



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2016 – 02:35 PM EST

PDB ID : 3TEH
Title : Crystal structure of Thermus thermophilus Phenylalanyl-tRNA synthetase complexed with L-dopa
Authors : Safro, M.; Klipcan, L.; Moor, N.
Deposited on : 2011-08-14
Resolution : 2.85 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

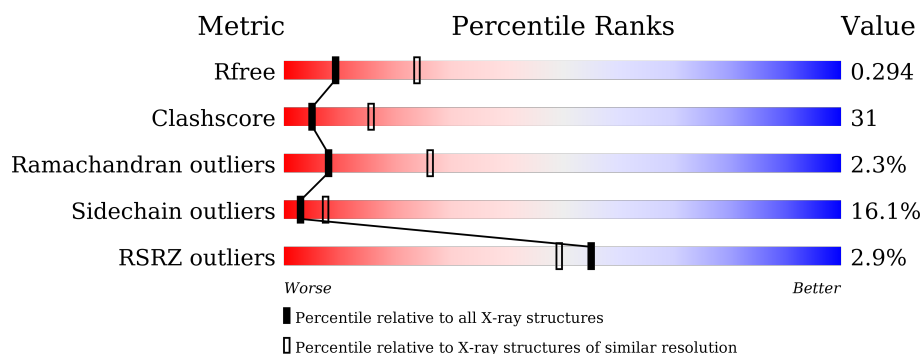
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	91344	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	350	<div> <div></div> <div>38%</div> <div>30%</div> <div>8%</div> <div>24%</div> </div>
2	B	785	<div> <div>3%</div> <div>51%</div> <div>40%</div> <div>8%</div> <div></div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DAH	A	351	-	-	X	-
3	DAH	B	786	-	-	X	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8670 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.

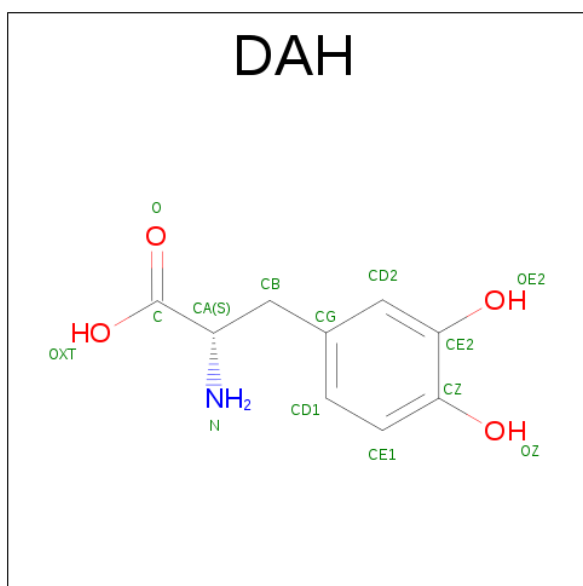
- Molecule 1 is a protein called Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	11	0	0
			2123	1388	363	365	7			

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	785	Total	C	N	O	S	46	0	0
			6127	3925	1091	1101	10			

- Molecule 3 is 3,4-DIHYDROXYPHENYLALANINE (three-letter code: DAH) (formula: $C_9H_{11}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	9	1	4		
3	B	1	Total	C	N	O	0	0
			14	9	1	4		

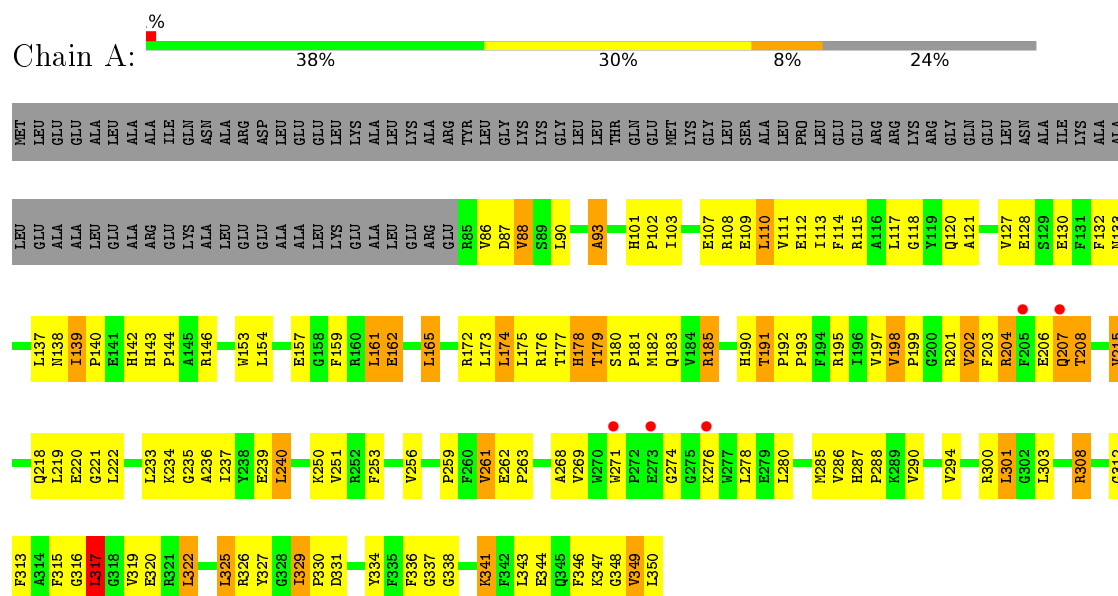
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	103	Total 103	O 103	0	0
4	B	289	Total 289	O 289	0	0

