64	0.47
1:A:294:ALA:HA	1:A:394:LEU:HD13	1.96	0.47
1:D:194:LEU:HD13	1:D:253:LEU:HD22	1.96	0.47
1:E:289:ALA:CA	1:E:316:ASN:H	2.27	0.47
1:B:174:THR:HG22	1:B:254:PHE:HE1	1.79	0.47
1:B:294:ALA:HA	1:B:394:LEU:HD13	1.96	0.47
1:E:469:TYR:O	1:E:472:THR:OG1	2.28	0.47
1:C:60:ARG:HD3	1:D:138:VAL:HG22	1.97	0.47
1:E:387:VAL:HB	1:F:69:TYR:HA	1.95	0.47
1:E:469:TYR:OH	1:E:513:LEU:O	2.28	0.47
1:F:116:SER:O	1:F:120:ASN:N	2.29	0.47
1:F:269:PRO:HB2	1:F:272:PRO:HD2	1.96	0.47
1:F:332:VAL:HG11	1:F:338:LEU:HD11	1.96	0.47
1:E:321:PHE:CZ	1:E:390:LEU:HD22	2.50	0.47
1:F:329:CYS:HB3	1:F:331:TRP:CZ3	2.50	0.47
1:A:28:ARG:NH2	1:B:40:ASP:OD1	2.48	0.47
1:C:262:THR:O	1:C:493:ARG:NH2	2.47	0.47
1:C:380:MET:HE2	1:C:380:MET:HB3	1.84	0.47
1:E:132:ALA:HA	1:E:373:PHE:CE1	2.50	0.47
1:E:299:GLU:HG3	1:E:300:PHE:CE2	2.50	0.46
1:E:400:MET:HB3	1:E:506:VAL:HG21	1.97	0.46
1:F:208:LYS:O	1:F:212:VAL:HG23	2.15	0.46
1:A:102:PRO:HG2	1:A:497:GLY:HA3	1.96	0.46
1:C:394:LEU:O	1:C:398:VAL:HG23	2.15	0.46
1:F:226:PHE:HB3	1:F:228:GLU:HG2	1.97	0.46
1:E:199:SER:OG	1:E:200:ASP:N	2.47	0.46
1:E:299:GLU:HG3	1:E:300:PHE:CD2	2.50	0.46
1:F:188:ARG:HD3	1:F:188:ARG:N	2.31	0.46
1:F:110:PHE:O	1:F:114:MET:HG2	2.16	0.46
1:F:404:PHE:CE1	1:F:408:ILE:HD11	2.50	0.46
1:D:132:ALA:HA	1:D:373:PHE:CE1	2.50	0.46
1:E:119:PHE:HB3	1:E:121:VAL:HG13	1.98	0.46
1:E:408:ILE:HG23	1:E:414:PHE:CB	2.45	0.46
1:F:264:SER:O	1:F:264:SER:OG	2.30	0.46
1:F:429:LEU:N	1:F:466:ASN:OD1	2.46	0.46
1:B:116:SER:OG	1:B:373:PHE:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:THR:O	1:F:120:ASN:HB2	2.15	0.46
1:F:362:TYR:HA	1:F:365:TRP:CD1	2.50	0.46
1:A:44:ASP:HB3	1:A:47:LYS:HE2	1.98	0.46
1:E:227:LYS:HA	1:E:227:LYS:HD2	1.86	0.46
1:A:99:ALA:CB	1:A:482:THR:HG23	2.44	0.46
1:D:348:TYR:CE1	1:E:520:ILE:HG21	2.51	0.46
1:D:468:VAL:O	1:D:472:THR:HG23	2.16	0.46
1:E:402:LYS:HA	1:E:405:GLU:HB3	1.98	0.46
1:F:259:VAL:HA	1:F:267:VAL:HG12	1.96	0.46
1:A:218:LYS:HA	1:A:218:LYS:HD3	1.58	0.46
1:A:325:LEU:HA	1:A:326:ASP:HA	1.65	0.46
1:A:465:LEU:HD13	1:A:524:PHE:HE1	1.81	0.46
1:F:463:ASN:ND2	1:F:490:TYR:H	2.13	0.46
1:D:111:LEU:HB2	1:D:380:MET:HE2	1.97	0.45
1:B:104:SER:O	1:B:323:THR:O	2.34	0.45
1:C:327:CYS:HB2	1:C:377:LYS:NZ	2.31	0.45
1:C:385:TYR:O	1:C:389:ASN:HB2	2.16	0.45
1:F:373:PHE:CE1	1:F:376:LEU:HG	2.51	0.45
1:E:110:PHE:CE2	1:E:111:LEU:HD21	2.52	0.45
1:E:146:MET:HE1	1:E:382:LEU:CD2	2.46	0.45
1:E:407:LEU:HD13	1:E:510:TRP:CD1	2.52	0.45
1:F:43:ARG:HG3	1:F:43:ARG:NH1	2.31	0.45
1:E:164:GLN:O	1:E:328:CYS:N	2.28	0.45
1:F:275:GLU:O	1:F:279:GLU:HG3	2.17	0.45
1:D:318:HIS:HA	1:D:323:THR:O	2.17	0.45
1:E:70:ASN:HB3	1:E:71:PRO:HD2	1.98	0.45
1:E:111:LEU:CD2	1:F:34:ILE:HG13	2.40	0.45
1:F:133:THR:HG22	1:F:360:VAL:HG23	1.99	0.45
1:F:519:LEU:C	1:F:519:LEU:CD1	2.85	0.45
1:F:127:MET:HE3	1:F:127:MET:O	2.16	0.45
1:F:271:SER:OG	1:F:272:PRO:HD3	2.17	0.45
1:E:147:LEU:HG	1:E:296:ILE:HG22	1.98	0.45
1:E:194:LEU:HB3	1:E:253:LEU:HD22	1.98	0.45
1:F:371:ARG:HH11	1:F:371:ARG:HB3	1.82	0.45
1:E:391:ARG:CB	1:E:391:ARG:HH21	2.30	0.45
1:E:473:VAL:HA	1:E:476:THR:HG23	1.99	0.45
