Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 10:05 PM EDT

PDB ID	:	3HWC / pdb_00003hwc
Title	:	Crystal Structure of Chlorophenol 4-Monooxygenase (TftD) of Burkholderia cepacia AC1100
Authors	:	Ballinger, J.W.; Kang, C.H.
Deposited on	:	2009-06-17
Resolution	:	2.50 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:

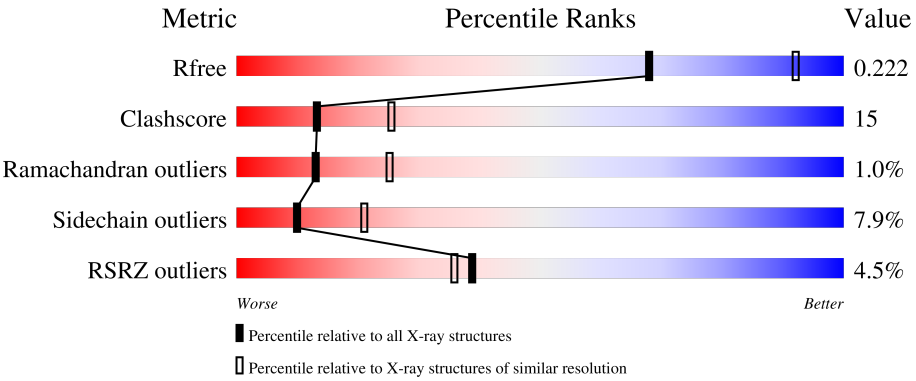
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.50 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}	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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	515	6% 64% 24% 5% 6%
1	B	515	6% 65% 25% • 6%
1	C	515	4% 63% 27% • 6%
1	D	515	% 70% 20% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 16516 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 Chlorophenol-4-monooxygenase component 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3834	2429	684	708	13			
1	B	482	Total	C	N	O	S	0	0	0
			3834	2429	684	708	13			
1	C	482	Total	C	N	O	S	0	0	0
			3834	2429	684	708	13			
1	D	482	Total	C	N	O	S	0	0	0
			3834	2429	684	708	13			

- Molecule 2 is water.

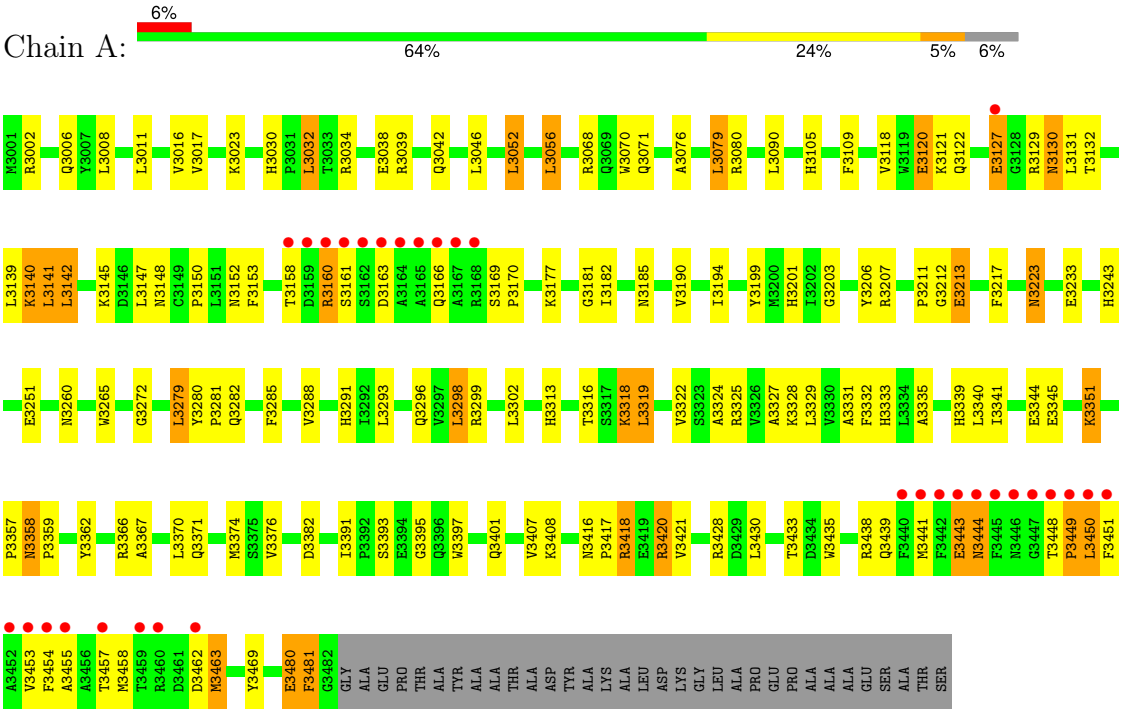
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	289	Total	O	0	0
			289	289		
2	B	271	Total	O	0	0
			271	271		
2	C	245	Total	O	0	0
			245	245		
2	D	375	Total	O	0	0
			375	375		

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.

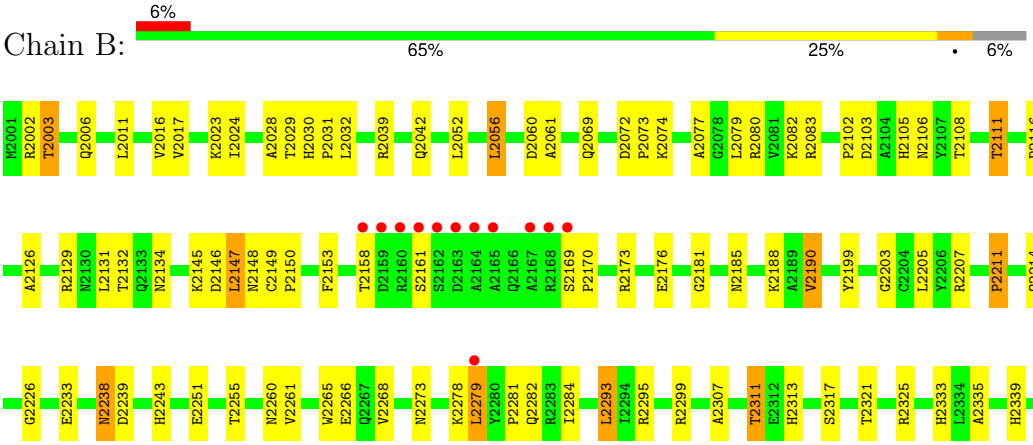
• Molecule 1: Chlorophenol-4-monooxygenase component 2

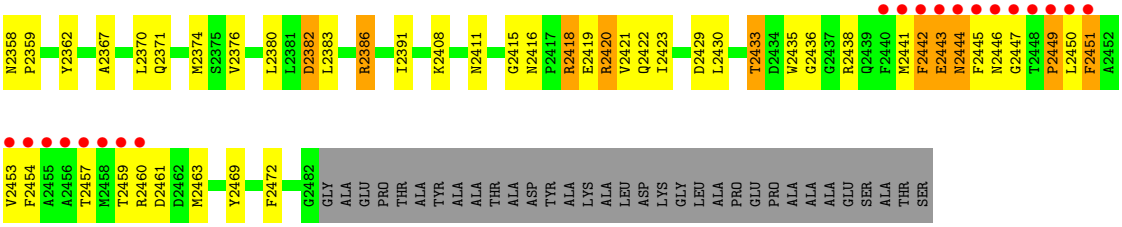
Chain A:

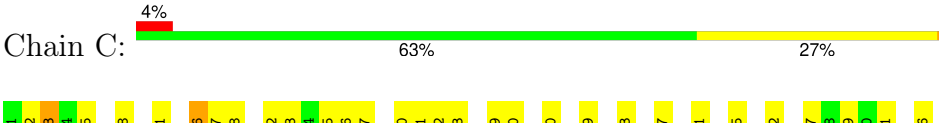


• Molecule 1: Chlorophenol-4-monooxygenase component 2

Chain B:

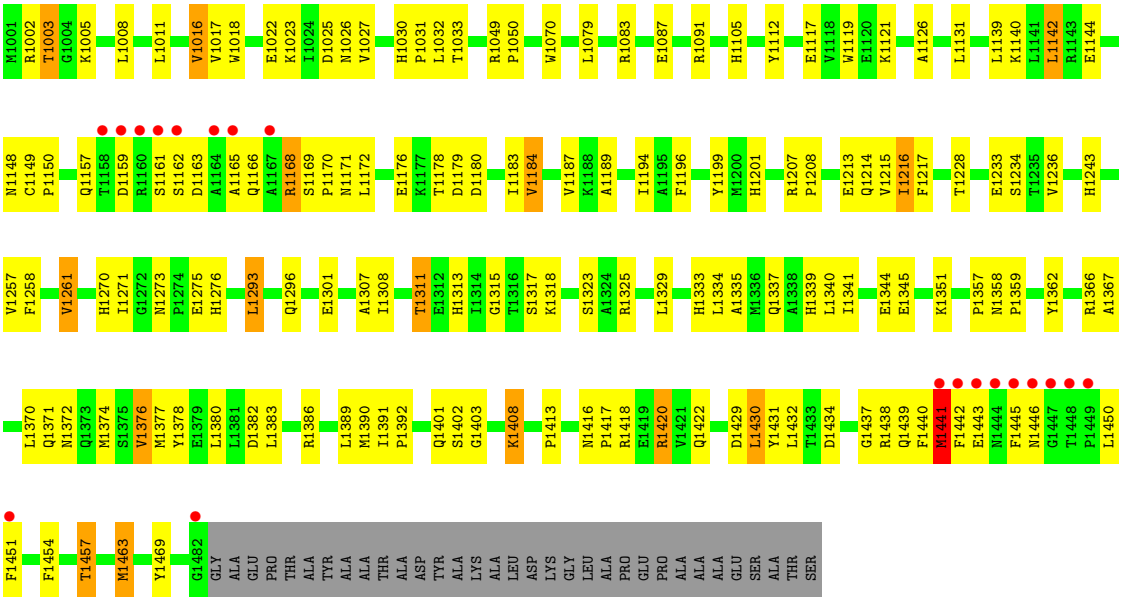






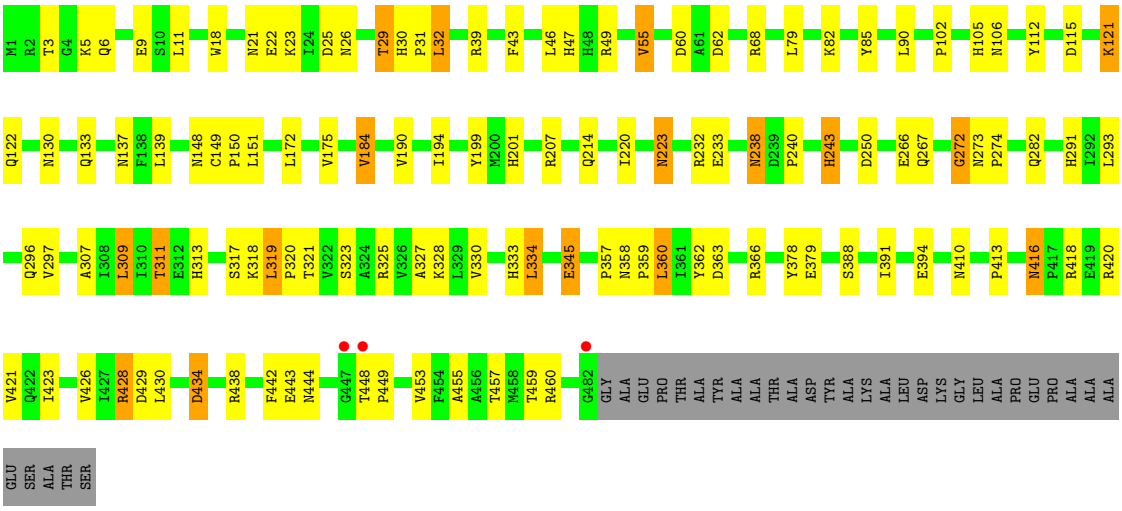
• Molecule 1: Chlorophenol-4-monooxygenase component 2

Chain C:



• Molecule 1: Chlorophenol-4-monooxygenase component 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	148.20Å 149.87Å 212.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.50 19.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.94-2.50) 97.8 (19.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.51 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.168 , 0.224 0.166 , 0.222	Depositor DCC
R_{free} test set	1030 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å^2)	23.7	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16516	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.32	0/3930	0.75	3/5335 (0.1%)
1	B	0.30	0/3930	0.75	2/5335 (0.0%)
1	C	0.30	0/3930	0.74	2/5335 (0.0%)
1	D	0.33	0/3930	0.75	7/5335 (0.1%)
All	All	0.32	0/15720	0.75	14/21340 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	416	ASN	CA-C-N	5.91	125.39	119.24
1	D	416	ASN	C-N-CA	5.91	125.39	119.24
1	A	3358	ASN	CA-C-N	5.84	125.21	118.85
1	A	3358	ASN	C-N-CA	5.84	125.21	118.85
1	A	3455	ALA	N-CA-C	-5.74	105.54	112.54
1	B	2149	CYS	CA-C-N	5.46	125.41	119.78
1	B	2149	CYS	C-N-CA	5.46	125.41	119.78
1	D	115	ASP	CA-C-N	5.28	124.60	118.85
1	D	115	ASP	C-N-CA	5.28	124.60	118.85
1	C	1149	CYS	CA-C-N	5.09	125.02	119.78
1	C	1149	CYS	C-N-CA	5.09	125.02	119.78
1	D	272	GLY	N-CA-C	5.08	121.81	115.21
1	D	243	HIS	CA-C-N	5.04	124.53	119.19
1	D	243	HIS	C-N-CA	5.04	124.53	119.19

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	3834	0	3734	132	0
1	B	3834	0	3734	131	0
1	C	3834	0	3734	124	0
1	D	3834	0	3737	97	0
2	A	289	0	0	6	0
2	B	271	0	0	8	0
2	C	245	0	0	3	0
2	D	375	0	0	5	0
All	All	16516	0	14939	443	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 15.