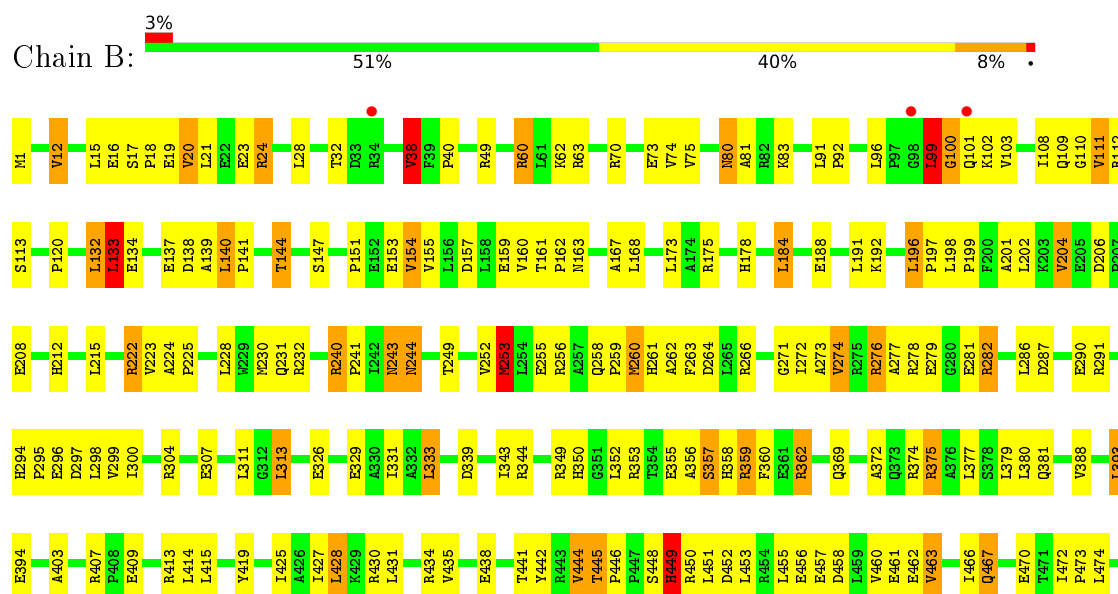
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Phenylalanyl-tRNA synthetase alpha chain



• Molecule 2: Phenylalanyl-tRNA synthetase beta chain



R767	V701	L622	L556	L557	P479
V768	P702	V626	K557	K558	D484
E770	A703	E627	E558	E559	E489
A771	P704	F631	L560	D561	A490
L772	Y707	P632	L562	L563	P491
R773	V710	F633	R564	R565	Y492
A774	L713	H635	P566	P567	R493
R775	V714	G637	R567	R568	K494
F776	A718	V638	L569	L570	R497
G777	Y721	S639	F571	F572	L498
F778	L722	G640	G574	R575	V501
G779	E723	R641	R576	F577	L502
L779	S724	V642	F578	E579	S503
R780	L725	E647	R580	R581	G504
F785	A726	G650	E582	E583	L505
	L727	F651	H584	F585	Q508
	F728	L652	I659	L585	E509
	D729	G653	A586	G587	V510
	L730	H556	Q661	L588	Y511
	Y731	P657	E662	L589	Y512
	Q732	E658	L663	F590	Y513
	G733	I659	L665	G593	S514
	P734	A660	V668	V594	F515
	L735	L736	H669	Q595	L532
	L736	Y737	L670	A599	L533
	P737	E738	F671	K600	L534
	E738	G739	E672	E601	N535
	R740	R741	L673	R602	P536
	S742	L743	L674	L603	L537
	L743	A744	L675	S604	
	F745	R746	D679	L608	A542
	L747	R748	K680	L609	A543
	R749	R750	P681	K610	L544
	R750	P751	L682	G611	R545
	P752	K753	P687	Y612	T546
	K753	R754	S688	L613	H547
	L755	Y755	R689	E614	L548
	L756	L757	H690	A615	F549
	R757	D758	P691	L616	P550
		V761	F694	F617	Q551
		E762	R695	A618	L552
		E763	D696	L620	V553
		A764	L697		R554
		V765			V555
		S766			

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	173.32Å 173.32Å 139.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.88 – 2.85 31.88 – 2.85	Depositor EDS
% Data completeness (in resolution range)	90.5 (31.88-2.85) 90.5 (31.88-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.85Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.235 , 0.297 0.235 , 0.294	Depositor DCC
R_{free} test set	2587 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8670	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAH

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2191	0.61	1/2971 (0.0%)
2	B	0.40	0/6280	0.62	2/8536 (0.0%)
All	All	0.40	0/8471	0.62	3/11507 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	LEU	CA-CB-CG	5.86	128.78	115.30
2	B	133	LEU	CA-CB-CG	5.76	128.55	115.30
2	B	38	VAL	N-CA-C	5.11	124.81	111.00

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	2123	0	2075	137	2
2	B	6127	0	6180	381	0
3	A	14	0	8	9	0
3	B	14	0	8	14	0
4	A	103	0	0	38	0
4	B	289	0	0	95	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8670	0	8271	507	3

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 31.