1:F:106:SER:OG	1:F:109:GLY:N	2.33	0.45
1:F:272:PRO:O	1:F:276:VAL:HG23	2.16	0.45
1:B:324:THR:HG22	1:B:325:LEU:O	2.18	0.44
1:E:386:GLY:HA2	1:F:68:PRO:HG2	1.98	0.44
1:E:32:HIS:HD2	1:F:32:HIS:ND1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LEU:C	1:F:115:LEU:CD2	2.89	0.44
1:A:369:LEU:HD13	1:B:203:HIS:HE1	1.81	0.44
1:F:290:TYR:OH	1:F:423:ALA:HB3	2.17	0.44
1:B:162:VAL:HB	1:B:365:TRP:CE3	2.53	0.44
1:E:124:PHE:CE1	1:E:363:LYS:HE2	2.53	0.44
1:E:224:LYS:HA	1:E:224:LYS:HD3	1.58	0.44
1:E:93:GLN:OE1	1:E:499:THR:HG21	2.17	0.44
1:E:373:PHE:CE1	1:E:376:LEU:HG	2.52	0.44
1:F:42:TYR:HA	1:F:45:VAL:HG23	2.00	0.44
1:F:116:SER:HA	1:F:119:PHE:CD2	2.53	0.44
1:F:139:VAL:O	1:F:142:TRP:HB2	2.18	0.44
1:F:372:ARG:CG	1:F:373:PHE:H	2.31	0.44
1:F:413:ARG:HA	1:F:413:ARG:CZ	2.48	0.44
1:B:104:SER:OG	1:B:322:PHE:HA	2.18	0.44
1:E:98:TYR:CD1	1:E:496:VAL:HG12	2.53	0.44
1:F:374:ARG:HG3	1:F:374:ARG:HH11	1.83	0.44
1:D:324:THR:N	1:D:377:LYS:HD3	2.32	0.44
1:E:114:MET:HG2	1:F:34:ILE:HG21	1.99	0.44
1:E:325:LEU:HA	1:E:326:ASP:HA	1.66	0.44
1:F:225:THR:HB	1:F:231:PHE:HA	1.99	0.44
1:B:150:PRO:HD2	1:B:153:PHE:CD2	2.52	0.44
1:B:314:SER:HA	1:B:329:CYS:O	2.18	0.44
1:C:325:LEU:HA	1:C:326:ASP:HA	1.65	0.44
1:E:70:ASN:CB	1:E:71:PRO:HD2	2.48	0.44
1:F:110:PHE:CD1	1:F:110:PHE:C	2.96	0.44
1:C:57:GLY:O	1:C:61:LYS:HG3	2.18	0.43
1:A:340:LYS:O	1:A:350:ARG:NH1	2.46	0.43
1:D:481:MET:HB3	1:D:493:ARG:O	2.18	0.43
1:F:427:PHE:CZ	1:F:492:ILE:CG2	3.01	0.43
1:C:397:HIS:HB3	1:C:496:VAL:O	2.18	0.43
1:C:426:CYS:HA	1:C:492:ILE:O	2.18	0.43
1:E:361:ASP:OD2	1:E:363:LYS:NZ	2.35	0.43
1:E:407:LEU:HB3	1:E:510:TRP:CD1	2.53	0.43
1:A:523:LYS:HD2	1:A:523:LYS:HA	1.79	0.43
1:B:322:PHE:CZ	1:B:393:PHE:HB3	2.53	0.43
1:C:132:ALA:HA	1:C:373:PHE:CE1	2.53	0.43
1:E:51:ARG:HB2	1:E:480:TYR:CG	2.53	0.43
1:F:200:ASP:HA	1:F:222:ALA:HB1	2.00	0.43
1:B:92:TRP:CE3	1:B:103:SER:HB2	2.53	0.43
1:B:275:GLU:HG3	1:B:276:VAL:N	2.32	0.43
1:D:185:LYS:HE3	1:D:185:LYS:HB2	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:GLU:HG2	1:F:300:PHE:CD1	2.52	0.43
1:A:308:GLU:CD	1:A:308:GLU:H	2.26	0.43
1:B:392:ASN:HA	1:B:395:ARG:HB2	2.01	0.43
1:B:508:TYR:CZ	1:B:512:ILE:HD11	2.54	0.43
1:D:348:TYR:H	1:D:348:TYR:HD1	1.66	0.43
1:E:44:ASP:O	1:E:47:LYS:HG2	2.18	0.43
1:E:107:VAL:HG12	1:F:21:PRO:O	2.18	0.43
1:B:376:LEU:O	1:B:380:MET:HG2	2.19	0.43
1:C:151:GLU:HG2	1:C:157:GLY:HA3	1.99	0.43
1:C:413:ARG:HD2	1:C:521:LEU:HD12	2.01	0.43
1:E:110:PHE:CE1	1:E:114:MET:HE1	2.53	0.43
1:E:170:ALA:O	1:E:174:THR:HG23	2.19	0.43
1:E:239:ARG:O	1:E:243:LEU:HG	2.18	0.43
1:F:299:GLU:OE2	1:F:299:GLU:N	2.48	0.43
1:A:51:ARG:NH2	1:A:471:GLU:OE2	2.40	0.43
1:E:133:THR:O	1:E:362:TYR:CE2	2.72	0.43
1:E:253:LEU:N	1:E:282:MET:HE3	2.34	0.43
1:F:136:GLU:HA	1:F:375:SER:HB3	2.00	0.43
1:A:51:ARG:HA	1:A:90:THR:HG23	2.01	0.43
1:C:316:ASN:ND2	2:C:602:HOH:O	2.51	0.43
1:C:424:MET:HE3	1:C:426:CYS:SG	2.59	0.43
1:A:121:VAL:HG12	1:B:92:TRP:HD1	1.84	0.43
1:B:99:ALA:HB1	1:B:482:THR:HG23	1.99	0.42
1:C:484:ALA:HB2	1:C:493:ARG:HD2	2.01	0.42
1:F:371:ARG:HB3	1:F:371:ARG:NH1	2.34	0.42
