Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 03:30 AM EDT

PDB ID	:	6LIU
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 (i) 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 (1)) were used in the production of this report:

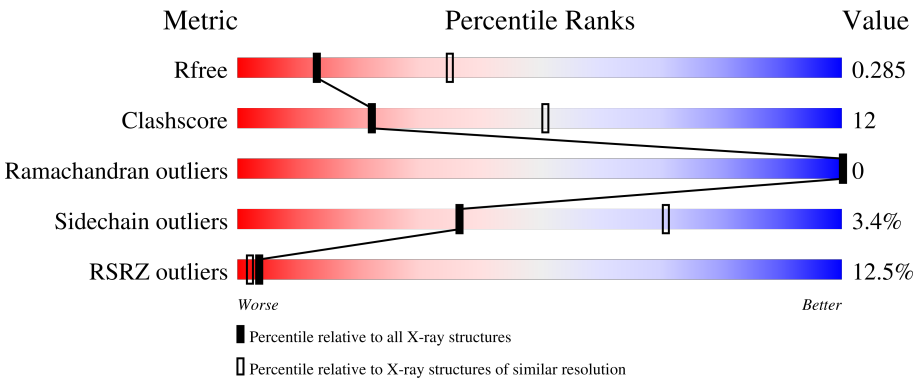
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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%, 75%, 15%, 10%
1	B	531	2%, 76%, 13%, 10%
1	C	531	2%, 77%, 12%, 11%
1	D	531	77%, 12%, •, 11%
1	E	531	34%, 47%, 37%, •, 14%

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Mol	Chain	Length	Quality of chain
1	F	531	26% 46% 30% • 21%

2 Entry composition (i)

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

- Molecule 2 is water.

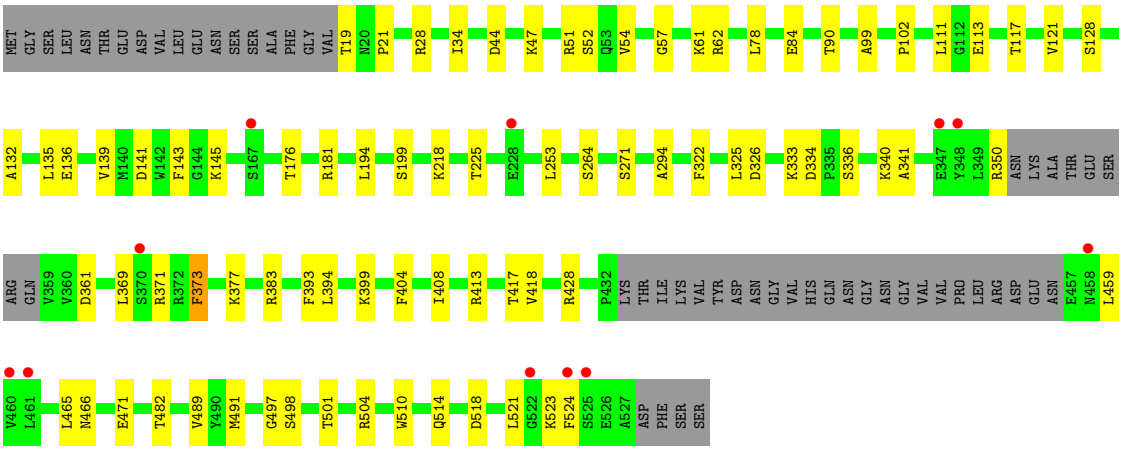
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	31	31	31	0	0
2	B	28	28	28	0	0
2	C	18	18	18	0	0
2	D	31	31	31	0	0
2	E	9	9	9	0	0
2	F	7	7	7	0	0

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.

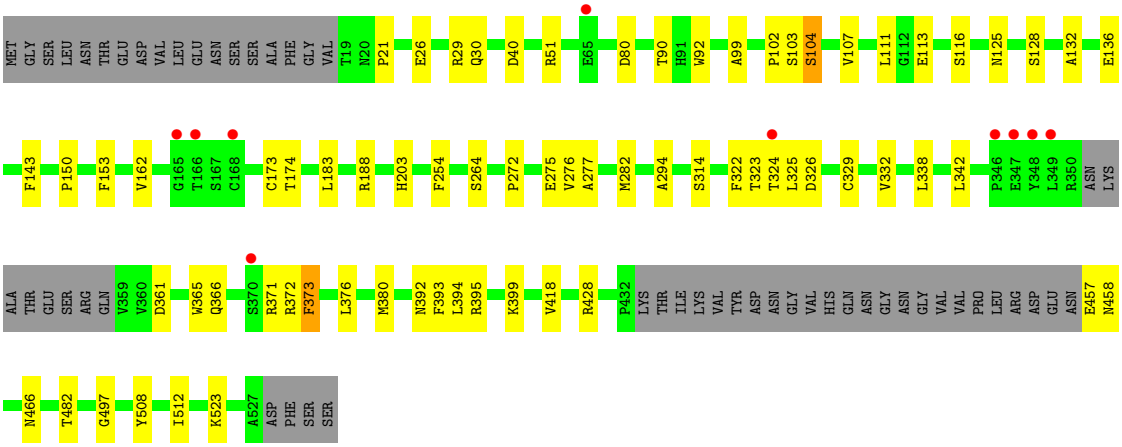
• Molecule 1: Tyrosine/DOPA decarboxylase 2