All (443) 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:C:1178:THR:HG22	1:C:1180:ASP:H	1.14	1.05
1:A:3079:LEU:HD11	1:A:3357:PRO:HG3	1.44	0.97
1:B:2433:THR:HG22	1:B:2436:GLY:H	1.31	0.96
1:A:3451:PHE:HD1	1:D:321:THR:HG1	1.00	0.95
1:A:3185:ASN:HD22	1:A:3260:ASN:H	1.13	0.92
1:D:172:LEU:HD11	1:D:184:VAL:HG13	1.57	0.86
1:B:2185:ASN:HD22	1:B:2260:ASN:H	1.21	0.85
1:C:1030:HIS:HD2	1:C:1032:LEU:H	1.26	0.84
1:C:1087:GLU:O	1:C:1091:ARG:HG3	1.77	0.83
1:B:2108:THR:O	1:B:2111:THR:HG23	1.79	0.82
1:D:79:LEU:HD21	1:D:357:PRO:HG3	1.62	0.82
1:C:1313:HIS:CD2	1:C:1420:ARG:HD3	2.14	0.81
1:D:30:HIS:HD2	1:D:32:LEU:H	1.29	0.81
1:C:1027:VAL:HG13	1:C:1033:THR:HG21	1.62	0.80
1:A:3313:HIS:CD2	1:A:3420:ARG:HD3	2.17	0.80
1:C:1371:GLN:HE22	1:C:1450:LEU:HD22	1.47	0.80
1:A:3345:GLU:HG3	1:C:1345:GLU:HG3	1.64	0.79
1:C:1176:GLU:HB3	1:C:1183:ILE:HB	1.63	0.79
1:D:313:HIS:HD2	1:D:420:ARG:HE	1.32	0.77
1:A:3457:THR:HG22	1:A:3463:MET:HG3	1.67	0.77
1:C:1079:LEU:HD21	1:C:1357:PRO:HG3	1.65	0.77
1:D:311:THR:HG23	1:D:317:SER:HB3	1.65	0.76
1:C:1126:ALA:HB2	1:C:1271:ILE:HD11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1296:GLN:HE22	1:C:1366:ARG:HA	1.51	0.75
1:D:410:ASN:HD22	1:D:420:ARG:HD2	1.52	0.74
1:B:2457:THR:HB	1:B:2463:MET:HE3	1.69	0.73
1:B:2450:LEU:HG	1:B:2451:PHE:HD2	1.51	0.73
1:B:2111:THR:HG21	1:B:2284:ILE:HA	1.71	0.73
1:B:2278:LYS:O	1:B:2279:LEU:HB2	1.87	0.73
1:C:1027:VAL:HG13	1:C:1033:THR:CG2	2.19	0.73
1:A:3185:ASN:ND2	1:A:3260:ASN:H	1.86	0.72
1:A:3448:THR:OG1	1:A:3449:PRO:HD2	1.89	0.72
1:A:3120:GLU:HG3	1:A:3132:THR:OG1	1.90	0.72
1:C:1311:THR:HG23	1:C:1317:SER:HB3	1.71	0.71
1:C:1315:GLY:HA3	1:C:1413:PRO:HG2	1.72	0.71
1:D:296:GLN:HE22	1:D:366:ARG:HA	1.55	0.71
1:B:2207:ARG:NH2	1:B:2214:GLN:HE22	1.89	0.71
1:C:1207:ARG:NH2	1:C:1214:GLN:HE22	1.88	0.70
1:D:313:HIS:CD2	1:D:420:ARG:HE	2.10	0.70
1:D:243:HIS:HD2	1:D:429:ASP:OD2	1.73	0.70
1:A:3441:MET:HA	1:A:3444:ASN:HB2	1.72	0.70
1:A:3079:LEU:HD13	1:A:3344:GLU:HG2	1.73	0.69
1:C:1313:HIS:HD2	1:C:1420:ARG:HH11	1.36	0.69
1:A:3313:HIS:HD2	1:A:3420:ARG:HD3	1.55	0.69
1:D:106:ASN:HD21	1:D:149:CYS:H	1.38	0.69
1:C:1243:HIS:HD2	1:C:1429:ASP:OD2	1.74	0.69
1:A:3030:HIS:HD2	1:A:3032:LEU:H	1.41	0.68
1:A:3120:GLU:HG2	1:A:3131:LEU:HB2	1.76	0.68
1:A:3393:SER:HB3	1:D:21:ASN:ND2	2.08	0.68
1:B:2003:THR:HG22	1:B:2006:GLN:H	1.58	0.68
1:B:2017:VAL:H	1:B:2023:LYS:HZ3	1.41	0.68
1:D:3:THR:H	1:D:6:GLN:HE21	1.40	0.68
1:A:3395:GLY:H	1:D:21:ASN:ND2	1.91	0.67
1:D:172:LEU:HD11	1:D:184:VAL:CG1	2.24	0.67
1:D:307:ALA:O	1:D:311:THR:HB	1.94	0.67
1:C:1176:GLU:HG2	1:C:1183:ILE:HD12	1.76	0.67
1:B:2052:LEU:HB3	1:B:2056:LEU:HD22	1.77	0.67
1:B:2311:THR:HG23	1:B:2317:SER:HB3	1.76	0.66
1:D:18:TRP:CZ2	1:D:23:LYS:HE3	2.31	0.66
1:A:3450:LEU:HD22	1:A:3453:VAL:HG21	1.77	0.66
1:B:2030:HIS:HD2	1:B:2032:LEU:H	1.44	0.66
1:B:2358:ASN:C	1:B:2358:ASN:HD22	2.02	0.66
1:A:3450:LEU:HD13	1:A:3453:VAL:HB	1.76	0.65
1:A:3358:ASN:C	1:A:3358:ASN:HD22	2.04	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1033:THR:HG23	1:C:1196:PHE:CZ	2.30	0.65
1:B:2190:VAL:HG11	1:B:2445:PHE:CZ	2.31	0.65
1:B:2313:HIS:CD2	1:B:2420:ARG:HD3	2.32	0.65
1:C:1313:HIS:HD2	1:C:1420:ARG:HD3	1.57	0.64
1:A:3462:ASP:OD1	1:A:3463:MET:N	2.31	0.64
1:C:1172:LEU:HD11	1:C:1184:VAL:HG13	1.77	0.64
1:A:3279:LEU:H	1:A:3279:LEU:HD12	1.63	0.64
1:A:3160:ARG:HG2	1:D:413:PRO:HG3	1.79	0.64
1:A:3016:VAL:HG13	1:A:3023:LYS:HE2	1.80	0.64
1:A:3454:PHE:HD2	1:C:1323:SER:HB2	1.63	0.63
1:A:3121:LYS:HD2	1:A:3122:GLN:HG2	1.80	0.63
1:A:3458:MET:HA	1:A:3463:MET:HB2	1.79	0.63
1:D:328:LYS:CE	1:D:379:GLU:HG3	2.28	0.62
1:A:3318:LYS:H	1:A:3318:LYS:HD2	1.64	0.62
1:C:1011:LEU:HD13	1:C:1027:VAL:HG12	1.80	0.62
1:D:207:ARG:HH12	1:D:214:GLN:NE2	1.96	0.62
1:B:2367:ALA:O	1:B:2371:GLN:HG3	2.00	0.62
1:A:3121:LYS:NZ	1:A:3122:GLN:HE21	1.96	0.62
1:B:2039:ARG:HE	1:B:2042:GLN:NE2	1.97	0.62
1:B:2391:ILE:HG23	1:B:2421:VAL:HG13	1.80	0.61
1:A:3177:LYS:HG3	1:A:3182:ILE:HG22	1.82	0.61
1:B:2449:PRO:O	1:B:2453:VAL:HG22	1.99	0.61
1:B:2313:HIS:HD2	1:B:2420:ARG:HH11	1.48	0.61
1:C:1168:ARG:HA	1:C:1168:ARG:NE	2.16	0.61
1:B:2185:ASN:ND2	1:B:2260:ASN:H	1.97	0.60
1:C:1371:GLN:NE2	1:C:1450:LEU:HB2	2.16	0.60
1:A:3002:ARG:HG3	1:A:3006:GLN:HE21	1.65	0.60
1:D:30:HIS:CD2	1:D:32:LEU:H	2.16	0.60
1:B:2030:HIS:CD2	1:B:2031:PRO:HD2	2.36	0.60
1:A:3118:VAL:HA	1:A:3121:LYS:HE3	1.84	0.60
1:B:2454:PHE:CG	1:D:327:ALA:HB2	2.37	0.60
1:B:2450:LEU:HG	1:B:2451:PHE:CD2	2.36	0.59
1:B:2453:VAL:O	1:B:2457:THR:HG23	2.01	0.59
1:C:1163:ASP:HA	1:C:1166:GLN:HB3	1.83	0.59
1:D:3:THR:H	1:D:6:GLN:NE2	2.00	0.59
1:A:3105:HIS:HE1	1:A:3148:ASN:ND2	2.00	0.59
1:A:3313:HIS:HE1	1:A:3416:ASN:O	1.85	0.59
1:C:1313:HIS:CD2	1:C:1420:ARG:HH11	2.19	0.59
1:B:2003:THR:HG22	1:B:2006:GLN:HG3	1.84	0.59
1:B:2079:LEU:HD21	1:B:2357:PRO:HG3	1.85	0.58
1:D:133:GLN:HE21	1:D:137:ASN:HD21	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3318:LYS:H	1:A:3318:LYS:CD	2.17	0.58
1:C:1440:PHE:HD1	1:C:1440:PHE:O	1.86	0.58
1:D:5:LYS:HE2	1:D:9:GLU:OE2	2.04	0.58
1:A:3393:SER:HB3	1:D:21:ASN:HD21	1.69	0.58
1:C:1307:ALA:O	1:C:1311:THR:HB	2.04	0.57