All (507) 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)
2:B:261:HIS:CD2	3:B:786:DAH:N	1.80	1.47
2:B:261:HIS:HD2	3:B:786:DAH:N	0.90	1.38
2:B:261:HIS:CD2	3:B:786:DAH:H	1.45	1.26
3:A:351:DAH:N	4:A:352:HOH:O	1.74	1.16
2:B:619:ARG:HG2	2:B:619:ARG:HH11	1.02	1.13
2:B:516:MET:HE3	2:B:546:THR:H	1.16	1.06
1:A:130:GLU:HB2	4:A:436:HOH:O	1.61	0.99
2:B:261:HIS:CD2	3:B:786:DAH:H2	1.71	0.99
2:B:553:VAL:HA	4:B:876:HOH:O	1.62	0.99
1:A:191:THR:HG23	2:B:484:ASP:OD2	1.64	0.98
1:A:278:LEU:HD11	1:A:325:LEU:HD22	1.43	0.95
1:A:88:VAL:HA	4:A:396:HOH:O	1.68	0.94
3:B:786:DAH:OE2	4:B:932:HOH:O	1.85	0.93
1:A:172:ARG:HB3	4:A:436:HOH:O	1.68	0.91
2:B:252:VAL:O	2:B:253:MET:HB2	1.68	0.91
2:B:619:ARG:HG2	2:B:619:ARG:NH1	1.78	0.90
2:B:192:LYS:H	2:B:381:GLN:HE22	1.20	0.89
2:B:313:LEU:HA	4:B:966:HOH:O	1.72	0.88
2:B:80:ASN:HD21	2:B:132:LEU:H	1.17	0.88
2:B:587:GLY:HA3	2:B:671:PHE:CE1	2.09	0.88
1:A:308:ARG:HE	1:A:308:ARG:HA	1.36	0.88
2:B:279:GLU:HG2	2:B:295:PRO:HG3	1.53	0.88
2:B:290:GLU:HG3	4:B:837:HOH:O	1.74	0.87
1:A:331:ASP:HB3	1:A:334:TYR:CE2	2.10	0.86
2:B:223:VAL:HA	2:B:244:ASN:HD22	1.41	0.86
1:A:198:VAL:HG13	1:A:220:GLU:HB2	1.57	0.85
2:B:272:ILE:HB	4:B:969:HOH:O	1.76	0.84
1:A:117:LEU:HD21	1:A:239:GLU:HG2	1.57	0.84
2:B:610:LYS:O	2:B:614:GLU:HG2	1.79	0.83
2:B:299:VAL:HA	4:B:966:HOH:O	1.77	0.83
2:B:409:GLU:OE1	2:B:413:ARG:HD3	1.79	0.83
2:B:460:VAL:HB	4:B:923:HOH:O	1.78	0.83
1:A:120:GLN:HG2	2:B:489:GLU:HB3	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:589:LEU:HD21	2:B:608:LEU:HD23	1.62	0.80
2:B:258:GLN:HE22	2:B:369:GLN:NE2	1.79	0.80
2:B:419:TYR:CE1	2:B:467:GLN:HG2	2.17	0.79
2:B:297:ASP:OD2	2:B:350:HIS:HE1	1.65	0.79
2:B:722:LEU:HB2	4:B:978:HOH:O	1.83	0.79
2:B:255:GLU:OE2	2:B:375:ARG:HD3	1.83	0.78
2:B:198:LEU:HD12	2:B:393:LEU:HD13	1.64	0.78
2:B:727:LEU:HG	4:B:866:HOH:O	1.83	0.78
1:A:235:GLY:HA2	4:A:443:HOH:O	1.84	0.78
1:A:331:ASP:HB3	1:A:334:TYR:CD2	2.19	0.77
1:A:139:ILE:HD13	1:A:259:PRO:HG2	1.67	0.77
1:A:202:VAL:HG23	4:A:446:HOH:O	1.84	0.76
2:B:204:VAL:HB	2:B:274:VAL:HG13	1.68	0.76
2:B:564:ARG:HD3	4:B:938:HOH:O	1.86	0.75
2:B:271:GLY:HA3	4:B:1049:HOH:O	1.85	0.75
2:B:445:THR:HG22	4:B:835:HOH:O	1.86	0.75
2:B:461:GLU:HG3	4:B:1017:HOH:O	1.85	0.75
1:A:326:ARG:HB2	4:A:427:HOH:O	1.87	0.75
2:B:448:SER:O	2:B:449:HIS:HB3	1.86	0.74
2:B:151:PRO:HD2	2:B:232:ARG:NE	2.02	0.74
2:B:356:ALA:HB2	3:B:786:DAH:HD1	1.68	0.74
2:B:680:LYS:HG3	4:B:955:HOH:O	1.87	0.74
2:B:431:LEU:HD13	2:B:462:GLU:HG3	1.69	0.73
1:A:278:LEU:HD11	1:A:325:LEU:CD2	2.19	0.73
2:B:615:ALA:HB1	4:B:817:HOH:O	1.89	0.72
1:A:233:LEU:HD12	4:A:429:HOH:O	1.88	0.72
1:A:178:HIS:HA	1:A:202:VAL:HG21	1.71	0.72
2:B:414:LEU:HD23	2:B:460:VAL:HG21	1.71	0.72
1:A:143:HIS:HB3	4:A:400:HOH:O	1.89	0.72
2:B:110:GLY:HA2	4:B:884:HOH:O	1.90	0.71
2:B:514:SER:O	2:B:545:ARG:HB2	1.90	0.71
1:A:300:ARG:HD2	4:A:423:HOH:O	1.91	0.71
1:A:271:TRP:HZ3	1:A:276:LYS:HE2	1.55	0.71
1:A:175:LEU:HB3	1:A:203:PHE:CD1	2.25	0.70
2:B:286:LEU:CD1	3:B:786:DAH:OXT	2.40	0.70
2:B:604:SER:HA	2:B:608:LEU:HD22	1.74	0.70
1:A:176:ARG:HD2	4:A:446:HOH:O	1.91	0.70
2:B:372:ALA:HA	4:B:1063:HOH:O	1.91	0.70
2:B:730:LEU:HA	4:B:933:HOH:O	1.92	0.70
2:B:575:ARG:HG3	4:B:1018:HOH:O	1.90	0.69
2:B:588:LEU:HD11	4:B:876:HOH:O	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:258:GLN:HE22	2:B:369:GLN:HE21	1.39	0.69