Chain A:



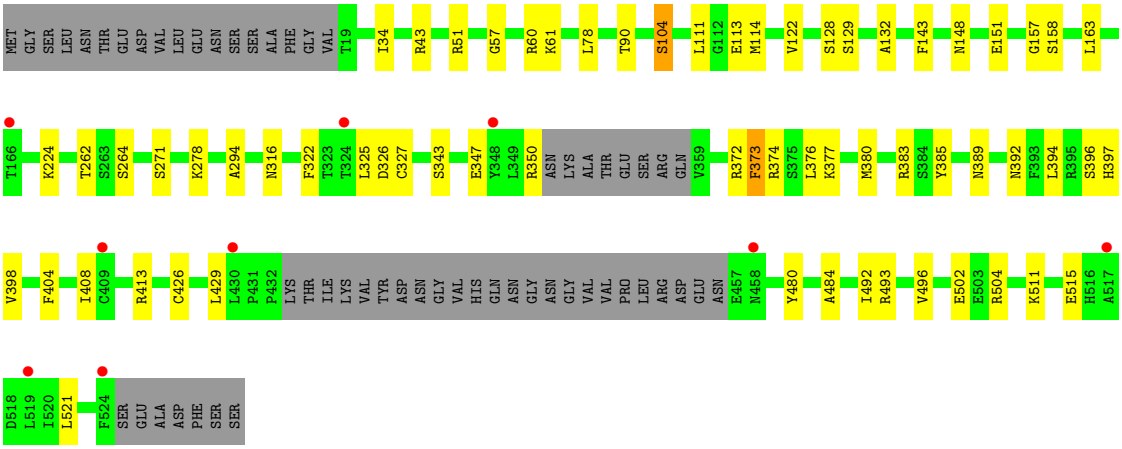
• Molecule 1: Tyrosine/DOPA decarboxylase 2

Chain B:



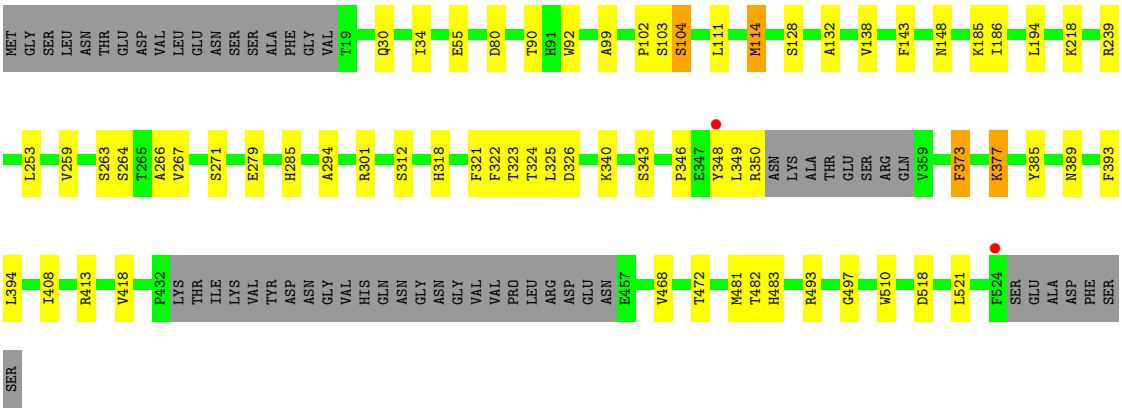
• Molecule 1: Tyrosine/DOPA decarboxylase 2

Chain C:



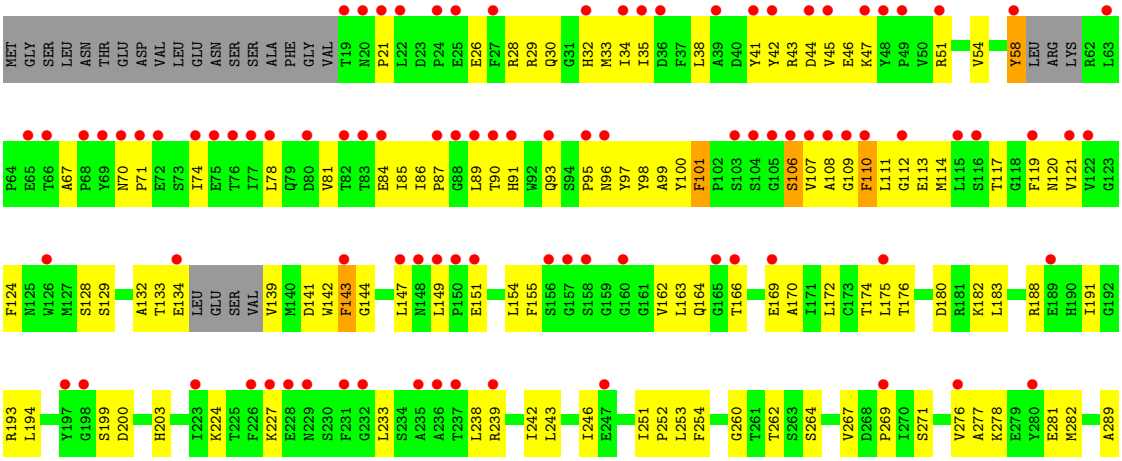
- Molecule 1: Tyrosine/DOPA decarboxylase 2

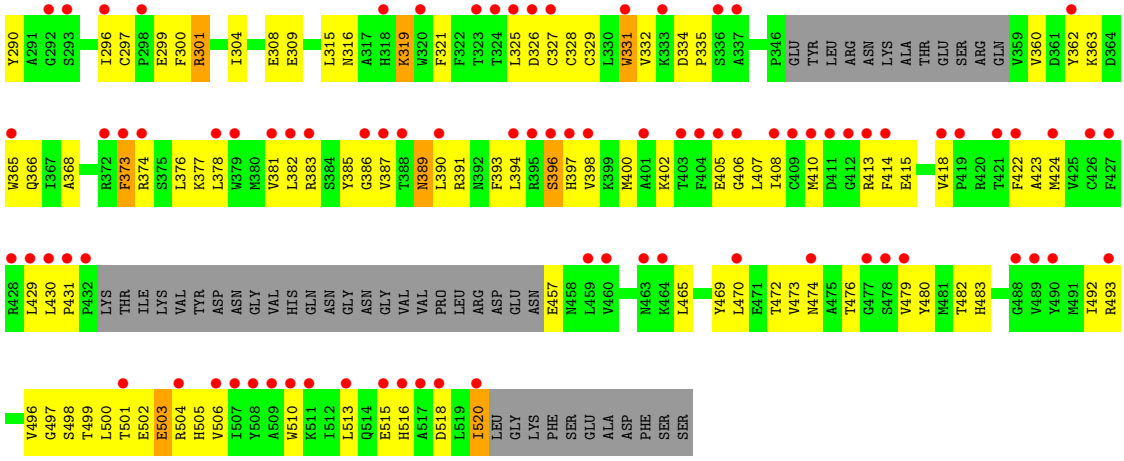
Chain D:



- Molecule 1: Tyrosine/DOPA decarboxylase 2

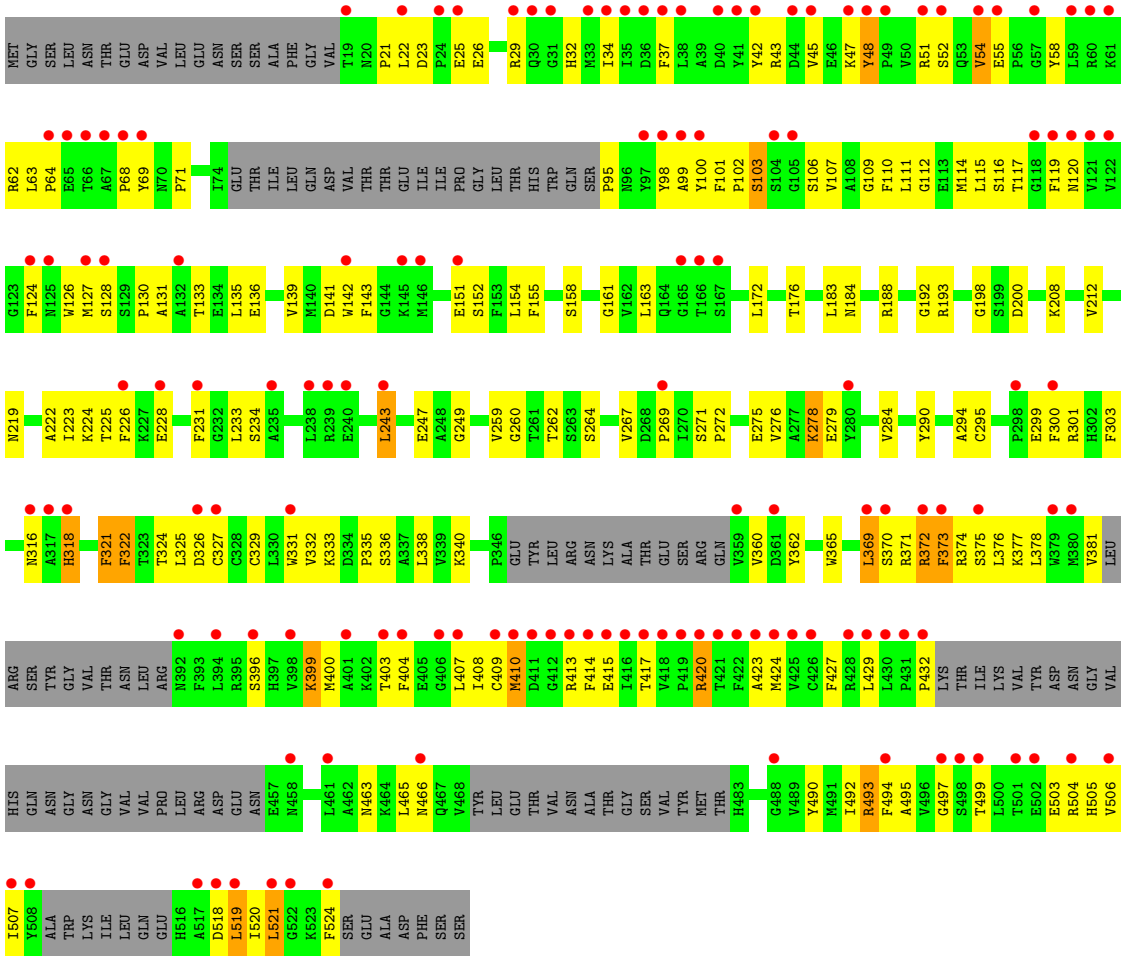
Chain E:





• Molecule 1: Tyrosine/DOPA decarboxylase 2

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	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 48.19 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.13-2.80) 93.9 (48.19-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.241 , 0.280 0.248 , 0.285	Depositor DCC
R_{free} test set	5754 reflections (5.01%)	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)	0.39 , 54.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[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 (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	0.42	0/3859	0.45	0/5241
1	B	0.36	0/3859	0.45	0/5241
1	C	0.34	0/3839	0.44	0/5214
1	D	0.37	0/3839	0.46	0/5214
1	E	0.32	0/3705	0.54	0/5033
1	F	0.30	0/3374	0.53	0/4570
All	All	0.36	0/22475	0.48	0/30513

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3766	0	3724	55	0
1	B	3766	0	3724	56	0
1	C	3746	0	3708	43	0
1	D	3746	0	3708	48	0
1	E	3616	0	3563	192	0
1	F	3295	0	3257	171	0
2	A	31	0	0	5	0
2	B	28	0	0	0	0
2	C	18	0	0	1	0
2	D	31	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	9	0	0	8	0
2	F	7	0	0	1	0
All	All	22059	0	21684	509	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 12.