1:B:2307:ALA:O	1:B:2311:THR:HB	2.05	0.57
1:B:2374:MET:HG3	1:C:1378:TYR:HB2	1.86	0.57
1:B:2207:ARG:HH21	1:B:2214:GLN:HE22	1.50	0.57
1:B:2411:ASN:HD21	1:B:2415:GLY:HA2	1.69	0.57
1:A:3367:ALA:O	1:A:3371:GLN:HG3	2.05	0.57
1:A:3391:ILE:HG23	1:A:3421:VAL:HG13	1.87	0.57
1:C:1454:PHE:HA	1:C:1457:THR:HB	1.86	0.57
1:A:3454:PHE:HA	1:A:3457:THR:HB	1.86	0.57
1:B:2161:SER:HB2	1:C:1413:PRO:HA	1.85	0.57
1:A:3145:LYS:HE3	1:A:3147:LEU:HD21	1.87	0.56
1:C:1335:ALA:O	1:C:1339:HIS:HD2	1.88	0.56
1:C:1372:ASN:O	1:C:1376:VAL:HG13	2.05	0.56
1:A:3056:LEU:C	1:A:3068:ARG:HG3	2.30	0.56
1:A:3279:LEU:HD13	1:A:3280:TYR:CD1	2.40	0.56
1:A:3030:HIS:CD2	1:A:3032:LEU:H	2.22	0.56
1:B:2017:VAL:H	1:B:2023:LYS:NZ	2.04	0.56
1:B:2111:THR:HG22	2:B:334:HOH:O	2.05	0.56
1:B:2371:GLN:HG2	1:B:2449:PRO:HG2	1.87	0.56
1:C:1119:TRP:CE3	1:C:1276:HIS:HE1	2.24	0.56
1:A:3039:ARG:HE	1:A:3042:GLN:NE2	2.04	0.56
1:C:1358:ASN:C	1:C:1358:ASN:HD22	2.13	0.55
1:D:30:HIS:CD2	1:D:32:LEU:HB2	2.41	0.55
1:D:172:LEU:CD1	1:D:184:VAL:HG13	2.35	0.55
1:D:293:LEU:HD22	1:D:362:TYR:HB2	1.89	0.55
1:D:428:ARG:HD2	2:D:864:HOH:O	2.07	0.55
1:C:1030:HIS:CD2	1:C:1032:LEU:H	2.15	0.55
1:D:328:LYS:HE2	1:D:379:GLU:HG3	1.89	0.55
1:B:2003:THR:CG2	1:B:2006:GLN:H	2.19	0.55
1:B:2238:ASN:C	1:B:2238:ASN:HD22	2.15	0.55
1:A:3140:LYS:HD2	1:A:3140:LYS:N	2.22	0.55
1:A:3441:MET:HA	1:A:3444:ASN:CB	2.35	0.55
1:A:3374:MET:HA	1:A:3374:MET:HE2	1.87	0.55
1:B:2313:HIS:HD2	1:B:2420:ARG:HD3	1.72	0.55
1:A:3450:LEU:HB3	2:A:997:HOH:O	2.08	0.54
1:B:2358:ASN:HD22	1:B:2359:PRO:N	2.05	0.54
1:C:1003:THR:HG22	1:C:1005:LYS:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:VAL:HG22	2:D:597:HOH:O	2.06	0.54
1:A:3296:GLN:HE22	1:A:3366:ARG:HA	1.72	0.54
1:B:2185:ASN:HD22	1:B:2260:ASN:N	1.98	0.54
1:D:309:LEU:HB3	1:D:423:ILE:HD13	1.88	0.54
1:A:3408:LYS:HD2	2:A:1072:HOH:O	2.08	0.54
1:B:2243:HIS:HD2	1:B:2429:ASP:OD2	1.90	0.54
1:A:3480:GLU:HG2	1:A:3481:PHE:N	2.23	0.54
1:C:1150:PRO:HB2	1:C:1194:ILE:HD13	1.89	0.54
1:C:1234:SER:OG	1:C:1236:VAL:HG23	2.08	0.54
1:C:1105:HIS:HE1	1:C:1148:ASN:OD1	1.90	0.54
1:A:3282:GLN:H	1:A:3282:GLN:NE2	2.06	0.53
1:C:1178:THR:CG2	1:C:1179:ASP:N	2.71	0.53
1:A:3374:MET:HG3	1:D:378:TYR:HB2	1.91	0.53
1:A:3395:GLY:H	1:D:21:ASN:HD21	1.55	0.53
1:C:1258:PHE:HB3	1:C:1261:VAL:HG13	1.90	0.53
1:C:1168:ARG:HA	1:C:1168:ARG:CZ	2.39	0.53
1:A:3435:TRP:O	1:A:3438:ARG:HG3	2.07	0.53
1:A:3313:HIS:HD2	1:A:3420:ARG:HH11	1.57	0.53
1:C:1311:THR:HG23	1:C:1317:SER:CB	2.37	0.53
1:C:1351:LYS:H	1:C:1351:LYS:HD2	1.73	0.53
1:C:1325:ARG:HH22	1:C:1382:ASP:HB3	1.73	0.53
1:A:3030:HIS:CD2	1:A:3032:LEU:HB2	2.44	0.52
1:A:3141:LEU:CD2	1:A:3145:LYS:HG3	2.40	0.52
1:A:3233:GLU:OE2	1:D:243:HIS:HE1	1.92	0.52
1:B:2454:PHE:CD2	1:D:327:ALA:HB2	2.44	0.52
1:A:3251:GLU:H	1:A:3438:ARG:NH2	2.07	0.52
1:D:60:ASP:HB3	1:D:62:ASP:OD2	2.09	0.52
1:A:3335:ALA:O	1:A:3339:HIS:HD2	1.93	0.52
1:B:2293:LEU:HD12	1:B:2362:TYR:HB2	1.91	0.52
1:B:2311:THR:HG23	1:B:2317:SER:CB	2.39	0.52
1:C:1418:ARG:O	1:C:1422:GLN:HG3	2.10	0.52
1:B:2069:GLN:HG2	2:B:299:HOH:O	2.09	0.52
1:B:2408:LYS:HB3	1:C:1170:PRO:HG3	1.91	0.52
1:B:2126:ALA:O	1:B:2129:ARG:HG2	2.09	0.52
1:B:2153:PHE:CZ	1:B:2203:GLY:HA3	2.45	0.51
1:B:2441:MET:HG2	1:C:1389:LEU:HG	1.92	0.51
1:A:3070:TRP:HH2	1:A:3142:LEU:HD22	1.76	0.51
1:A:3211:PRO:HB2	1:A:3213:GLU:HG3	1.92	0.51
1:D:243:HIS:CD2	1:D:429:ASP:OD2	2.61	0.51
1:A:3121:LYS:HZ2	1:A:3122:GLN:HE21	1.59	0.51
1:A:3030:HIS:HD2	1:A:3032:LEU:HB2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3441:MET:HE3	1:D:388:SER:OG	2.10	0.51
1:A:3469:TYR:OH	1:C:1333:HIS:CD2	2.64	0.51
1:B:2002:ARG:HB2	1:B:2146:ASP:HB3	1.93	0.51
1:B:2023:LYS:HD3	1:B:2024:ILE:N	2.26	0.51
1:D:105:HIS:HE1	1:D:148:ASN:OD1	1.94	0.50
1:A:3105:HIS:HE1	1:A:3148:ASN:HD21	1.60	0.50
1:A:3469:TYR:OH	1:C:1333:HIS:HD2	1.94	0.50
1:D:313:HIS:HE1	1:D:416:ASN:O	1.94	0.50
1:D:444:ASN:OD1	1:D:449:PRO:HG3	2.11	0.50
1:A:3034:ARG:O	1:A:3038:GLU:HG3	2.11	0.50
1:B:2217:PHE:HZ	1:B:2281:PRO:HG3	1.75	0.50
1:C:1437:GLY:HA2	1:C:1440:PHE:CZ	2.46	0.50
1:D:220:ILE:HG22	1:D:267:GLN:NE2	2.27	0.50
1:A:3351:LYS:HE3	1:A:3351:LYS:HA	1.94	0.50
1:C:1159:ASP:O	1:C:1165:ALA:HB2	2.11	0.50
1:D:121:LYS:HE2	1:D:122:GLN:HE21	1.77	0.50
1:C:1150:PRO:HD2	1:C:1199:TYR:O	2.12	0.49
1:C:1430:LEU:HB3	1:C:1431:TYR:CD1	2.46	0.49
1:A:3358:ASN:HD22	1:A:3359:PRO:N	2.10	0.49
1:B:2170:PRO:HG3	1:C:1408:LYS:HD2	1.92	0.49
1:A:3105:HIS:CE1	1:A:3148:ASN:HD21	2.30	0.49
1:B:2169:SER:H	1:B:2173:ARG:NH2	2.09	0.49
1:C:1243:HIS:CD2	1:C:1429:ASP:OD2	2.62	0.49
1:B:2386:ARG:HD2	2:C:720:HOH:O	2.11	0.49
1:D:112:TYR:OH	1:D:201:HIS:HE1	1.96	0.49
1:A:3150:PRO:HB2	1:A:3194:ILE:HD13	1.95	0.49
1:C:1273:ASN:C	1:C:1273:ASN:HD22	2.21	0.49
1:A:3233:GLU:OE2	1:D:243:HIS:CE1	2.65	0.49
1:B:2003:THR:H	1:B:2006:GLN:HE21	1.60	0.49
1:A:3150:PRO:HD2	1:A:3199:TYR:O	2.12	0.49
1:A:3332:PHE:CD2	1:A:3376:VAL:HG21	2.48	0.49
1:B:2454:PHE:HD1	1:D:323:SER:HB3	1.76	0.49
1:B:2461:ASP:HB2	1:B:2463:MET:HE1	1.93	0.49
1:A:3316:THR:HB	1:A:3322:VAL:HG21	1.93	0.49
1:D:151:LEU:HA	1:D:201:HIS:HB3	1.95	0.49
1:A:3160:ARG:H	1:A:3160:ARG:HE	1.60	0.49