1:F:126:TRP:HD1	1:F:133:THR:HB	1.83	0.42
1:D:385:TYR:O	1:D:389:ASN:HB2	2.19	0.42
1:E:144:GLY:HA2	1:E:149:LEU:HD12	1.99	0.42
1:E:520:ILE:H	1:E:520:ILE:HG13	1.73	0.42
1:F:163:LEU:HD23	1:F:163:LEU:HA	1.92	0.42
1:A:132:ALA:HA	1:A:373:PHE:CE1	2.55	0.42
1:F:325:LEU:HA	1:F:326:ASP:HA	1.69	0.42
1:F:432:PRO:HG3	1:F:521:LEU:HD11	2.01	0.42
1:E:58:TYR:OH	1:F:131:ALA:HB2	2.20	0.42
1:C:278:LYS:N	1:C:278:LYS:HD3	2.35	0.42
1:C:383:ARG:NH1	1:D:80:ASP:OD2	2.40	0.42
1:E:175:LEU:HD13	1:E:254:PHE:CG	2.55	0.42
1:E:335:PRO:HB3	1:E:365:TRP:CH2	2.55	0.42
1:F:172:LEU:O	1:F:176:THR:OG1	2.34	0.42
1:C:114:MET:HA	1:D:114:MET:HE2	2.02	0.42
1:C:511:LYS:HE3	1:C:511:LYS:HB3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:38:LEU:HD23	1:E:38:LEU:HA	1.90	0.42
1:E:95:PRO:HB2	1:E:505:HIS:CD2	2.55	0.42
1:E:203:HIS:CE1	1:F:369:LEU:HD11	2.36	0.42
1:E:242:ILE:O	1:E:246:ILE:HG13	2.19	0.42
1:E:316:ASN:CB	1:E:319:LYS:HB2	2.50	0.42
1:E:470:LEU:CD2	1:E:483:HIS:HB3	2.50	0.42
1:F:126:TRP:CZ2	1:F:130:PRO:HB3	2.55	0.42
1:F:335:PRO:HB3	1:F:365:TRP:CH2	2.54	0.42
1:E:21:PRO:HD2	1:F:499:THR:HG21	2.01	0.42
1:E:239:ARG:CZ	1:E:276:VAL:HG22	2.49	0.42
1:A:265:THR:OG1	1:A:424:MET:HE2	2.19	0.42
1:C:122:VAL:O	1:C:128:SER:HB3	2.20	0.42
1:D:408:ILE:CD1	1:D:510:TRP:HZ3	2.32	0.42
1:E:260:GLY:H	1:E:267:VAL:HG22	1.85	0.42
1:E:308:GLU:HG2	1:E:309:GLU:HG2	2.01	0.42
1:F:29:ARG:HD2	1:F:29:ARG:HA	1.82	0.42
1:E:402:LYS:HB3	1:E:402:LYS:HE2	1.77	0.41
1:F:23:ASP:HB3	1:F:26:GLU:HB2	2.02	0.41
1:F:151:GLU:O	1:F:151:GLU:HG2	2.19	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.91	0.41
1:C:374:ARG:HG2	1:C:377:LYS:HZ2	1.85	0.41
1:E:197:TYR:HD1	1:E:282:MET:HE1	1.82	0.41
1:C:374:ARG:HG2	1:C:377:LYS:NZ	2.35	0.41
1:E:86:ILE:N	1:E:87:PRO:HD2	2.36	0.41
1:E:129:SER:N	2:E:601:HOH:O	2.53	0.41
1:F:193:ARG:HD2	1:F:249:GLY:O	2.21	0.41
1:F:400:MET:HA	1:F:403:THR:OG1	2.20	0.41
1:A:111:LEU:HD11	1:B:30:GLN:HB3	2.01	0.41
1:A:408:ILE:HG12	1:A:510:TRP:CZ3	2.55	0.41
1:D:349:LEU:C	1:D:350:ARG:HG2	2.45	0.41
1:E:385:TYR:CD2	1:E:393:PHE:HE2	2.38	0.41
1:B:132:ALA:HA	1:B:373:PHE:CE1	2.54	0.41
1:D:140:MET:HE1	1:D:329:CYS:HB3	2.03	0.41
1:D:408:ILE:CD1	1:D:510:TRP:CZ3	3.02	0.41
1:E:151:GLU:CA	1:E:154:LEU:HB2	2.49	0.41
1:E:316:ASN:HB3	1:E:319:LYS:HB2	2.02	0.41
1:E:385:TYR:HB3	1:E:389:ASN:CB	2.51	0.41
1:F:107:VAL:O	1:F:111:LEU:HG	2.20	0.41
1:F:183:LEU:HD13	1:F:188:ARG:HA	2.03	0.41
1:F:188:ARG:HD3	1:F:188:ARG:H	1.86	0.41
1:F:372:ARG:HA	1:F:372:ARG:NE	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:ALA:HA	2:D:612:HOH:O	2.19	0.41
1:E:473:VAL:HG12	1:E:516:HIS:CE1	2.47	0.41
1:F:404:PHE:HD2	1:F:407:LEU:HD12	1.85	0.41
1:A:383:ARG:NH1	1:B:80:ASP:OD2	2.40	0.41
1:C:511:LYS:HD3	1:C:515:GLU:OE2	2.21	0.41
1:E:499:THR:H	1:E:499:THR:HG23	1.49	0.41
1:E:499:THR:HB	1:F:22:LEU:HD22	2.02	0.41
1:F:62:ARG:HE	1:F:62:ARG:HB3	1.65	0.41
1:F:151:GLU:HA	1:F:154:LEU:HG	2.03	0.41
1:A:383:ARG:HH21	1:B:72:GLU:CD	2.28	0.41
1:B:325:LEU:HA	1:B:326:ASP:HA	1.65	0.41
1:C:51:ARG:HD3	1:C:480:TYR:CE1	2.56	0.41