All (509) 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	1.05
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	1.02
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
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: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:F:102:PRO:HG3	1:F:497:GLY:HA3	1.64	0.76
1:F:278:LYS:HZ3	1:F:284:VAL:HG23	1.51	0.76
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:285:HIS:HD1	1:D:312:SER:HG	1.37	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:F:519:LEU:HD12	1:F:519:LEU:C	2.12	0.69
1:E:51:ARG:HA	1:E:90:THR:HG23	1.73	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:F:100:TYR:N	1:F:493:ARG:HH22	1.92	0.68
1:F:278:LYS:HZ3	1:F:284:VAL:CG2	2.06	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:116:SER:HB2	1:F:376:LEU:HD12	1.77	0.66
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:F:396:SER:O	1:F:400:MET:HG2	1.97	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: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:E:325:LEU:HD22	1:F:372:ARG:HD2	1.81	0.62
1:E:301:ARG:HD3	1:E:304:ILE:HG13	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:THR:HG21	1:E:516:HIS:HE1	1.65	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: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
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: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:C:325:LEU:HG	1:C:326:ASP:HB3	1.83	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: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:28:ARG:HG2	1:E:32:HIS:CE1	2.38	0.59
1:E:30:GLN:HA	1:E:33:MET:HE3	1.84	0.59
1:F:278:LYS:NZ	1:F:284:VAL:HG21	2.19	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:A:399:LYS:NZ	2:A:602:HOH:O	2.32	0.58
1:B:104:SER:HG	1:B:322:PHE:H	1.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:420:ARG:HD3	1:F:420:ARG:H	1.69	0.56
1:A:417:THR:HG21	1:A:491:MET:HG2	1.87	0.56
1:E:134:GLU:C	2:E:605:HOH:O	2.44	0.56
1:E:111:LEU:HD23	1:E:114:MET:HE3	1.88	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:F:116:SER:HG	1:F:373:PHE:HD2	1.52	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:C:114:MET:HA	1:D:114:MET:HE1	1.89	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:43:ARG:HG3	1:F:43:ARG:HH11	1.72	0.53
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:111:LEU:C	1:E:114:MET:H	2.11	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: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:F:278:LYS:HZ1	1:F:284:VAL:HG21	1.75	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:193:ARG:NH1	1:E:251:ILE:HD11	2.25	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:103:SER:O	1:F:103:SER:OG	2.26	0.50
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:E:111:LEU:CD2	1:E:114:MET:HE3	2.42	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:OG	1:E:264:SER:O	2.25	0.50
1:F:294:ALA:HB1	1:F:300:PHE:CD2	2.47	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: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
1:A:393:PHE:CZ	1:B:21:PRO:HG3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:LYS:NZ	2:A:605:HOH:O	2.44	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: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: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: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:F:243:LEU:O	1:F:247:GLU:HG3	2.13	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:TYR:CD1	1:E:58:TYR:C	2.85	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:F:127:MET:HE3	1:F:127:MET:O	2.15	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:278:LYS:HZ1	1:F:284:VAL:CG2	2.25	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:180:ASP:CG	1:E:188:ARG:HH22	2.21	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
1:F:99:ALA:C	1:F:493:ARG:NH2	2.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:275:GLU:HG3	1:B:276:VAL:N	2.32	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: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: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:D:185:LYS:HE3	1:D:185:LYS:HB2	1.84	0.43
1:F:299:GLU:HG2	1:F:300:PHE:CD1	2.52	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:C:392:ASN:O	1:C:396:SER:OG	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ARG:HD2	1:C:521:LEU:HD12	2.01	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: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:F:519:LEU:C	1:F:519:LEU:CD1	2.85	0.43
1:A:121:VAL:HG12	1:B:92:TRP:HD1	1.84	0.43
1:A:136:GLU:CD	1:A:371:ARG:HH22	2.19	0.42
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:F:151:GLU:O	1:F:151:GLU:HG2	2.19	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:B:277:ALA:HA	1:B:282:MET:HE2	2.02	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:511:LYS:HE3	1:C:511:LYS:HB3	1.88	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:ARG:CZ	1:E:276:VAL:HG22	2.49	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:110:PHE:CE1	1:E:114:MET:HE1	2.54	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: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: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: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: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
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:HB	1:F:22:LEU:HD22	2.02	0.41
1:E:499:THR:H	1:E:499:THR:HG23	1.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:35:ILE:HD13	1:F:114:MET:HE1	2.03	0.41
1:E:128:SER:HB2	2:E:601:HOH:O	2.19	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: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: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
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

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%)	403 (98%)	6 (2%)	65	89
1	B	409/456 (90%)	405 (99%)	4 (1%)	76	93
1	C	407/456 (89%)	397 (98%)	10 (2%)	47	80
1	D	407/456 (89%)	397 (98%)	10 (2%)	47	80
1	E	393/456 (86%)	371 (94%)	22 (6%)	21	51
1	F	357/456 (78%)	328 (92%)	29 (8%)	11	33
All	All	2382/2736 (87%)	2301 (97%)	81 (3%)	37	71

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	PHE
1	A	199	SER
1	A	271	SER
1	A	361	ASP
1	A	373	PHE
1	A	504	ARG
1	B	104	SER

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Mol	Chain	Res	Type
1	B	143	PHE
1	B	361	ASP
1	B	373	PHE
1	C	43	ARG
1	C	104	SER
1	C	129	SER
1	C	143	PHE
1	C	148	ASN
1	C	158	SER
1	C	224	LYS
1	C	264	SER
1	C	271	SER
1	C	373	PHE
1	D	103	SER
1	D	104	SER
1	D	114	MET
1	D	143	PHE
1	D	263	SER
1	D	271	SER
1	D	321	PHE
1	D	343	SER
1	D	373	PHE
1	D	377	LYS
1	E	43	ARG
1	E	58	TYR
1	E	101	PHE
1	E	106	SER
1	E	110	PHE
1	E	143	PHE
1	E	182	LYS
1	E	271	SER
1	E	278	LYS
1	E	281	GLU
1	E	301	ARG
1	E	319	LYS
1	E	331	TRP
1	E	373	PHE
1	E	389	ASN
1	E	396	SER
1	E	413	ARG
1	E	422	PHE
1	E	503	GLU