1:A:3333:HIS:HE1	2:A:219:HOH:O	1.96	0.49
1:B:2238:ASN:HD22	1:B:2239:ASP:N	2.11	0.49
1:C:1440:PHE:O	1:C:1440:PHE:CD1	2.66	0.49
1:A:3285:PHE:HA	1:A:3288:VAL:HG12	1.95	0.48
1:B:2433:THR:HG22	1:B:2436:GLY:N	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1178:THR:HG22	1:C:1180:ASP:N	2.00	0.48
1:D:133:GLN:HE21	1:D:137:ASN:ND2	2.10	0.48
1:B:2039:ARG:HE	1:B:2042:GLN:HE21	1.61	0.48
1:A:3341:ILE:O	1:A:3345:GLU:HG2	2.14	0.48
1:C:1178:THR:HG22	1:C:1179:ASP:N	2.28	0.48
1:C:1215:VAL:O	1:C:1271:ILE:HA	2.13	0.48
1:A:3448:THR:O	1:A:3449:PRO:C	2.56	0.48
1:B:2105:HIS:HE1	1:B:2148:ASN:OD1	1.95	0.48
1:A:3169:SER:HB2	1:A:3170:PRO:CD	2.43	0.48
1:C:1033:THR:HG23	1:C:1196:PHE:CE1	2.49	0.48
1:C:1377:MET:HG3	1:C:1431:TYR:CD2	2.49	0.48
1:C:1408:LYS:O	1:C:1408:LYS:HD3	2.14	0.48
1:B:2345:GLU:CD	1:D:345:GLU:HG2	2.39	0.47
1:A:3068:ARG:HE	1:A:3071:GLN:HE22	1.62	0.47
1:C:1207:ARG:HH21	1:C:1214:GLN:HE22	1.58	0.47
1:C:1441:MET:HE2	1:C:1441:MET:O	2.13	0.47
1:B:2190:VAL:HG22	1:C:1390:MET:HG3	1.95	0.47
1:B:2441:MET:HE3	1:B:2441:MET:HA	1.97	0.47
1:A:3327:ALA:HB2	1:C:1454:PHE:CD1	2.49	0.47
1:C:1070:TRP:HH2	1:C:1142:LEU:HD22	1.79	0.47
1:C:1454:PHE:CZ	1:C:1463:MET:HG2	2.50	0.47
1:D:291:HIS:HE1	2:D:608:HOH:O	1.97	0.47
1:A:3324:ALA:HB2	1:C:1451:PHE:CD1	2.50	0.47
1:A:3052:LEU:HB3	1:A:3056:LEU:HD22	1.96	0.47
1:A:3324:ALA:HB2	1:C:1451:PHE:HD1	1.80	0.47
1:C:1439:GLN:O	1:C:1443:GLU:HG3	2.15	0.47
1:B:2333:HIS:HE1	2:B:159:HOH:O	1.97	0.47
1:D:55:VAL:O	1:D:68:ARG:HD2	2.15	0.47
1:A:3153:PHE:CZ	1:A:3203:GLY:HA3	2.50	0.46
1:A:3181:GLY:HA2	1:A:3265:TRP:CD1	2.50	0.46
1:B:2082:LYS:HG3	2:B:408:HOH:O	2.14	0.46
1:B:2233:GLU:OE2	1:C:1243:HIS:HE1	1.98	0.46
1:D:273:ASN:C	1:D:273:ASN:HD22	2.23	0.46
1:D:453:VAL:O	1:D:457:THR:HG23	2.15	0.46
1:A:3331:ALA:HB2	1:C:1450:LEU:HD11	1.96	0.46
1:A:3370:LEU:HD21	1:A:3443:GLU:HB2	1.96	0.46
1:A:3279:LEU:HD12	1:A:3279:LEU:N	2.28	0.46
1:B:2457:THR:C	1:B:2459:THR:H	2.24	0.46
1:C:1091:ARG:NH2	1:C:1301:GLU:OE2	2.47	0.46
1:B:2145:LYS:HB3	1:B:2147:LEU:HD13	1.96	0.46
1:A:3293:LEU:HD22	1:A:3362:TYR:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2003:THR:HG22	1:B:2006:GLN:CG	2.45	0.46
1:C:1293:LEU:HD12	1:C:1362:TYR:HB2	1.97	0.46
1:D:282:GLN:NE2	1:D:460:ARG:HD2	2.31	0.46
1:C:1187:VAL:HG22	1:C:1257:VAL:HG12	1.98	0.46
1:B:2190:VAL:HG11	1:B:2445:PHE:HZ	1.79	0.46
1:D:30:HIS:HD2	1:D:32:LEU:HB2	1.79	0.46
1:D:39:ARG:HA	1:D:39:ARG:NE	2.31	0.46
1:B:2391:ILE:CG2	1:B:2421:VAL:HG13	2.44	0.46
1:C:1367:ALA:O	1:C:1371:GLN:HG3	2.16	0.46
1:A:3333:HIS:HD2	1:C:1469:TYR:OH	1.98	0.45
1:C:1003:THR:HG22	1:C:1005:LYS:H	1.81	0.45
1:C:1083:ARG:HD2	1:C:1340:LEU:HD21	1.98	0.45
1:C:1216:ILE:HD12	1:C:1217:PHE:N	2.32	0.45
1:A:3109:PHE:HB3	1:A:3139:LEU:HD21	1.98	0.45
1:B:2131:LEU:O	1:B:2134:ASN:HB2	2.16	0.45
1:C:1025:ASP:OD2	1:C:1026:ASN:N	2.48	0.45
1:C:1318:LYS:HB2	2:C:871:HOH:O	2.16	0.45
1:C:1389:LEU:HA	2:C:586:HOH:O	2.16	0.45
1:B:2116:PRO:HB2	1:B:2132:THR:HG23	1.97	0.45
1:B:2150:PRO:HD2	1:B:2199:TYR:O	2.16	0.45
1:B:2226:GLY:HA3	1:B:2261:VAL:HG12	1.98	0.45
1:C:1083:ARG:HD3	1:C:1344:GLU:OE2	2.16	0.45
1:C:1207:ARG:HH21	1:C:1214:GLN:NE2	2.14	0.45
1:A:3080:ARG:HG2	2:A:725:HOH:O	2.16	0.45
1:B:2371:GLN:CG	1:B:2449:PRO:HG2	2.47	0.45
1:C:1049:ARG:HA	1:C:1050:PRO:HD3	1.85	0.45
1:D:22:GLU:OE2	1:D:30:HIS:HE1	1.99	0.45
1:B:2205:LEU:N	1:B:2205:LEU:HD22	2.31	0.45
1:B:2217:PHE:CZ	1:B:2281:PRO:HG3	2.51	0.45
1:B:2358:ASN:C	1:B:2358:ASN:ND2	2.73	0.45
1:C:1018:TRP:CZ2	1:C:1023:LYS:HE2	2.52	0.45
1:A:3318:LYS:HD3	1:A:3319:LEU:N	2.31	0.45
1:D:455:ALA:O	1:D:459:THR:HG23	2.17	0.45
1:B:2003:THR:H	1:B:2006:GLN:NE2	2.13	0.45
1:D:47:HIS:HE1	1:D:85:TYR:OH	1.99	0.45
1:D:333:HIS:HD2	1:D:334:LEU:HD13	1.82	0.45
1:C:1313:HIS:HE1	1:C:1416:ASN:O	2.00	0.45
1:C:1454:PHE:CE2	1:C:1463:MET:HG2	2.52	0.45
1:A:3120:GLU:OE2	1:A:3130:ASN:HA	2.16	0.44
1:A:3333:HIS:CD2	1:C:1469:TYR:OH	2.70	0.44
1:B:2273:ASN:C	1:B:2273:ASN:HD22	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1359:PRO:HA	1:C:1362:TYR:CZ	2.53	0.44
1:B:2433:THR:CG2	1:B:2435:TRP:HB3	2.47	0.44
1:C:1308:ILE:O	1:C:1311:THR:HG22	2.17	0.44
1:A:3243:HIS:NE2	1:D:233:GLU:OE1	2.49	0.44
1:A:3358:ASN:C	1:A:3358:ASN:ND2	2.75	0.44
1:B:2459:THR:HG23	1:B:2460:ARG:N	2.31	0.44
1:A:3299:ARG:HH12	1:A:3439:GLN:NE2	2.16	0.44
1:D:293:LEU:O	1:D:297:VAL:HG23	2.18	0.44
1:C:1273:ASN:ND2	1:C:1275:GLU:H	2.15	0.44
1:D:26:ASN:C	1:D:26:ASN:HD22	2.24	0.44
1:A:3039:ARG:HE	1:A:3042:GLN:HE21	1.65	0.44
1:A:3318:LYS:CD	1:A:3318:LYS:N	2.81	0.44
1:B:2188:LYS:HD3	1:B:2188:LYS:HA	1.87	0.44
1:D:410:ASN:ND2	1:D:420:ARG:HD2	2.28	0.44
1:A:3163:ASP:HB2	1:A:3166:GLN:HB3	2.00	0.43
1:B:2358:ASN:HA	1:B:2359:PRO:HD3	1.82	0.43
1:C:1016:VAL:HG22	1:C:1228:THR:HG23	2.01	0.43
1:D:238:ASN:O	1:D:240:PRO:HD3	2.18	0.43
1:A:3070:TRP:CH2	1:A:3142:LEU:HD22	2.51	0.43
1:B:2441:MET:HE3	1:B:2444:ASN:HD22	1.82	0.43
1:D:30:HIS:CD2	1:D:31:PRO:HD2	2.53	0.43
1:D:359:PRO:O	1:D:363:ASP:HB2	2.18	0.43
1:B:2011:LEU:HD12	1:B:2028:ALA:HB2	1.99	0.43
1:B:2321:THR:HG22	1:B:2325:ARG:HH21	1.83	0.43
1:D:223:ASN:C	1:D:223:ASN:HD22	2.26	0.43
1:B:2386:ARG:HH21	1:C:1189:ALA:HB1	1.83	0.43