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.92	0.41
1:D:340:LYS:O	1:D:350:ARG:NH1	2.52	0.41
1:A:141:ASP:O	1:A:145:LYS:HG3	2.20	0.41
1:C:376:LEU:O	1:C:380:MET:HG3	2.19	0.41
1:D:33:MET:HE3	1:D:33:MET:HB2	1.95	0.41
1:E:111:LEU:C	1:E:113:GLU:N	2.78	0.41
1:E:128:SER:HB2	2:E:601:HOH:O	2.19	0.41
1:E:140:MET:HE1	1:E:329:CYS:SG	2.61	0.41
1:E:183:LEU:HB3	1:E:188:ARG:HG2	2.02	0.41
1:F:198:GLY:O	1:F:223:ILE:HG12	2.20	0.41
1:A:347:GLU:CD	1:D:523:LYS:HD2	2.46	0.41
1:A:404:PHE:CE2	1:A:408:ILE:HD11	2.56	0.41
1:B:162:VAL:HB	1:B:365:TRP:HE3	1.86	0.41
1:C:397:HIS:HA	1:C:400:MET:HE3	2.03	0.41
1:D:55:GLU:OE2	1:D:55:GLU:N	2.54	0.41
1:E:163:LEU:HD23	1:E:329:CYS:HA	2.03	0.41
1:F:413:ARG:HH11	1:F:521:LEU:HD13	1.85	0.41
1:F:424:MET:HB2	1:F:495:ALA:HB2	2.03	0.41
1:B:399:LYS:HD3	1:B:399:LYS:HA	1.79	0.40
1:E:143:PHE:HE1	1:E:296:ILE:HG21	1.86	0.40
1:A:52:SER:OG	1:A:54:VAL:HG22	2.21	0.40
1:E:227:LYS:NZ	1:E:418:VAL:HG12	2.36	0.40
1:E:431:PRO:HB3	1:E:465:LEU:HD22	2.03	0.40
1:C:104:SER:HB3	1:C:322:PHE:H	1.86	0.40
1:F:294:ALA:O	1:F:300:PHE:HD2	2.04	0.40
1:A:498:SER:HB3	1:A:501:THR:OG1	2.22	0.40
1:A:510:TRP:O	1:A:514:GLN:HG2	2.22	0.40
1:B:173:CYS:HB3	1:B:342:LEU:HD11	2.03	0.40
1:A:369:LEU:HD13	1:B:203:HIS:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:LYS:HB2	1:C:377:LYS:HE2	1.70	0.40
1:E:78:LEU:HD12	1:E:78:LEU:HA	1.85	0.40
1:E:107:VAL:HG23	1:E:110:PHE:CD2	2.56	0.40
1:E:121:VAL:HG21	1:E:373:PHE:HB2	2.03	0.40
1:F:114:MET:HE3	1:F:114:MET:HB2	1.99	0.40
1:F:502:GLU:CD	1:F:502:GLU:H	2.28	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	471/531 (89%)	458 (97%)	13 (3%)	0	100	100
1	B	471/531 (89%)	461 (98%)	10 (2%)	0	100	100
1	C	468/531 (88%)	460 (98%)	8 (2%)	0	100	100
1	D	468/531 (88%)	455 (97%)	13 (3%)	0	100	100
1	E	449/531 (85%)	429 (96%)	20 (4%)	0	100	100
1	F	405/531 (76%)	386 (95%)	19 (5%)	0	100	100
All	All	2732/3186 (86%)	2649 (97%)	83 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	409/456 (90%)	409 (100%)	0	100	100
1	B	409/456 (90%)	408 (100%)	1 (0%)	87	96
1	C	407/456 (89%)	406 (100%)	1 (0%)	87	96
1	D	407/456 (89%)	405 (100%)	2 (0%)	81	93
1	E	393/456 (86%)	390 (99%)	3 (1%)	73	90
1	F	357/456 (78%)	352 (99%)	5 (1%)	59	85
All	All	2382/2736 (87%)	2370 (100%)	12 (0%)	81	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	104	SER
1	C	104	SER
1	D	90	THR
1	D	104	SER
1	E	58	TYR
1	E	518	ASP
1	E	520	ILE
1	F	54	VAL
1	F	55	GLU
1	F	518	ASP
1	F	519	LEU
1	F	520	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	GLN
1	A	96	ASN
1	A	467	GLN
1	B	96	ASN
1	B	392	ASN
1	B	516	HIS
1	C	30	GLN
1	C	93	GLN
1	C	96	ASN
1	C	467	GLN
1	D	30	GLN
1	D	96	ASN
1	D	207	GLN

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Mol	Chain	Res	Type
1	D	211	GLN
1	D	467	GLN
1	D	516	HIS
1	E	30	GLN
1	E	32	HIS
1	E	120	ASN
1	E	203	HIS
1	E	302	HIS
1	E	345	ASN
1	E	463	ASN
1	F	229	ASN
1	F	318	HIS
1	F	345	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	477/531 (89%)	0.25	13 (2%) 56 46	28, 41, 59, 99	0
1	B	477/531 (89%)	0.20	19 (3%) 42 33	28, 38, 58, 107	0