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Mol	Chain	Res	Type
1	E	515	GLU
1	E	518	ASP
1	E	520	ILE
1	F	37	PHE
1	F	47	LYS
1	F	48	TYR
1	F	51	ARG
1	F	54	VAL
1	F	55	GLU
1	F	103	SER
1	F	124	PHE
1	F	143	PHE
1	F	158	SER
1	F	234	SER
1	F	243	LEU
1	F	278	LYS
1	F	318	HIS
1	F	321	PHE
1	F	322	PHE
1	F	369	LEU
1	F	372	ARG
1	F	373	PHE
1	F	399	LYS
1	F	409	CYS
1	F	410	MET
1	F	420	ARG
1	F	493	ARG
1	F	518	ASP
1	F	519	LEU
1	F	520	ILE
1	F	521	LEU
1	F	524	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	392	ASN
1	C	93	GLN
1	E	32	HIS
1	E	120	ASN
1	E	203	HIS
1	E	366	GLN

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Mol	Chain	Res	Type
1	E	463	ASN
1	F	318	HIS

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 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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.08	11 (2%)	60	51	28, 41, 59, 99	0
1	B	477/531 (89%)	0.01	10 (2%)	63	54	28, 38, 58, 107	0
1	C	474/531 (89%)	0.07	9 (1%)	66	59	29, 41, 63, 86	0
1	D	474/531 (89%)	-0.07	2 (0%)	92	91	28, 37, 57, 92	0
1	E	459/531 (86%)	1.86	179 (38%)	0	0	67, 90, 106, 120	0
1	F	419/531 (78%)	1.56	137 (32%)	0	0	51, 88, 108, 124	0
All	All	2780/3186 (87%)	0.56	348 (12%)	3	2	28, 44, 101, 124	0

All (348) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	22	LEU	13.5
1	F	49	PRO	6.7
1	F	41	TYR	6.6
1	E	379	TRP	6.2
1	F	37	PHE	6.2
1	F	518	ASP	6.2
1	F	522	GLY	6.2
1	E	404	PHE	6.1
1	F	406	GLY	6.0
1	F	521	LEU	5.9
1	E	19	THR	5.9
1	E	509	ALA	5.7
1	B	348	TYR	5.7
1	E	478	SER	5.6
1	E	42	TYR	5.6
1	E	65	GLU	5.6
1	E	383	ARG	5.5
1	E	83	THR	5.4
1	F	33	MET	5.3