1:C:1112:TYR:OH	1:C:1201:HIS:HE1	2.01	0.43
1:A:3217:PHE:HZ	1:A:3281:PRO:HG3	1.84	0.43
1:B:2370:LEU:HD21	1:B:2443:GLU:HB3	2.00	0.43
1:D:223:ASN:C	1:D:223:ASN:ND2	2.73	0.43
1:D:313:HIS:HD2	1:D:420:ARG:NE	2.09	0.43
1:B:2438:ARG:O	1:B:2442:PHE:HD1	2.00	0.43
1:B:2469:TYR:OH	1:D:333:HIS:CD2	2.71	0.43
1:C:1359:PRO:HA	1:C:1362:TYR:CE2	2.54	0.43
1:D:330:VAL:HG12	1:D:334:LEU:HD22	2.00	0.43
1:A:3109:PHE:CZ	1:A:3201:HIS:CD2	3.07	0.43
1:B:2359:PRO:HA	1:B:2362:TYR:CZ	2.53	0.43
1:C:1416:ASN:N	1:C:1417:PRO:HD3	2.33	0.43
1:B:2083:ARG:HD3	1:B:2344:GLU:OE1	2.19	0.43
1:B:2382:ASP:HB3	2:B:355:HOH:O	2.18	0.43
1:B:2419:GLU:O	1:B:2423:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3120:GLU:HG3	1:A:3132:THR:N	2.34	0.43
1:A:3129:ARG:O	1:A:3130:ASN:C	2.62	0.42
1:B:2072:ASP:HA	1:B:2073:PRO:HD3	1.84	0.42
1:C:1070:TRP:CH2	1:C:1142:LEU:HD22	2.54	0.42
1:A:3397:TRP:CZ2	1:A:3418:ARG:HG2	2.53	0.42
1:A:3206:TYR:CG	1:A:3207:ARG:N	2.86	0.42
1:A:3358:ASN:HA	1:A:3359:PRO:HD3	1.81	0.42
1:B:2211:PRO:HG2	1:B:2214:GLN:CD	2.44	0.42
1:B:2443:GLU:OE2	1:B:2446:ASN:HB2	2.20	0.42
1:B:2454:PHE:CE2	1:B:2463:MET:HG2	2.53	0.42
1:C:1207:ARG:NH2	1:C:1214:GLN:NE2	2.61	0.42
1:D:232:ARG:NH2	1:D:250:ASP:OD1	2.52	0.42
1:D:82:LYS:O	1:D:85:TYR:HB3	2.19	0.42
1:C:1027:VAL:O	1:C:1033:THR:HG22	2.19	0.42
1:B:2282:GLN:OE1	1:B:2460:ARG:HD3	2.19	0.42
1:C:1391:ILE:HA	1:C:1392:PRO:HD3	1.91	0.42
1:D:325:ARG:O	1:D:328:LYS:HG3	2.20	0.42
1:B:2150:PRO:HG3	2:B:763:HOH:O	2.19	0.42
1:D:102:PRO:HA	1:D:105:HIS:CE1	2.55	0.42
1:B:2449:PRO:HA	1:B:2453:VAL:HG13	2.02	0.42
1:D:319:LEU:HA	1:D:320:PRO:HD3	1.92	0.42
1:A:3359:PRO:HA	1:A:3362:TYR:CZ	2.55	0.42
1:B:2077:ALA:HA	1:B:2080:ARG:NH1	2.35	0.42
1:B:2359:PRO:HA	1:B:2362:TYR:CE2	2.55	0.42
1:B:2449:PRO:O	1:B:2450:LEU:C	2.62	0.42
1:A:3291:HIS:HE1	2:A:225:HOH:O	2.03	0.42
1:C:1140:LYS:O	1:C:1144:GLU:HG3	2.20	0.42
1:D:328:LYS:HD2	2:D:1022:HOH:O	2.20	0.42
1:A:3223:ASN:C	1:A:3223:ASN:HD22	2.27	0.41
2:A:187:HOH:O	1:C:1339:HIS:HE1	2.01	0.41
1:B:2181:GLY:HA2	1:B:2265:TRP:CD1	2.55	0.41
1:B:2313:HIS:HE1	1:B:2416:ASN:O	2.03	0.41
1:B:2418:ARG:O	1:B:2422:GLN:HG3	2.20	0.41
1:C:1441:MET:CE	1:C:1445:PHE:HB3	2.50	0.41
1:D:360:LEU:HD23	1:D:360:LEU:HA	1.92	0.41
1:A:3212:GLY:O	1:A:3272:GLY:HA2	2.20	0.41
1:C:1184:VAL:HG12	1:C:1261:VAL:HG22	2.01	0.41
1:D:313:HIS:CD2	1:D:420:ARG:HB2	2.55	0.41
1:A:3223:ASN:C	1:A:3223:ASN:ND2	2.79	0.41
1:A:3374:MET:HG3	1:D:378:TYR:CB	2.50	0.41
1:B:2279:LEU:O	1:B:2282:GLN:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:GLU:H	1:D:266:GLU:CD	2.28	0.41
1:D:358:ASN:HA	1:D:359:PRO:HD3	1.87	0.41
1:B:2069:GLN:HG3	1:B:2103:ASP:HA	2.03	0.41
1:C:1358:ASN:HA	1:C:1359:PRO:HD3	1.88	0.41
1:B:2335:ALA:O	1:B:2339:HIS:HD2	2.04	0.41
1:B:2454:PHE:HE2	1:B:2463:MET:HG2	1.85	0.41
1:C:1030:HIS:HA	1:C:1031:PRO:HD3	1.95	0.41
1:D:29:THR:HG21	2:D:922:HOH:O	2.20	0.41
1:A:3068:ARG:HE	1:A:3071:GLN:NE2	2.19	0.41
1:A:3076:ALA:HB1	1:A:3080:ARG:NH2	2.36	0.41
1:B:2169:SER:OG	1:C:1408:LYS:HE2	2.21	0.41
1:B:2345:GLU:HG2	1:D:345:GLU:HG2	2.03	0.41
1:D:220:ILE:HG22	1:D:267:GLN:HE21	1.85	0.41
1:A:3127:GLU:N	1:A:3127:GLU:CD	2.79	0.41
1:A:3407:VAL:HG13	1:A:3417:PRO:HG2	2.01	0.41
1:A:3433:THR:HA	1:D:434:ASP:HB3	2.03	0.41
1:A:3450:LEU:HD22	1:A:3453:VAL:CG2	2.48	0.41
1:A:3462:ASP:CG	1:A:3463:MET:H	2.27	0.41
1:B:2169:SER:HA	1:B:2173:ARG:NH2	2.36	0.41
1:B:2435:TRP:O	1:B:2438:ARG:HG3	2.21	0.41
1:B:2438:ARG:O	1:B:2442:PHE:CD1	2.74	0.41
1:C:1337:GLN:O	1:C:1341:ILE:HG12	2.21	0.41
1:C:1402:SER:O	1:C:1403:GLY:C	2.63	0.41
1:D:328:LYS:NZ	1:D:379:GLU:HG3	2.35	0.41
1:A:3328:LYS:HA	1:C:1450:LEU:HD21	2.02	0.41
1:B:2459:THR:HG23	1:B:2460:ARG:H	1.84	0.41
1:C:1207:ARG:O	1:C:1208:PRO:C	2.64	0.41
1:D:150:PRO:HB2	1:D:194:ILE:HD13	2.02	0.41
1:D:207:ARG:HH12	1:D:214:GLN:HE22	1.68	0.41
1:B:2472:PHE:HB3	2:B:246:HOH:O	2.20	0.40
1:B:2243:HIS:HE1	1:C:1233:GLU:OE1	2.04	0.40
1:B:2251:GLU:H	1:B:2438:ARG:NH2	2.20	0.40
1:B:2266:GLU:HB3	2:B:631:HOH:O	2.21	0.40
1:C:1441:MET:HE2	1:C:1441:MET:C	2.46	0.40
1:D:391:ILE:HG23	1:D:421:VAL:HG13	2.02	0.40
1:A:3298:LEU:HD12	1:A:3298:LEU:HA	1.90	0.40
1:B:2243:HIS:CE1	1:C:1233:GLU:OE1	2.75	0.40
1:C:1169:SER:HB3	1:C:1171:ASN:OD1	2.21	0.40
1:D:272:GLY:O	1:D:274:PRO:HD3	2.22	0.40
1:B:2060:ASP:OD2	1:B:2061:ALA:N	2.47	0.40
1:B:2102:PRO:O	1:B:2106:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2118:VAL:HA	1:B:2121:LYS:HG2	2.04	0.40
1:B:2359:PRO:HB2	1:B:2460:ARG:NH2	2.36	0.40
1:C:1117:GLU:O	1:C:1121:LYS:HD3	2.21	0.40
1:C:1270:HIS:CD2	1:C:1270:HIS:C	2.97	0.40
1:D:442:PHE:CE2	1:D:443:GLU:HG3	2.56	0.40
1:A:3017:VAL:H	1:A:3023:LYS:NZ	2.20	0.40
1:A:3325:ARG:HH12	1:A:3382:ASP:HB3	1.86	0.40
1:A:3325:ARG:HH22	1:A:3382:ASP:CG	2.28	0.40
1:D:43:PHE:O	1:D:47:HIS:CD2	2.74	0.40
1:D:150:PRO:HD2	1:D:199:TYR:O	2.22	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	480/515 (93%)	453 (94%)	22 (5%)	5 (1%)	13 25
1	B	480/515 (93%)	446 (93%)	24 (5%)	10 (2%)	5 10
1	C	480/515 (93%)	458 (95%)	19 (4%)	3 (1%)	22 39
1	D	480/515 (93%)	472 (98%)	7 (2%)	1 (0%)	44 64
All	All	1920/2060 (93%)	1829 (95%)	72 (4%)	19 (1%)	13 25