2:B:294:HIS:CE1	2:B:296:GLU:HB2	2.27	0.69
2:B:681:PRO:HD2	4:B:955:HOH:O	1.92	0.69
1:A:153:TRP:HZ3	4:A:436:HOH:O	1.75	0.69
2:B:252:VAL:O	2:B:253:MET:CB	2.41	0.69
1:A:173:LEU:HB3	4:A:449:HOH:O	1.93	0.69
1:A:179:THR:OG1	1:A:220:GLU:HG2	1.93	0.69
2:B:362:ARG:HG3	4:B:891:HOH:O	1.92	0.68
2:B:286:LEU:HD11	3:B:786:DAH:OXT	1.93	0.68
2:B:297:ASP:OD2	2:B:350:HIS:CE1	2.46	0.68
2:B:12:VAL:HG22	2:B:15:LEU:HG	1.75	0.68
2:B:393:LEU:HB2	4:B:959:HOH:O	1.94	0.68
2:B:593:GLY:HA3	2:B:604:SER:HB3	1.75	0.68
2:B:141:PRO:HG2	2:B:144:THR:HG21	1.76	0.67
1:A:133:ASN:HA	1:A:181:PRO:HG3	1.76	0.67
2:B:313:LEU:HD23	4:B:966:HOH:O	1.94	0.67
2:B:713:LEU:CD2	2:B:775:ARG:HD3	2.24	0.67
3:A:351:DAH:CA	4:A:352:HOH:O	2.30	0.67
1:A:240:LEU:HB2	4:A:392:HOH:O	1.94	0.67
2:B:751:HIS:HB2	2:B:756:LEU:HD13	1.77	0.67
1:A:327:TYR:HB3	1:A:346:PHE:HE2	1.61	0.66
2:B:192:LYS:H	2:B:381:GLN:NE2	1.93	0.66
2:B:256:ARG:HD3	4:B:1063:HOH:O	1.95	0.66
1:A:161:LEU:HD22	1:A:161:LEU:C	2.16	0.66
2:B:261:HIS:HB3	4:B:932:HOH:O	1.96	0.66
2:B:253:MET:CG	2:B:259:PRO:HA	2.25	0.66
2:B:294:HIS:CD2	4:B:1054:HOH:O	2.48	0.66
2:B:505:LEU:HD13	2:B:612:TYR:HD1	1.60	0.65
1:A:263:PRO:O	4:A:411:HOH:O	2.15	0.65
1:A:220:GLU:HB3	4:A:437:HOH:O	1.97	0.65
2:B:18:PRO:CG	2:B:154:VAL:HG21	2.26	0.65
1:A:236:ALA:HB3	4:A:429:HOH:O	1.96	0.64
2:B:509:GLU:HB3	2:B:571:PHE:CE1	2.32	0.64
2:B:141:PRO:O	2:B:144:THR:HG22	1.98	0.64
2:B:721:TYR:CE1	2:B:751:HIS:CD2	2.85	0.64
2:B:120:PRO:HG3	2:B:133:LEU:HD13	1.80	0.64
2:B:294:HIS:HD2	4:B:1054:HOH:O	1.80	0.64
2:B:502:LEU:HD23	2:B:571:PHE:CD2	2.33	0.64
2:B:261:HIS:HD2	3:B:786:DAH:H	0.64	0.64
2:B:357:SER:O	2:B:358:HIS:HB3	1.98	0.64
2:B:1:MET:HE2	4:B:893:HOH:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLU:HG2	1:A:347:LYS:HE3	1.80	0.63
1:A:349:VAL:HG12	1:A:350:LEU:HG	1.80	0.63
1:A:138:ASN:O	1:A:140:PRO:HD3	1.99	0.63
2:B:188:GLU:HB3	4:B:1041:HOH:O	1.96	0.63
2:B:743:LEU:HD23	4:B:933:HOH:O	1.98	0.63
2:B:517:ASP:O	2:B:520:ASP:HB2	1.99	0.63
2:B:502:LEU:HD23	2:B:571:PHE:CE2	2.34	0.62
2:B:567:ARG:NH1	2:B:594:VAL:HG12	2.14	0.62
2:B:230:MET:HG2	4:B:962:HOH:O	1.99	0.62
2:B:96:LEU:HB2	2:B:99:LEU:HD12	1.81	0.62
2:B:178:HIS:CD2	2:B:184:LEU:HB2	2.34	0.62
1:A:261:VAL:HG13	4:A:411:HOH:O	1.99	0.62
1:A:234:LYS:HE2	2:B:474:LEU:HD11	1.81	0.61
3:A:351:DAH:HA	4:A:352:HOH:O	1.97	0.61
1:A:208:THR:HG22	1:A:208:THR:O	2.00	0.61
1:A:316:GLY:HA3	3:A:351:DAH:HB3	1.82	0.61
2:B:298:LEU:HD21	4:B:975:HOH:O	2.00	0.61
2:B:635:HIS:HB3	2:B:638:VAL:H	1.66	0.61
2:B:635:HIS:O	2:B:639:SER:HB2	2.00	0.61
2:B:141:PRO:O	2:B:144:THR:CG2	2.48	0.61
2:B:38:VAL:O	2:B:40:PRO:HD3	2.01	0.60
2:B:552:LEU:O	2:B:555:VAL:HG12	2.01	0.60
2:B:516:MET:HE3	2:B:546:THR:N	2.02	0.60
2:B:407:ARG:HG3	2:B:456:GLU:OE2	2.02	0.60
2:B:530:ARG:HG3	4:B:952:HOH:O	2.03	0.59
2:B:753:LYS:HE3	4:B:860:HOH:O	2.01	0.59
2:B:725:LEU:HD11	2:B:745:PHE:CD1	2.38	0.59
2:B:631:PHE:HB2	2:B:634:LEU:HD12	1.84	0.59
2:B:714:VAL:O	2:B:718:ALA:HB2	2.03	0.58
2:B:769:ALA:HA	4:B:874:HOH:O	2.02	0.58
2:B:261:HIS:CG	3:B:786:DAH:H2	2.20	0.58
2:B:356:ALA:CB	3:B:786:DAH:HD1	2.33	0.58
1:A:101:HIS:CG	1:A:102:PRO:HD2	2.39	0.58
1:A:251:VAL:HG12	1:A:269:VAL:HG12	1.85	0.58
2:B:151:PRO:HD2	2:B:232:ARG:HE	1.69	0.58
2:B:509:GLU:HA	2:B:571:PHE:O	2.03	0.58