1	C	474/531 (89%)	0.27	9 (1%) 66 57	29, 41, 63, 86	0
1	D	474/531 (89%)	0.15	11 (2%) 61 51	28, 37, 57, 92	0
1	E	459/531 (86%)	3.12	354 (77%) 0 0	67, 90, 106, 120	0
1	F	419/531 (78%)	2.89	274 (65%) 0 0	51, 88, 108, 124	0
All	All	2780/3186 (87%)	1.10	680 (24%) 2 1	28, 44, 101, 124	0

All (680) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	11.3
1	F	50	VAL	8.7
1	F	41	TYR	8.5
1	E	379	TRP	8.1
1	F	37	PHE	7.6
1	E	42	TYR	7.6
1	F	49	PRO	7.5
1	F	97	TYR	7.4
1	F	497	GLY	7.1
1	E	122	VAL	7.1
1	E	139	VAL	7.1
1	B	349	LEU	7.0
1	E	115	LEU	7.0
1	F	22	LEU	7.0
1	F	74	ILE	7.0
1	F	59	LEU	6.8
1	E	45	VAL	6.7
1	F	393	PHE	6.6
1	E	68	PRO	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	527	ALA	6.5
1	E	24	PRO	6.4
1	F	404	PHE	6.4
1	F	369	LEU	6.4
1	E	105	GLY	6.4
1	E	107	VAL	6.3
1	E	41	TYR	6.3
1	E	383	ARG	6.3
1	E	500	LEU	6.2
1	E	82	THR	6.2
1	E	48	TYR	6.2
1	F	99	ALA	6.1
1	F	381	VAL	6.1
1	F	423	ALA	6.1
1	E	58	TYR	6.0
1	E	397	HIS	6.0
1	F	38	LEU	5.9
1	E	509	ALA	5.9
1	F	506	VAL	5.9
1	E	507	ILE	5.9
1	F	298	PRO	5.9
1	F	500	LEU	5.9
1	F	417	THR	5.8
1	E	474	ASN	5.8
1	F	380	MET	5.8
1	F	401	ALA	5.8
1	E	478	SER	5.8
1	F	498	SER	5.8
1	E	119	PHE	5.8
1	F	124	PHE	5.8
1	F	521	LEU	5.7
1	E	390	LEU	5.7
1	F	45	VAL	5.7
1	F	42	TYR	5.7
1	E	27	PHE	5.7
1	F	48	TYR	5.6
1	E	296	ILE	5.6
1	E	110	PHE	5.6
1	E	19	THR	5.6
1	F	296	ILE	5.5
1	E	121	VAL	5.5
1	E	422	PHE	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	479	VAL	5.5
1	F	359	VAL	5.5
1	E	39	ALA	5.5
1	E	473	VAL	5.4
1	E	506	VAL	5.4
1	F	414	PHE	5.4
1	F	33	MET	5.4
1	F	24	PRO	5.4
1	E	134	GLU	5.4
1	F	54	VAL	5.4
1	F	373	PHE	5.4
1	E	106	SER	5.4
1	E	362	TYR	5.4
1	E	394	LEU	5.4
1	E	365	TRP	5.3
1	F	321	PHE	5.3
1	F	422	PHE	5.3
1	F	524	PHE	5.3
1	E	403	THR	5.3
1	F	507	ILE	5.3
1	F	517	ALA	5.3
1	E	89	LEU	5.3
1	E	404	PHE	5.3
1	F	58	TYR	5.2
1	F	132	ALA	5.2
1	E	21	PRO	5.2
1	E	504	ARG	5.2
1	E	87	PRO	5.2
1	E	23	ASP	5.1
1	F	403	THR	5.1
1	E	512	ILE	5.1
1	F	421	THR	5.1
1	E	378	LEU	5.1
1	E	108	ALA	5.1
1	E	143	PHE	5.1
1	E	112	GLY	5.1
1	F	127	MET	5.1
1	E	78	LEU	5.0
1	E	393	PHE	5.0
1	E	381	VAL	5.0
1	E	325	LEU	5.0
1	F	19	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	F	119	PHE	5.0
1	F	69	TYR	5.0
1	E	20	ASN	5.0
1	F	142	TRP	5.0
1	F	375	SER	5.0
1	F	426	CYS	5.0
1	F	95	PRO	5.0
1	F	406	GLY	4.9
1	F	122	VAL	4.9
1	E	516	HIS	4.9
1	C	524	PHE	4.9
1	E	292	GLY	4.9
1	F	317	ALA	4.9
1	A	348	TYR	4.9
1	E	401	ALA	4.8
1	F	394	LEU	4.8
1	E	54	VAL	4.8
1	E	69	TYR	4.8
1	E	44	ASP	4.8
1	E	51	ARG	4.8
1	E	426	CYS	4.8
1	F	47	LYS	4.7
1	F	52	SER	4.7
1	F	118	GLY	4.7
1	F	35	ILE	4.7
1	F	396	SER	4.7
1	F	429	LEU	4.7
1	F	418	VAL	4.7
1	E	86	ILE	4.7
1	D	348	TYR	4.6
1	F	494	PHE	4.6
1	F	67	ALA	4.6
1	F	128	SER	4.6
1	E	374	ARG	4.6
1	B	348	TYR	4.6
1	F	73	SER	4.6
1	E	163	LEU	4.6
1	E	519	LEU	4.6
1	F	496	VAL	4.6
1	F	300	PHE	4.6
1	F	499	THR	4.6
1	F	51	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	143	PHE	4.5
1	E	508	TYR	4.5
1	F	104	SER	4.5
1	F	32	HIS	4.5
1	F	416	ILE	4.5
1	F	379	TRP	4.5
1	E	83	THR	4.5
1	E	324	THR	4.5
1	F	66	THR	4.5
1	E	493	ARG	4.5
1	F	98	TYR	4.4