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Mol	Chain	Res	Type	RSRZ
1	F	418	VAL	5.3
1	E	507	ILE	5.2
1	F	66	THR	5.1
1	E	87	PRO	5.1
1	F	379	TRP	5.1
1	E	431	PRO	5.1
1	F	404	PHE	5.1
1	F	431	PRO	5.1
1	E	66	THR	5.1
1	E	516	HIS	5.1
1	F	132	ALA	5.0
1	F	48	TYR	5.0
1	F	416	ILE	5.0
1	F	59	LEU	5.0
1	E	41	TYR	4.9
1	F	38	LEU	4.9
1	E	27	PHE	4.9
1	E	119	PHE	4.8
1	E	24	PRO	4.8
1	F	409	CYS	4.8
1	F	69	TYR	4.7
1	E	474	ASN	4.7
1	E	422	PHE	4.6
1	E	68	PRO	4.6
1	E	115	LEU	4.5
1	F	121	VAL	4.5
1	E	511	LYS	4.5
1	F	68	PRO	4.5
1	F	65	GLU	4.4
1	E	91	HIS	4.4
1	E	44	ASP	4.4
1	F	413	ARG	4.4
1	E	418	VAL	4.3
1	E	518	ASP	4.3
1	E	88	GLY	4.2
1	F	119	PHE	4.2
1	E	506	VAL	4.2
1	E	510	TRP	4.2
1	D	348	TYR	4.1
1	F	414	PHE	4.1
1	E	148	ASN	4.1
1	E	121	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	108	ALA	4.1
1	E	390	LEU	4.1
1	F	45	VAL	4.0
1	A	348	TYR	4.0
1	E	430	LEU	4.0
1	F	60	ARG	4.0
1	E	20	ASN	4.0
1	F	415	GLU	4.0
1	E	82	THR	4.0
1	E	36	ASP	3.9
1	F	127	MET	3.9
1	E	414	PHE	3.9
1	F	499	THR	3.9
1	E	110	PHE	3.9
1	F	380	MET	3.9
1	E	63	LEU	3.9
1	F	298	PRO	3.9
1	E	39	ALA	3.9
1	E	408	ILE	3.8
1	E	51	ARG	3.8
1	F	42	TYR	3.8
1	E	58	TYR	3.8
1	E	410	MET	3.8
1	A	347	GLU	3.8
1	F	403	THR	3.7
1	E	460	VAL	3.7
1	F	373	PHE	3.6
1	E	166	THR	3.6
1	E	157	GLY	3.6
1	F	425	VAL	3.6
1	E	479	VAL	3.5
1	E	336	SER	3.5
1	E	165	GLY	3.5
1	E	236	ALA	3.5
1	F	497	GLY	3.5
1	F	502	GLU	3.5
1	B	349	LEU	3.4
1	E	34	ILE	3.4
1	F	40	ASP	3.4
1	E	69	TYR	3.4
1	E	96	ASN	3.4
1	C	409	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	413	ARG	3.4
1	F	31	GLY	3.4
1	E	296	ILE	3.4
1	F	432	PRO	3.4
1	F	508	TYR	3.4
1	E	504	ARG	3.4
1	F	506	VAL	3.4
1	F	120	ASN	3.4
1	F	517	ALA	3.3
1	F	97	TYR	3.3
1	E	426	CYS	3.3
1	F	64	PRO	3.3
1	F	458	ASN	3.3
1	E	106	SER	3.3
1	E	411	ASP	3.3
1	F	369	LEU	3.3
1	E	71	PRO	3.3
1	F	61	LYS	3.3
1	F	145	LYS	3.3
1	F	411	ASP	3.3
1	E	103	SER	3.2
1	E	107	VAL	3.2
1	E	327	CYS	3.2
1	E	78	LEU	3.2
1	E	394	LEU	3.2
1	A	458	ASN	3.2
1	F	122	VAL	3.2
1	E	432	PRO	3.2
1	F	47	LYS	3.2
1	F	36	ASP	3.2
1	E	47	LYS	3.2
1	E	134	GLU	3.2
1	E	158	SER	3.1
1	F	498	SER	3.1
1	E	160	GLY	3.1
1	E	470	LEU	3.1
1	F	104	SER	3.1
1	F	422	PHE	3.1
1	E	331	TRP	3.1
1	B	347	GLU	3.1
1	E	325	LEU	3.1
1	F	430	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	463	ASN	3.1
1	E	75	GLU	3.1
1	E	513	LEU	3.0
1	F	423	ALA	3.0
1	F	426	CYS	3.0
1	E	32	HIS	3.0
1	F	401	ALA	3.0
1	E	520	ILE	3.0
1	E	93	GLN	3.0
1	F	228	GLU	3.0
1	F	238	LEU	3.0
1	F	524	PHE	3.0
1	E	45	VAL	3.0
1	E	398	VAL	3.0
1	F	99	ALA	3.0
1	E	378	LEU	3.0
1	E	428	ARG	3.0
1	F	300	PHE	2.9
1	F	466	ASN	2.9
1	F	428	ARG	2.9
1	F	504	ARG	2.9
1	F	392	ASN	2.9
1	E	489	VAL	2.9
1	E	372	ARG	2.9
1	E	459	LEU	2.9
1	E	397	HIS	2.9
1	F	128	SER	2.9
1	F	165	GLY	2.9
1	F	226	PHE	2.9
1	F	429	LEU	2.9
1	F	488	GLY	2.9
1	E	77	ILE	2.9
1	F	316	ASN	2.9
1	E	150	PRO	2.9
1	F	30	GLN	2.9
1	E	490	TYR	2.8
1	F	54	VAL	2.8
1	E	493	ARG	2.8
1	E	401	ALA	2.8