2:B:669:HIS:HD2	4:B:814:HOH:O	1.86	0.58
2:B:688:SER:HB3	2:B:750:ARG:HD3	1.84	0.58
2:B:201:ALA:HB3	4:B:1049:HOH:O	2.04	0.58
2:B:589:LEU:HB2	2:B:609:LEU:HD22	1.85	0.58
2:B:589:LEU:HB2	2:B:609:LEU:CD2	2.33	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:619:ARG:CG	2:B:619:ARG:NH1	2.60	0.58
2:B:713:LEU:HD21	2:B:775:ARG:HD3	1.85	0.58
2:B:224:ALA:N	2:B:244:ASN:ND2	2.52	0.58
2:B:609:LEU:HG	4:B:913:HOH:O	2.02	0.58
1:A:162:GLU:O	1:A:185:ARG:NH2	2.36	0.58
2:B:494:LYS:HE3	2:B:679:ASP:OD1	2.04	0.58
2:B:554:ARG:O	2:B:558:GLU:HG3	2.04	0.58
2:B:620:LEU:CB	2:B:622:LEU:HD22	2.34	0.57
2:B:710:VAL:HA	4:B:974:HOH:O	2.03	0.57
1:A:176:ARG:HD3	4:A:368:HOH:O	2.04	0.57
2:B:192:LYS:N	2:B:381:GLN:HE22	1.97	0.57
2:B:431:LEU:CD1	2:B:462:GLU:HG3	2.35	0.57
2:B:721:TYR:HE1	2:B:751:HIS:CD2	2.22	0.57
2:B:585:LEU:O	2:B:673:LEU:HD23	2.04	0.57
2:B:730:LEU:HD23	4:B:933:HOH:O	2.05	0.57
2:B:141:PRO:HG2	2:B:144:THR:CG2	2.34	0.57
2:B:278:ARG:O	2:B:281:GLU:HB2	2.04	0.57
2:B:497:ARG:HB3	4:B:1025:HOH:O	2.03	0.56
2:B:583:THR:HG23	4:B:1018:HOH:O	2.05	0.56
2:B:695:ARG:HD3	2:B:761:VAL:HG11	1.85	0.56
2:B:740:HIS:O	2:B:741:LYS:HB3	2.06	0.56
2:B:763:GLU:O	2:B:767:ARG:HG2	2.06	0.56
2:B:755:THR:HG23	4:B:1034:HOH:O	2.06	0.56
2:B:356:ALA:CB	3:B:786:DAH:CD1	2.83	0.56
1:A:336:PHE:HB3	2:B:513:TYR:CE2	2.39	0.56
2:B:20:VAL:O	2:B:24:ARG:HB2	2.05	0.56
2:B:224:ALA:H	2:B:244:ASN:ND2	2.03	0.56
2:B:356:ALA:HB1	3:B:786:DAH:CE1	2.36	0.56
2:B:751:HIS:HB2	2:B:756:LEU:CD1	2.35	0.56
1:A:331:ASP:O	1:A:334:TYR:HD2	1.89	0.56
2:B:581:GLU:HG2	4:B:937:HOH:O	2.05	0.56
2:B:255:GLU:OE1	2:B:375:ARG:NH1	2.39	0.55
2:B:701:VAL:HG13	2:B:702:PRO:HD2	1.88	0.55
2:B:356:ALA:C	2:B:357:SER:O	2.42	0.55
2:B:616:LEU:N	4:B:920:HOH:O	2.38	0.55
1:A:261:VAL:HG22	4:A:411:HOH:O	2.05	0.55
2:B:673:LEU:HD23	2:B:673:LEU:N	2.22	0.55
2:B:20:VAL:HA	2:B:23:GLU:HG2	1.88	0.55
2:B:415:LEU:HG	4:B:923:HOH:O	2.05	0.55
2:B:710:VAL:HG23	4:B:1019:HOH:O	2.07	0.55
2:B:243:ASN:HA	4:B:819:HOH:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:CA	1:A:202:VAL:HG21	2.37	0.54
2:B:350:HIS:HD2	4:B:904:HOH:O	1.90	0.54
2:B:536:PRO:HB3	2:B:542:ALA:HA	1.89	0.54
2:B:178:HIS:CD2	2:B:430:ARG:HH12	2.25	0.54
2:B:253:MET:HG3	2:B:259:PRO:HA	1.88	0.54
2:B:516:MET:HB3	4:B:843:HOH:O	2.06	0.54
1:A:154:LEU:HD12	4:A:449:HOH:O	2.05	0.54
2:B:694:PHE:CD1	2:B:694:PHE:N	2.76	0.54
2:B:670:LEU:HB3	4:B:1053:HOH:O	2.08	0.54
2:B:80:ASN:ND2	2:B:132:LEU:H	1.98	0.54
2:B:548:LEU:HD22	2:B:584:HIS:HB3	1.89	0.54
2:B:579:GLU:N	4:B:952:HOH:O	2.38	0.54
2:B:691:PRO:HG3	4:B:916:HOH:O	2.08	0.53
2:B:490:ALA:HB3	2:B:491:PRO:HD3	1.88	0.53
2:B:202:LEU:HA	4:B:969:HOH:O	2.07	0.53
2:B:12:VAL:HG22	2:B:12:VAL:O	2.09	0.53
2:B:524:PHE:CZ	2:B:663:LEU:HD11	2.44	0.53
2:B:691:PRO:HB3	4:B:994:HOH:O	2.09	0.53
2:B:588:LEU:HD23	2:B:588:LEU:C	2.29	0.53
1:A:93:ALA:HA	2:B:595:GLY:O	2.08	0.53
2:B:501:VAL:HB	4:B:1046:HOH:O	2.08	0.53
4:A:447:HOH:O	2:B:594:VAL:HA	2.07	0.53
2:B:633:PHE:CD1	2:B:634:LEU:HG	2.43	0.53
1:A:117:LEU:HD21	1:A:239:GLU:CG	2.33	0.52
2:B:642:VAL:HG23	2:B:650:GLY:C	2.29	0.52
2:B:696:ASP:OD2	2:B:746:HIS:CD2	2.62	0.52
2:B:419:TYR:CZ	2:B:467:GLN:HG2	2.45	0.52
2:B:761:VAL:O	2:B:765:VAL:HG13	2.09	0.52
1:A:142:HIS:HA	2:B:344:ARG:NH2	2.23	0.52
2:B:357:SER:O	2:B:358:HIS:CB	2.58	0.52
2:B:428:LEU:HD13	4:B:889:HOH:O	2.09	0.52