1	E	477	GLY	4.4
1	F	105	GLY	4.4
1	F	121	VAL	4.4
1	F	413	ARG	4.4
1	E	331	TRP	4.4
1	F	425	VAL	4.4
1	F	120	ASN	4.4
1	E	423	ALA	4.4
1	E	147	LEU	4.4
1	E	419	PRO	4.4
1	F	21	PRO	4.4
1	F	96	ASN	4.4
1	F	374	ARG	4.4
1	E	91	HIS	4.4
1	F	146	MET	4.3
1	F	39	ALA	4.3
1	E	96	ASN	4.3
1	E	320	TRP	4.3
1	F	100	TYR	4.3
1	E	25	GLU	4.3
1	E	501	THR	4.3
1	F	407	LEU	4.3
1	F	318	HIS	4.3
1	F	138	VAL	4.3
1	E	377	LYS	4.3
1	E	126	TRP	4.3
1	E	35	ILE	4.3
1	F	368	ALA	4.3
1	F	398	VAL	4.3
1	F	468	VAL	4.3
1	F	503	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
1	F	400	MET	4.2
1	E	289	ALA	4.2
1	E	111	LEU	4.2
1	F	501	THR	4.2
1	E	395	ARG	4.2
1	E	118	GLY	4.2
1	E	360	VAL	4.2
1	E	407	LEU	4.2
1	F	107	VAL	4.2
1	F	57	GLY	4.2
1	E	226	PHE	4.2
1	E	142	TRP	4.2
1	E	330	LEU	4.2
1	E	387	VAL	4.2
1	F	56	PRO	4.2
1	F	325	LEU	4.2
1	E	388	THR	4.1
1	F	519	LEU	4.1
1	E	97	TYR	4.1
1	E	469	TYR	4.1
1	E	88	GLY	4.1
1	E	396	SER	4.1
1	F	134	GLU	4.1
1	E	150	PRO	4.1
1	E	293	SER	4.1
1	E	373	PHE	4.1
1	E	175	LEU	4.0
1	E	418	VAL	4.0
1	E	67	ALA	4.0
1	E	399	LYS	4.0
1	E	109	GLY	4.0
1	F	135	LEU	4.0
1	E	66	THR	4.0
1	F	141	ASP	4.0
1	E	511	LYS	4.0
1	E	427	PHE	4.0
1	E	93	GLN	4.0
1	E	513	LEU	4.0
1	F	36	ASP	4.0
1	E	481	MET	4.0
1	F	331	TRP	4.0
1	E	103	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	165	GLY	4.0
1	C	348	TYR	4.0
1	E	382	LEU	4.0
1	F	114	MET	4.0
1	E	131	ALA	3.9
1	E	43	ARG	3.9
1	B	457	GLU	3.9
1	F	115	LEU	3.9
1	E	94	SER	3.9
1	E	398	VAL	3.9
1	F	251	ILE	3.9
1	F	294	ALA	3.9
1	F	46	GLU	3.9
1	F	502	GLU	3.9
1	A	523	LYS	3.9
1	E	74	ILE	3.9
1	E	72	GLU	3.9
1	F	290	TYR	3.9
1	F	64	PRO	3.9
1	F	419	PRO	3.9
1	E	127	MET	3.8
1	F	140	MET	3.8
1	E	56	PRO	3.8
1	F	293	SER	3.8
1	E	123	GLY	3.8
1	E	154	LEU	3.8
1	E	376	LEU	3.8
1	E	259	VAL	3.8
1	E	290	TYR	3.8
1	E	233	LEU	3.8
1	E	113	GLU	3.8
1	F	106	SER	3.8
1	F	457	GLU	3.8
1	E	28	ARG	3.8
1	F	372	ARG	3.8
1	E	47	LYS	3.8
1	F	125	ASN	3.8
1	E	130	PRO	3.7
1	E	141	ASP	3.7
1	F	295	CYS	3.7
1	E	510	TRP	3.7
1	E	380	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	124	PHE	3.7
1	E	165	GLY	3.7
1	B	347	GLU	3.7
1	E	76	THR	3.7
1	E	429	LEU	3.7
1	E	37	PHE	3.7
1	F	139	VAL	3.7
1	F	319	LYS	3.7
1	E	294	ALA	3.7
1	F	28	ARG	3.7
1	F	291	ALA	3.7
1	E	267	VAL	3.7
1	E	421	THR	3.7
1	E	38	LEU	3.6
1	F	131	ALA	3.6
1	F	316	ASN	3.6
1	E	77	ILE	3.6
1	E	514	GLN	3.6
1	E	384	SER	3.6
1	A	347	GLU	3.6
1	F	392	ASN	3.6
1	E	327	CYS	3.6
1	F	329	CYS	3.6
1	E	133	THR	3.6
1	E	49	PRO	3.6
1	E	465	LEU	3.6
1	F	147	LEU	3.6
1	E	62	ARG	3.6
1	F	161	GLY	3.6
1	F	360	VAL	3.6
1	F	327	CYS	3.6
1	E	116	SER	3.6
1	E	370	SER	3.6
1	E	498	SER	3.6
1	F	103	SER	3.5
1	F	129	SER	3.5
1	E	503	GLU	3.5
1	F	424	MET	3.5
1	E	64	PRO	3.5
1	E	258	THR	3.5
1	F	378	LEU	3.5
1	E	490	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	431	PRO	3.5
1	E	32	HIS	3.5
1	F	108	ALA	3.5
1	E	307	VAL	3.5
1	F	361	ASP	3.5
1	E	466	ASN	3.5
1	F	412	GLY	3.5
1	E	140	MET	3.5
1	F	315	LEU	3.5
1	E	90	THR	3.5
1	E	291	ALA	3.5
1	E	322	PHE	3.4
1	F	493	ARG	3.4
1	D	129	SER	3.4
1	F	102	PRO	3.4
1	F	432	PRO	3.4
1	E	30	GLN	3.4
1	E	369	LEU	3.4
1	E	261	THR	3.4