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3449	PRO
1	A	3463	MET
1	A	3480	GLU
1	A	3481	PHE
1	B	2190	VAL

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Mol	Chain	Res	Type
1	A	3161	SER
1	B	2158	THR
1	B	2442	PHE
1	B	2449	PRO
1	C	1162	SER
1	B	2279	LEU
1	C	1161	SER
1	C	1441	MET
1	B	2451	PHE
1	B	2176	GLU
1	B	2444	ASN
1	D	448	THR
1	B	2211	PRO
1	B	2447	GLY

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	406/425 (96%)	370 (91%)	36 (9%)	8 17
1	B	406/425 (96%)	381 (94%)	25 (6%)	15 31
1	C	406/425 (96%)	369 (91%)	37 (9%)	7 16
1	D	406/425 (96%)	376 (93%)	30 (7%)	11 23
All	All	1624/1700 (96%)	1496 (92%)	128 (8%)	10 21

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3008	LEU
1	A	3011	LEU
1	A	3032	LEU
1	A	3046	LEU
1	A	3052	LEU
1	A	3056	LEU
1	A	3079	LEU

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Mol	Chain	Res	Type
1	A	3090	LEU
1	A	3120	GLU
1	A	3127	GLU
1	A	3130	ASN
1	A	3140	LYS
1	A	3141	LEU
1	A	3142	LEU
1	A	3152	ASN
1	A	3158	THR
1	A	3160	ARG
1	A	3190	VAL
1	A	3213	GLU
1	A	3223	ASN
1	A	3279	LEU
1	A	3298	LEU
1	A	3302	LEU
1	A	3318	LYS
1	A	3319	LEU
1	A	3329	LEU
1	A	3340	LEU
1	A	3351	LYS
1	A	3401	GLN
1	A	3418	ARG
1	A	3420	ARG
1	A	3428	ARG
1	A	3430	LEU
1	A	3443	GLU
1	A	3444	ASN
1	A	3450	LEU
1	B	2003	THR
1	B	2016	VAL
1	B	2029	THR
1	B	2056	LEU
1	B	2074	LYS
1	B	2111	THR
1	B	2147	LEU
1	B	2223	ASN
1	B	2238	ASN
1	B	2255	THR
1	B	2268	VAL
1	B	2293	LEU
1	B	2295	ARG

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Mol	Chain	Res	Type
1	B	2299	ARG
1	B	2311	THR
1	B	2376	VAL
1	B	2380	LEU
1	B	2382	ASP
1	B	2383	LEU
1	B	2386	ARG
1	B	2418	ARG
1	B	2420	ARG
1	B	2430	LEU
1	B	2433	THR
1	B	2443	GLU
1	C	1002	ARG
1	C	1003	THR
1	C	1008	LEU
1	C	1016	VAL
1	C	1017	VAL
1	C	1022	GLU
1	C	1131	LEU
1	C	1139	LEU
1	C	1142	LEU
1	C	1157	GLN
1	C	1168	ARG
1	C	1184	VAL
1	C	1213	GLU
1	C	1216	ILE
1	C	1261	VAL
1	C	1293	LEU
1	C	1311	THR
1	C	1329	LEU
1	C	1334	LEU
1	C	1370	LEU
1	C	1374	MET
1	C	1376	VAL
1	C	1380	LEU
1	C	1383	LEU
1	C	1386	ARG
1	C	1401	GLN
1	C	1408	LYS
1	C	1420	ARG
1	C	1430	LEU
1	C	1432	LEU