2:B:509:GLU:CB	2:B:571:PHE:CE1	2.92	0.52
1:A:338:GLY:HA3	2:B:555:VAL:CG2	2.40	0.52
1:A:237:ILE:HA	4:A:392:HOH:O	2.09	0.52
1:A:237:ILE:HD13	4:A:392:HOH:O	2.10	0.52
2:B:62:LYS:NZ	2:B:62:LYS:HB2	2.25	0.52
2:B:102:LYS:HG3	2:B:103:VAL:H	1.75	0.51
2:B:253:MET:HG2	2:B:259:PRO:HA	1.91	0.51
1:A:144:PRO:HB2	4:B:891:HOH:O	2.09	0.51
1:A:341:LYS:HB3	4:A:453:HOH:O	2.09	0.51
2:B:620:LEU:HB2	2:B:622:LEU:HD22	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:CZ3	1:A:276:LYS:HE2	2.41	0.51
1:A:316:GLY:HA3	3:A:351:DAH:CD2	2.40	0.51
1:A:262:GLU:OE2	2:B:461:GLU:OE1	2.29	0.51
1:A:278:LEU:HA	4:A:431:HOH:O	2.10	0.51
2:B:163:ASN:O	2:B:452:ASP:HB3	2.11	0.51
2:B:599:ALA:HB1	4:B:879:HOH:O	2.10	0.51
2:B:713:LEU:HB3	4:B:974:HOH:O	2.10	0.51
1:A:322:LEU:HB2	4:A:445:HOH:O	2.10	0.51
2:B:175:ARG:HD2	4:B:822:HOH:O	2.10	0.51
2:B:212:HIS:HE1	2:B:394:GLU:OE2	1.92	0.51
2:B:427:ILE:HG23	2:B:466:ILE:HG21	1.92	0.51
2:B:722:LEU:HD12	2:B:748:ARG:O	2.11	0.51
2:B:273:ALA:HB1	4:B:970:HOH:O	2.10	0.51
2:B:505:LEU:HD13	2:B:612:TYR:CD1	2.43	0.51
2:B:627:GLU:OE1	2:B:641:ARG:NH2	2.44	0.51
1:A:178:HIS:HB2	3:A:351:DAH:H	1.76	0.51
1:A:338:GLY:HA3	2:B:555:VAL:HG21	1.93	0.51
1:A:165:LEU:HD21	1:A:303:LEU:HD11	1.93	0.50
2:B:99:LEU:HD13	2:B:100:GLY:N	2.26	0.50
2:B:339:ASP:O	2:B:343:ILE:HG12	2.10	0.50
1:A:343:LEU:HD13	2:B:509:GLU:O	2.12	0.50
2:B:703:ALA:HB3	2:B:704:PRO:HD3	1.94	0.50
1:A:180:SER:O	1:A:183:GLN:HG2	2.10	0.50
1:A:193:PRO:HB2	2:B:479:PHE:CD1	2.46	0.50
2:B:575:ARG:NE	4:B:1018:HOH:O	2.44	0.50
2:B:749:PHE:O	2:B:750:ARG:HB2	2.12	0.50
1:A:317:LEU:HD23	1:A:317:LEU:C	2.32	0.50
2:B:533:LEU:HB2	2:B:536:PRO:HG3	1.93	0.50
2:B:153:GLU:HG3	2:B:154:VAL:N	2.27	0.50
2:B:710:VAL:O	2:B:714:VAL:HG23	2.12	0.50
1:A:308:ARG:CA	1:A:308:ARG:HE	2.18	0.49
2:B:656:HIS:CE1	2:B:658:GLU:HB2	2.47	0.49
2:B:725:LEU:HD11	2:B:745:PHE:HD1	1.75	0.49
1:A:215:VAL:HG22	1:A:336:PHE:CE2	2.47	0.49
2:B:674:ARG:NH1	4:B:864:HOH:O	2.44	0.49
2:B:771:ALA:O	2:B:775:ARG:HG3	2.12	0.49
2:B:724:SER:HB2	2:B:748:ARG:HD3	1.95	0.49
2:B:223:VAL:CA	2:B:244:ASN:HD22	2.18	0.49
2:B:779:LEU:N	2:B:779:LEU:HD12	2.28	0.49
2:B:736:LEU:HD23	4:B:896:HOH:O	2.11	0.49
2:B:601:GLU:O	2:B:602:ARG:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:768:VAL:O	2:B:772:LEU:HB2	2.13	0.49
2:B:282:ARG:HG2	4:B:980:HOH:O	2.13	0.49
1:A:288:PRO:CG	2:B:457:GLU:HG3	2.43	0.49
2:B:80:ASN:N	2:B:80:ASN:HD22	2.09	0.49
1:A:103:ILE:HD11	1:A:320:GLU:HG3	1.94	0.48
2:B:556:LEU:HB3	4:B:876:HOH:O	2.13	0.48
1:A:179:THR:C	1:A:181:PRO:HD2	2.34	0.48
2:B:764:ALA:O	2:B:768:VAL:HG23	2.13	0.48
2:B:160:VAL:CG1	2:B:167:ALA:HB3	2.44	0.48
2:B:727:LEU:HD23	2:B:727:LEU:O	2.12	0.48
2:B:524:PHE:N	2:B:524:PHE:CD2	2.82	0.48
1:A:108:ARG:O	1:A:112:GLU:HG2	2.13	0.48
2:B:428:LEU:N	4:B:889:HOH:O	2.46	0.48
2:B:425:ILE:HD11	2:B:442:TYR:CZ	2.47	0.48
2:B:467:GLN:HA	2:B:467:GLN:HE21	1.78	0.48
2:B:757:ARG:HD2	2:B:758:ASP:H	1.78	0.48
1:A:280:LEU:HD21	1:A:322:LEU:HD23	1.95	0.48
2:B:75:VAL:HG23	2:B:111:VAL:HG22	1.95	0.48
2:B:627:GLU:O	2:B:640:GLY:HA2	2.14	0.48
2:B:710:VAL:CG2	4:B:1019:HOH:O	2.61	0.48
1:A:182:MET:HG2	1:A:198:VAL:HG21	1.95	0.48
1:A:331:ASP:HB3	1:A:334:TYR:HE2	1.71	0.48
2:B:191:LEU:HD23	2:B:381:GLN:NE2	2.28	0.48
2:B:355:GLU:HB3	2:B:359:ARG:NH1	2.29	0.47