1	F	166	THR	3.4
1	E	385	TYR	3.4
1	E	389	ASN	3.4
1	E	257	PRO	3.4
1	E	265	THR	3.4
1	E	149	LEU	3.3
1	E	335	PRO	3.3
1	F	397	HIS	3.3
1	E	156	SER	3.3
1	E	263	SER	3.3
1	F	30	GLN	3.3
1	E	286	VAL	3.3
1	E	475	ALA	3.3
1	F	428	ARG	3.3
1	F	31	GLY	3.3
1	E	63	LEU	3.3
1	E	470	LEU	3.3
1	E	494	PHE	3.3
1	F	111	LEU	3.3
1	E	391	ARG	3.3
1	E	412	GLY	3.3
1	F	278	LYS	3.3
1	F	363	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	95	PRO	3.3
1	E	269	PRO	3.3
1	F	410	MET	3.3
1	E	201	GLN	3.3
1	E	336	SER	3.3
1	A	457	GLU	3.2
1	E	36	ASP	3.2
1	E	520	ILE	3.2
1	E	323	THR	3.2
1	F	123	GLY	3.2
1	E	463	ASN	3.2
1	F	20	ASN	3.2
1	F	34	ILE	3.2
1	E	317	ALA	3.2
1	E	425	VAL	3.2
1	E	166	THR	3.2
1	F	25	GLU	3.2
1	E	191	ILE	3.2
1	F	133	THR	3.2
1	E	84	GLU	3.2
1	E	100	TYR	3.2
1	F	518	ASP	3.2
1	F	504	ARG	3.2
1	E	313	PHE	3.2
1	E	410	MET	3.2
1	F	71	PRO	3.2
1	E	104	SER	3.1
1	E	430	LEU	3.1
1	F	27	PHE	3.1
1	E	366	GLN	3.1
1	F	72	GLU	3.1
1	E	171	ILE	3.1
1	E	372	ARG	3.1
1	F	322	PHE	3.1
1	F	324	THR	3.1
1	F	508	TYR	3.1
1	E	329	CYS	3.1
1	F	110	PHE	3.1
1	F	137	SER	3.1
1	F	292	GLY	3.1
1	F	522	GLY	3.1
1	B	346	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	399	LYS	3.1
1	E	368	ALA	3.1
1	E	489	VAL	3.1
1	F	101	PHE	3.1
1	D	349	LEU	3.1
1	E	46	GLU	3.1
1	E	227	LYS	3.1
1	E	346	PRO	3.1
1	E	98	TYR	3.0
1	F	458	ASN	3.0
1	E	386	GLY	3.0
1	E	71	PRO	3.0
1	E	238	LEU	3.0
1	E	499	THR	3.0
1	E	101	PHE	3.0
1	E	120	ASN	3.0
1	E	287	ASP	3.0
1	B	350	ARG	3.0
1	E	408	ILE	3.0
1	F	136	GLU	3.0
1	E	359	VAL	3.0
1	E	198	GLY	3.0
1	E	319	LYS	3.0
1	E	518	ASP	3.0
1	F	116	SER	3.0
1	E	190	HIS	3.0
1	E	270	ILE	3.0
1	F	263	SER	3.0
1	F	326	ASP	3.0
1	E	464	LYS	2.9
1	F	126	TRP	2.9
1	E	85	ILE	2.9
1	A	349	LEU	2.9
1	F	488	GLY	2.9
1	E	515	GLU	2.9
1	E	204	CYS	2.9
1	C	323	THR	2.9
1	F	520	ILE	2.9
1	F	430	LEU	2.9
1	F	465	LEU	2.9
1	E	102	PRO	2.9
1	E	128	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	361	ASP	2.9
1	F	156	SER	2.9
1	A	524	PHE	2.9
1	F	485	VAL	2.9
1	E	326	ASP	2.9
1	E	337	ALA	2.9
1	F	266	ALA	2.9
1	E	482	THR	2.9
1	F	249	GLY	2.9
1	E	216	ASN	2.9
1	E	268	ASP	2.9
1	F	411	ASP	2.9
1	E	129	SER	2.9
1	E	153	PHE	2.9
1	E	181	ARG	2.9
1	E	264	SER	2.9
1	E	314	SER	2.9
1	B	324	THR	2.9
1	E	232	GLY	2.8
1	E	65	GLU	2.8
1	E	197	TYR	2.8
1	F	231	PHE	2.8
1	F	262	THR	2.8
1	F	346	PRO	2.8
1	E	26	GLU	2.8
1	F	299	GLU	2.8
1	F	483	HIS	2.8
1	E	117	THR	2.8
1	E	160	GLY	2.8
1	E	92	TRP	2.8
1	E	132	ALA	2.8
1	E	484	ALA	2.8
1	E	73	SER	2.8
1	F	402	LYS	2.8
1	F	112	GLY	2.8
1	E	298	PRO	2.8
1	F	366	GLN	2.8
1	A	275	GLU	2.8
1	F	195	VAL	2.8
1	F	367	ILE	2.8
1	E	158	SER	2.8
1	F	269	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	65	GLU	2.7
1	E	274	CYS	2.7
1	F	320	TRP	2.7
1	F	427	PHE	2.7
1	E	206	LEU	2.7
1	F	304	ILE	2.7
1	F	461	LEU	2.7
1	F	466	ASN	2.7
1	E	192	GLY	2.7
1	E	312	SER	2.7
1	B	124	PHE	2.7
1	E	321	PHE	2.7
1	F	408	ILE	2.7
1	E	161	GLY	2.7
1	E	334	ASP	2.7
1	E	164	GLN	2.7
1	E	492	ILE	2.7
1	E	316	ASN	2.7
1	E	431	PRO	2.7
1	F	40	ASP	2.7
1	E	375	SER	2.7
1	F	264	SER	2.7
1	E	222	ALA	2.7
1	E	304	ILE	2.7
1	E	328	CYS	2.7
1	E	432	PRO	2.7