1	E	365	TRP	2.8
1	E	298	PRO	2.8
1	E	373	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	501	THR	2.8
1	C	348	TYR	2.8
1	B	370	SER	2.8
1	E	292	GLY	2.8
1	F	44	ASP	2.8
1	F	100	TYR	2.8
1	E	293	SER	2.8
1	E	90	THR	2.8
1	E	151	GLU	2.7
1	E	156	SER	2.7
1	E	396	SER	2.7
1	E	280	TYR	2.7
1	E	386	GLY	2.7
1	F	359	VAL	2.7
1	F	410	MET	2.7
1	F	398	VAL	2.7
1	E	337	ALA	2.7
1	F	235	ALA	2.7
1	E	35	ILE	2.7
1	E	49	PRO	2.7
1	A	524	PHE	2.7
1	E	403	THR	2.7
1	E	421	THR	2.7
1	E	237	THR	2.7
1	F	19	THR	2.6
1	E	84	GLU	2.6
1	E	122	VAL	2.6
1	B	324	THR	2.6
1	E	112	GLY	2.6
1	F	142	TRP	2.6
1	F	25	GLU	2.6
1	E	226	PHE	2.6
1	C	458	ASN	2.6
1	C	430	LEU	2.6
1	E	104	SER	2.6
1	F	29	ARG	2.6
1	F	35	ILE	2.6
1	E	80	ASP	2.6
1	E	381	VAL	2.6
1	E	239	ARG	2.5
1	E	412	GLY	2.5
1	F	421	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	74	ILE	2.5
1	F	375	SER	2.5
1	E	395	ARG	2.5
1	E	387	VAL	2.5
1	F	361	ASP	2.5
1	E	70	ASN	2.5
1	F	239	ARG	2.5
1	E	76	THR	2.5
1	E	147	LEU	2.5
1	F	370	SER	2.5
1	F	396	SER	2.5
1	E	235	ALA	2.5
1	F	327	CYS	2.5
1	E	501	THR	2.5
1	E	429	LEU	2.5
1	E	427	PHE	2.4
1	F	417	THR	2.4
1	E	169	GLU	2.4
1	F	98	TYR	2.4
1	F	412	GLY	2.4
1	E	72	GLU	2.4
1	F	243	LEU	2.4
1	F	124	PHE	2.4
1	C	324	THR	2.4
1	E	231	PHE	2.4
1	E	105	GLY	2.4
1	E	247	GLU	2.4
1	E	517	ALA	2.4
1	E	223	ILE	2.4
1	E	109	GLY	2.4
1	E	419	PRO	2.4
1	E	382	LEU	2.4
1	E	95	PRO	2.4
1	E	405	GLU	2.3
1	E	116	SER	2.3
1	F	394	LEU	2.3
1	E	228	GLU	2.3
1	B	346	PRO	2.3
1	F	51	ARG	2.3
1	F	67	ALA	2.3
1	E	406	GLY	2.3
1	F	57	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	409	CYS	2.3
1	E	189	GLU	2.3
1	F	34	ILE	2.3
1	F	519	LEU	2.3
1	A	370	SER	2.3
1	B	65	GLU	2.3
1	F	24	PRO	2.3
1	F	269	PRO	2.3
1	E	198	GLY	2.3
1	F	118	GLY	2.3
1	F	318	HIS	2.3
1	E	362	TYR	2.3
1	F	424	MET	2.3
1	F	166	THR	2.3
1	E	515	GLU	2.3
1	E	326	ASP	2.3
1	F	419	PRO	2.3
1	F	461	LEU	2.3
1	F	507	ILE	2.3
1	E	333	LYS	2.3
1	C	517	ALA	2.2
1	E	149	LEU	2.2
1	E	323	THR	2.2
1	E	324	THR	2.2
1	E	175	LEU	2.2
1	E	320	TRP	2.2
1	E	276	VAL	2.2
1	F	167	SER	2.2
1	F	231	PHE	2.2
1	F	22	LEU	2.2
1	F	55	GLU	2.2
1	E	143	PHE	2.2
1	B	168	CYS	2.2
1	F	331	TRP	2.2
1	E	25	GLU	2.2
1	F	420	ARG	2.2
1	D	524	PHE	2.2
1	F	280	TYR	2.2
1	F	407	LEU	2.2
1	F	372	ARG	2.2
1	C	524	PHE	2.2
1	A	228	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	166	THR	2.1
1	F	494	PHE	2.1
1	E	269	PRO	2.1
1	A	167	SER	2.1
1	E	318	HIS	2.1
1	E	488	GLY	2.1
1	F	326	ASP	2.1
1	F	317	ALA	2.1
1	F	125	ASN	2.1
1	B	166	THR	2.1
1	E	388	THR	2.1
1	E	89	LEU	2.1
1	F	240	GLU	2.1
1	E	464	LYS	2.1
1	A	522	GLY	2.1
1	E	21	PRO	2.1
1	E	232	GLY	2.1
1	A	461	LEU	2.1
1	F	105	GLY	2.1
1	C	519	LEU	2.1
1	F	146	MET	2.1
1	F	151	GLU	2.1
1	E	477	GLY	2.1
1	F	52	SER	2.0
1	E	229	ASN	2.0
1	E	508	TYR	2.0
1	A	460	VAL	2.0
1	E	424	MET	2.0
1	E	48	TYR	2.0
1	E	197	TYR	2.0
1	E	227	LYS	2.0
1	B	165	GLY	2.0
1	A	525	SER	2.0
1	E	126	TRP	2.0
1	E	374	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.