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Mol	Chain	Res	Type
1	C	1434	ASP
1	C	1438	ARG
1	C	1441	MET
1	C	1442	PHE
1	C	1446	ASN
1	C	1457	THR
1	C	1463	MET
1	D	11	LEU
1	D	25	ASP
1	D	29	THR
1	D	32	LEU
1	D	46	LEU
1	D	49	ARG
1	D	55	VAL
1	D	90	LEU
1	D	121	LYS
1	D	130	ASN
1	D	139	LEU
1	D	175	VAL
1	D	184	VAL
1	D	190	VAL
1	D	223	ASN
1	D	238	ASN
1	D	309	LEU
1	D	311	THR
1	D	318	LYS
1	D	319	LEU
1	D	334	LEU
1	D	345	GLU
1	D	360	LEU
1	D	394	GLU
1	D	418	ARG
1	D	426	VAL
1	D	428	ARG
1	D	430	LEU
1	D	434	ASP
1	D	438	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (110) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3006	GLN

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Mol	Chain	Res	Type
1	A	3026	ASN
1	A	3030	HIS
1	A	3042	GLN
1	A	3048	HIS
1	A	3071	GLN
1	A	3105	HIS
1	A	3122	GLN
1	A	3134	ASN
1	A	3136	HIS
1	A	3137	ASN
1	A	3148	ASN
1	A	3152	ASN
1	A	3157	GLN
1	A	3171	ASN
1	A	3185	ASN
1	A	3201	HIS
1	A	3223	ASN
1	A	3282	GLN
1	A	3291	HIS
1	A	3296	GLN
1	A	3313	HIS
1	A	3333	HIS
1	A	3339	HIS
1	A	3358	ASN
1	A	3368	HIS
1	A	3371	GLN
1	A	3372	ASN
1	A	3373	GLN
1	A	3396	GLN
1	A	3410	ASN
1	A	3439	GLN
1	A	3444	ASN
1	A	3446	ASN
1	A	3475	GLN
1	B	2006	GLN
1	B	2030	HIS
1	B	2042	GLN
1	B	2105	HIS
1	B	2133	GLN
1	B	2134	ASN
1	B	2137	ASN
1	B	2166	GLN

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Mol	Chain	Res	Type
1	B	2185	ASN
1	B	2214	GLN
1	B	2223	ASN
1	B	2238	ASN
1	B	2243	HIS
1	B	2248	GLN
1	B	2260	ASN
1	B	2273	ASN
1	B	2313	HIS
1	B	2333	HIS
1	B	2339	HIS
1	B	2358	ASN
1	B	2371	GLN
1	B	2372	ASN
1	B	2396	GLN
1	B	2411	ASN
1	C	1030	HIS
1	C	1105	HIS
1	C	1122	GLN
1	C	1133	GLN
1	C	1157	GLN
1	C	1201	HIS
1	C	1214	GLN
1	C	1243	HIS
1	C	1248	GLN
1	C	1267	GLN
1	C	1270	HIS
1	C	1273	ASN
1	C	1276	HIS
1	C	1296	GLN
1	C	1313	HIS
1	C	1333	HIS
1	C	1339	HIS
1	C	1358	ASN
1	C	1368	HIS
1	C	1371	GLN
1	C	1372	ASN
1	C	1396	GLN
1	D	6	GLN
1	D	21	ASN
1	D	26	ASN
1	D	30	HIS

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Mol	Chain	Res	Type
1	D	47	HIS
1	D	48	HIS
1	D	105	HIS
1	D	106	ASN
1	D	122	GLN
1	D	130	ASN
1	D	137	ASN
1	D	201	HIS
1	D	214	GLN
1	D	223	ASN
1	D	243	HIS
1	D	267	GLN
1	D	273	ASN
1	D	282	GLN
1	D	289	HIS
1	D	291	HIS
1	D	296	GLN
1	D	313	HIS
1	D	333	HIS
1	D	368	HIS
1	D	396	GLN
1	D	401	GLN
1	D	410	ASN
1	D	422	GLN
1	D	446	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	482/515 (93%)	-0.40	32 (6%)	26	24	14, 28, 87, 134	0
1	B	482/515 (93%)	-0.34	32 (6%)	26	24	15, 30, 92, 129	0
1	C	482/515 (93%)	-0.33	19 (3%)	44	40	16, 33, 69, 119	0
1	D	482/515 (93%)	-0.77	3 (0%)	85	83	12, 22, 45, 68	0
All	All	1928/2060 (93%)	-0.46	86 (4%)	39	36	12, 29, 69, 134	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2164	ALA	7.4
1	B	2450	LEU	6.2
1	A	3444	ASN	5.6
1	C	1164	ALA	5.5
1	A	3450	LEU	5.3
1	C	1165	ALA	5.0
1	A	3459	THR	4.9
1	A	3165	ALA	4.9
1	B	2165	ALA	4.9
1	B	2448	THR	4.6
1	B	2454	PHE	4.4
1	A	3162	SER	4.3
1	A	3164	ALA	4.3
1	A	3451	PHE	4.2
1	C	1167	ALA	4.1
1	B	2158	THR	4.1
1	B	2162	SER	4.0
1	B	2451	PHE	4.0
1	B	2442	PHE	3.9
1	B	2160	ARG	3.9
1	C	1159	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	3161	SER	3.8
1	C	1442	PHE	3.7
1	A	3448	THR	3.7
1	B	2163	ASP	3.7
1	B	2459	THR	3.7
1	B	2169	SER	3.6
1	B	2456	ALA	3.6
1	A	3452	ALA	3.5
1	A	3159	ASP	3.5
1	D	482	GLY	3.4
1	C	1161	SER	3.4
1	C	1449	PRO	3.3
1	D	447	GLY	3.3
1	A	3167	ALA	3.3
1	C	1162	SER	3.3
1	A	3454	PHE	3.3
1	A	3453	VAL	3.2
1	A	3442	PHE	3.2
1	A	3158	THR	3.1
1	C	1451	PHE	3.1
1	C	1448	THR	3.1
1	B	2458	MET	3.1
1	B	2453	VAL	3.0
1	B	2441	MET	3.0
1	B	2161	SER	3.0
1	B	2159	ASP	3.0
1	A	3455	ALA	3.0
1	B	2443	GLU	3.0
1	B	2460	ARG	2.9
1	B	2279	LEU	2.9
1	C	1443	GLU	2.8
1	C	1446	ASN	2.8
1	B	2447	GLY	2.8
1	A	3449	PRO	2.8
1	A	3160	ARG	2.8
1	C	1447	GLY	2.8
1	A	3446	ASN	2.7
1	D	448	THR	2.7
1	B	2167	ALA	2.7
1	A	3443	GLU	2.7
1	A	3163	ASP	2.6
1	A	3441	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2455	ALA	2.6
1	A	3447	GLY	2.6
1	B	2440	PHE	2.6
1	C	1482	GLY	2.5
1	B	2168	ARG	2.5
1	A	3166	GLN	2.4
1	C	1160	ARG	2.4
1	C	1158	THR	2.4
1	B	2444	ASN	2.4
1	B	2446	ASN	2.4
1	C	1441	MET	2.3
1	A	3457	THR	2.2
1	C	1445	PHE	2.2
1	A	3440	PHE	2.2
1	B	2457	THR	2.2
1	A	3460	ARG	2.2
1	A	3127	GLU	2.2
1	B	2445	PHE	2.2
1	A	3168	ARG	2.1
1	A	3445	PHE	2.1
1	C	1444	ASN	2.1
1	B	2449	PRO	2.1
1	A	3462	ASP	2.1

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.