1	B	278	LYS	2.6
1	F	43	ARG	2.6
1	E	497	GLY	2.6
1	F	68	PRO	2.6
1	B	125	ASN	2.6
1	E	167	SER	2.6
1	E	505	HIS	2.6
1	E	224	LYS	2.6
1	E	33	MET	2.6
1	E	220	PHE	2.6
1	B	128	SER	2.6
1	F	188	ARG	2.6
1	F	395	ARG	2.6
1	E	295	CYS	2.6
1	E	215	ILE	2.6
1	E	284	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	323	THR	2.6
1	F	460	VAL	2.6
1	E	502	GLU	2.6
1	F	248	ALA	2.6
1	C	43	ARG	2.6
1	E	363	LYS	2.6
1	A	329	CYS	2.6
1	B	247	GLU	2.6
1	E	99	ALA	2.6
1	F	145	LYS	2.5
1	E	157	GLY	2.5
1	E	480	TYR	2.5
1	E	332	VAL	2.5
1	F	287	ASP	2.5
1	F	505	HIS	2.5
1	F	516	HIS	2.5
1	E	333	LYS	2.5
1	F	149	LEU	2.5
1	E	114	MET	2.5
1	E	162	VAL	2.5
1	E	169	GLU	2.5
1	E	205	ALA	2.5
1	F	345	ASN	2.5
1	A	218	LYS	2.5
1	E	40	ASP	2.5
1	F	305	ASP	2.5
1	F	377	LYS	2.5
1	F	523	LYS	2.5
1	C	124	PHE	2.5
1	E	176	THR	2.5
1	E	517	ALA	2.5
1	E	29	ARG	2.5
1	F	376	LEU	2.5
1	E	34	ILE	2.5
1	E	283	TRP	2.5
1	E	414	PHE	2.5
1	F	155	PHE	2.5
1	B	527	ALA	2.5
1	F	328	CYS	2.5
1	C	349	LEU	2.4
1	C	346	PRO	2.4
1	E	50	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	260	GLY	2.4
1	F	232	GLY	2.4
1	F	420	ARG	2.4
1	E	225	THR	2.4
1	F	63	LEU	2.4
1	F	250	LEU	2.4
1	B	361	ASP	2.4
1	E	186	ILE	2.4
1	E	230	SER	2.4
1	E	413	ARG	2.4
1	F	164	GLN	2.4
1	E	183	LEU	2.4
1	E	392	ASN	2.4
1	E	255	VAL	2.4
1	D	61	LYS	2.4
1	F	29	ARG	2.4
1	F	226	PHE	2.4
1	F	365	TRP	2.4
1	F	362	TYR	2.4
1	E	57	GLY	2.4
1	E	182	LYS	2.4
1	E	420	ARG	2.4
1	F	495	ALA	2.4
1	E	146	MET	2.4
1	E	262	THR	2.4
1	E	229	ASN	2.3
1	F	53	GLN	2.3
1	F	61	LYS	2.3
1	F	227	LYS	2.3
1	D	524	PHE	2.3
1	F	303	PHE	2.3
1	F	297	CYS	2.3
1	E	31	GLY	2.3
1	E	303	PHE	2.3
1	F	313	PHE	2.3
1	F	491	MET	2.3
1	E	79	GLN	2.3
1	C	523	LYS	2.3
1	F	230	SER	2.3
1	E	202	THR	2.3
1	E	241	VAL	2.3
1	E	300	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	463	ASN	2.3
1	F	415	GLU	2.3
1	E	218	LYS	2.3
1	E	318	HIS	2.3
1	F	370	SER	2.3
1	E	75	GLU	2.2
1	E	189	GLU	2.2
1	E	194	LEU	2.2
1	B	399	LYS	2.2
1	F	492	ILE	2.2
1	E	256	CYS	2.2
1	E	472	THR	2.2
1	F	55	GLU	2.2
1	F	289	ALA	2.2
1	E	148	ASN	2.2
1	E	174	THR	2.2
1	F	265	THR	2.2
1	E	159	GLY	2.2
1	F	288	ALA	2.2
1	F	308	GLU	2.2
1	F	70	ASN	2.2
1	F	184	ASN	2.2
1	A	432	PRO	2.2
1	F	258	THR	2.2
1	E	152	SER	2.2
1	E	199	SER	2.2
1	F	260	GLY	2.2
1	D	278	LYS	2.2
1	D	368	ALA	2.2
1	D	457	GLU	2.2
1	E	483	HIS	2.2
1	E	196	VAL	2.2
1	F	237	THR	2.2
1	E	168	CYS	2.2
1	E	173	CYS	2.2
1	E	278	LYS	2.2
1	F	464	LYS	2.2
1	F	203	HIS	2.1
1	B	129	SER	2.1
1	E	52	SER	2.1
1	D	350	ARG	2.1
1	B	345	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	80	ASP	2.1
1	E	236	ALA	2.1
1	F	62	ARG	2.1
1	F	158	SER	2.1
1	E	53	GLN	2.1
1	E	491	MET	2.1
1	F	194	LEU	2.1
1	C	19	THR	2.1
1	A	55	GLU	2.1
1	E	299	GLU	2.1
1	F	272	PRO	2.1
1	D	367	ILE	2.1
1	E	251	ILE	2.1
1	E	240	GLU	2.1
1	E	203	HIS	2.0
1	E	272	PRO	2.0
1	A	461	LEU	2.0
1	B	458	ASN	2.0
1	E	125	ASN	2.0
1	F	459	LEU	2.0
1	E	254	PHE	2.0
1	E	467	GLN	2.0
1	F	271	SER	2.0
1	F	144	GLY	2.0
1	F	153	PHE	2.0
1	E	242	ILE	2.0
1	E	273	ILE	2.0
1	B	323	THR	2.0
1	F	261	THR	2.0
1	D	275	GLU	2.0
1	E	281	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.