2:B:549:PHE:CG	2:B:550:PRO:HD3	2.49	0.47
1:A:139:ILE:HG22	1:A:146:ARG:HG2	1.95	0.47
1:A:271:TRP:CZ3	1:A:274:GLY:HA3	2.48	0.47
2:B:621:GLY:C	2:B:622:LEU:HD13	2.35	0.47
2:B:775:ARG:HG2	4:B:821:HOH:O	2.13	0.47
2:B:99:LEU:O	2:B:101:GLN:N	2.44	0.47
1:A:268:ALA:HA	1:A:278:LEU:O	2.14	0.47
1:A:280:LEU:HD22	4:A:445:HOH:O	2.14	0.47
2:B:578:ARG:O	2:B:579:GLU:HB2	2.15	0.47
1:A:183:GLN:NE2	4:A:444:HOH:O	2.48	0.47
2:B:671:PHE:HB3	4:B:913:HOH:O	2.14	0.47
2:B:764:ALA:HA	2:B:767:ARG:CG	2.44	0.47
2:B:620:LEU:HB3	2:B:622:LEU:HD22	1.95	0.47
1:A:262:GLU:HA	1:A:263:PRO:C	2.34	0.47
2:B:533:LEU:C	2:B:535:ASN:H	2.18	0.47
1:A:308:ARG:NE	1:A:308:ARG:HA	2.16	0.47
2:B:450:ARG:HB3	2:B:453:LEU:HG	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:722:LEU:HD12	2:B:723:GLU:H	1.80	0.47
2:B:713:LEU:HD22	2:B:775:ARG:HD3	1.97	0.47
2:B:701:VAL:HG22	2:B:777:PHE:CD1	2.49	0.47
1:A:130:GLU:HB3	4:A:438:HOH:O	2.14	0.47
2:B:457:GLU:O	2:B:460:VAL:HG22	2.15	0.47
2:B:291:ARG:NH2	2:B:352:LEU:HD21	2.31	0.46
2:B:407:ARG:NH1	2:B:456:GLU:OE1	2.48	0.46
2:B:731:TYR:HD2	4:B:1023:HOH:O	1.98	0.46
1:A:117:LEU:CD2	1:A:239:GLU:HG2	2.36	0.46
2:B:264:ASP:OD2	2:B:266:ARG:HD3	2.16	0.46
2:B:178:HIS:NE2	2:B:430:ARG:NH1	2.63	0.46
2:B:642:VAL:HG23	2:B:650:GLY:O	2.14	0.46
1:A:316:GLY:HA3	3:A:351:DAH:HD2	1.97	0.46
2:B:355:GLU:HB3	2:B:359:ARG:HH11	1.80	0.46
2:B:501:VAL:HG13	2:B:619:ARG:HD3	1.97	0.46
2:B:615:ALA:O	2:B:618:ALA:HB3	2.15	0.46
2:B:729:ASP:HB3	2:B:744:ALA:CB	2.46	0.46
1:A:206:GLU:HG3	1:A:207:GLN:H	1.81	0.46
1:A:162:GLU:H	1:A:162:GLU:HG2	1.59	0.46
1:A:285:MET:N	4:A:411:HOH:O	2.48	0.46
2:B:548:LEU:HD21	2:B:574:GLY:H	1.80	0.46
2:B:569:LEU:HD13	2:B:589:LEU:HD13	1.97	0.46
2:B:696:ASP:C	2:B:697:LEU:HD13	2.36	0.46
2:B:549:PHE:C	2:B:549:PHE:CD1	2.89	0.46
2:B:718:ALA:HA	2:B:768:VAL:HG22	1.96	0.46
2:B:635:HIS:ND1	2:B:637:GLY:N	2.60	0.45
2:B:765:VAL:HA	2:B:768:VAL:HG23	1.98	0.45
1:A:201:ARG:HD2	1:A:336:PHE:HZ	1.81	0.45
2:B:49:ARG:HD2	2:B:137:GLU:HG3	1.97	0.45
2:B:139:ALA:O	2:B:140:LEU:HD13	2.16	0.45
2:B:356:ALA:HB1	3:B:786:DAH:CD1	2.46	0.45
2:B:549:PHE:CD2	2:B:651:PHE:HZ	2.35	0.45
1:A:127:VAL:HG13	4:A:449:HOH:O	2.15	0.45
2:B:549:PHE:CD1	2:B:550:PRO:N	2.85	0.45
2:B:206:ASP:OD1	2:B:208:GLU:HB2	2.16	0.45
2:B:455:LEU:O	2:B:458:ASP:HB2	2.17	0.45
2:B:634:LEU:O	2:B:656:HIS:CD2	2.69	0.45
1:A:109:GLU:O	1:A:113:ILE:HG13	2.17	0.45
2:B:188:GLU:O	2:B:188:GLU:HG3	2.16	0.45
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.70	0.45
2:B:570:LEU:HG	2:B:588:LEU:HD22	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:569:LEU:HD12	2:B:588:LEU:O	2.17	0.45
2:B:773:ARG:HG3	4:B:874:HOH:O	2.16	0.45
1:A:179:THR:OG1	1:A:220:GLU:CG	2.64	0.45
2:B:240:ARG:HA	2:B:241:PRO:HD3	1.82	0.45
2:B:223:VAL:CG1	2:B:326:GLU:HA	2.47	0.45
1:A:343:LEU:HB2	4:A:419:HOH:O	2.17	0.45
2:B:457:GLU:HA	2:B:460:VAL:HG13	1.99	0.45
2:B:549:PHE:HB2	2:B:670:LEU:HD22	1.99	0.45
2:B:196:LEU:HB2	2:B:197:PRO:CD	2.48	0.44
2:B:656:HIS:HB3	2:B:659:ILE:HG13	1.99	0.44
2:B:74:VAL:HA	2:B:113:SER:HA	1.97	0.44
2:B:261:HIS:CB	4:B:932:HOH:O	2.61	0.44
1:A:110:LEU:HD12	1:A:110:LEU:HA	1.84	0.44
1:A:240:LEU:HD11	1:A:317:LEU:HD11	1.98	0.44
2:B:588:LEU:HG	4:B:1053:HOH:O	2.18	0.44
2:B:590:PHE:HA	4:B:814:HOH:O	2.17	0.44
1:A:107:GLU:O	1:A:111:VAL:HG13	2.17	0.44
2:B:668:VAL:HG12	4:B:1053:HOH:O	2.16	0.44
2:B:707:TYR:CE1	2:B:727:LEU:HD13	2.53	0.44
2:B:63:ARG:NH1	2:B:73:GLU:OE2	2.44	0.44
2:B:206:ASP:CG	2:B:276:ARG:HH11	2.21	0.44
2:B:512:THR:HG22	2:B:513:TYR:O	2.18	0.44
2:B:615:ALA:C	4:B:920:HOH:O	2.55	0.44
2:B:761:VAL:O	2:B:765:VAL:CG1	2.66	0.44
1:A:114:PHE:CZ	1:A:240:LEU:HG	2.53	0.44
1:A:190:HIS:HB3	2:B:484:ASP:OD1	2.18	0.44
2:B:543:ALA:HB3	4:B:843:HOH:O	2.17	0.44
2:B:722:LEU:HD21	2:B:725:LEU:HB2	2.00	0.44
1:A:165:LEU:HD22	1:A:301:LEU:HD23	2.00	0.43
2:B:445:THR:HA	2:B:446:PRO:HD3	1.83	0.43
1:A:174:LEU:HD13	1:A:174:LEU:N	2.34	0.43
2:B:544:LEU:O	2:B:545:ARG:C	2.56	0.43
2:B:505:LEU:CD1	2:B:612:TYR:HD1	2.29	0.43
1:A:177:THR:O	1:A:204:ARG:NH2	2.51	0.43
2:B:204:VAL:CB	2:B:274:VAL:HG13	2.45	0.43
2:B:294:HIS:CG	2:B:295:PRO:HD2	2.53	0.43
2:B:215:LEU:HA	2:B:333:LEU:O	2.19	0.43
2:B:262:ALA:HB1	2:B:331:ILE:HD12	2.00	0.43
2:B:259:PRO:HB2	2:B:360:PHE:CE2	2.53	0.43
2:B:178:HIS:CD2	2:B:430:ARG:NH1	2.86	0.43
2:B:548:LEU:HD22	2:B:584:HIS:CB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:HIS:HB2	1:A:218:GLN:HE22	1.84	0.43
2:B:160:VAL:HA	4:B:793:HOH:O	2.19	0.43
2:B:740:HIS:HB3	2:B:741:LYS:H	1.54	0.43
1:A:344:GLU:HG2	1:A:347:LYS:CE	2.48	0.43
2:B:743:LEU:HA	4:B:933:HOH:O	2.19	0.43
1:A:87:ASP:HB3	1:A:90:LEU:HD22	2.01	0.43
2:B:91:LEU:HB3	2:B:92:PRO:HD2	2.00	0.43
1:A:198:VAL:HA	1:A:199:PRO:HD3	1.76	0.43
1:A:233:LEU:HA	4:A:429:HOH:O	2.18	0.43
1:A:287:HIS:ND1	1:A:288:PRO:HD2	2.33	0.43
4:A:419:HOH:O	2:B:508:GLN:HG2	2.18	0.43
1:A:197:VAL:HG13	1:A:219:LEU:HD21	2.00	0.42
2:B:304:ARG:O	2:B:307:GLU:HB2	2.18	0.42
2:B:559:ASN:O	2:B:565:PRO:HD2	2.19	0.42
2:B:589:LEU:O	2:B:590:PHE:CB	2.67	0.42
2:B:524:PHE:O	2:B:633:PHE:HB3	2.19	0.42
2:B:670:LEU:C	4:B:913:HOH:O	2.57	0.42
2:B:80:ASN:H	2:B:80:ASN:HD22	1.65	0.42
2:B:168:LEU:HD13	2:B:359:ARG:HG3	2.01	0.42
2:B:224:ALA:HB1	2:B:225:PRO:HD2	2.00	0.42
2:B:718:ALA:HA	2:B:768:VAL:CG2	2.50	0.42
2:B:728:PHE:O	2:B:729:ASP:HB2	2.20	0.42
2:B:222:ARG:CG	2:B:222:ARG:HH21	2.32	0.42
2:B:380:LEU:HD23	2:B:380:LEU:HA	1.84	0.42
2:B:763:GLU:HG3	4:B:928:HOH:O	2.20	0.42
1:A:329:ILE:HA	1:A:330:PRO:HD3	1.86	0.42
2:B:198:LEU:HA	2:B:199:PRO:HD3	1.89	0.42
2:B:279:GLU:CG	2:B:295:PRO:HG3	2.37	0.42
2:B:463:VAL:O	2:B:467:GLN:HB2	2.19	0.42
2:B:707:TYR:HA	4:B:1019:HOH:O	2.19	0.42
2:B:754:ARG:HG2	2:B:754:ARG:H	1.61	0.42
1:A:201:ARG:HG2	4:B:946:HOH:O	2.20	0.42
1:A:113:ILE:HG21	1:A:240:LEU:HD23	2.02	0.42
2:B:349:ARG:HG2	2:B:350:HIS:ND1	2.34	0.42
2:B:353:ARG:C	2:B:353:ARG:HD3	2.40	0.42
2:B:355:GLU:OE1	2:B:359:ARG:NH1	2.52	0.42
1:A:161:LEU:C	1:A:161:LEU:CD2	2.87	0.42
2:B:764:ALA:HA	2:B:767:ARG:HG3	2.02	0.42
2:B:249:THR:HB	2:B:260:MET:HG2	2.02	0.42
2:B:461:GLU:CG	4:B:1017:HOH:O	2.56	0.42
2:B:81:ALA:HB2	2:B:132:LEU:HD22	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:GLU:CG	1:A:207:GLN:N	2.83	0.41
2:B:472:ILE:HA	2:B:473:PRO:HD3	1.90	0.41
1:A:137:LEU:HD23	1:A:137:LEU:HA	1.86	0.41
2:B:600:LYS:HG2	4:B:879:HOH:O	2.21	0.41
1:A:128:GLU:OE1	1:A:132:PHE:HB2	2.20	0.41
1:A:285:MET:HA	1:A:312:GLY:O	2.21	0.41
1:A:159:PHE:HD1	4:B:952:HOH:O	2.01	0.41
1:A:287:HIS:CG	1:A:288:PRO:HD2	2.56	0.41
2:B:263:PHE:CZ	2:B:300:ILE:HG21	2.55	0.41
2:B:326:GLU:CD	2:B:326:GLU:H	2.24	0.41
2:B:60:ARG:H	2:B:60:ARG:HG3	1.74	0.41
2:B:701:VAL:CG1	2:B:702:PRO:HD2	2.49	0.41
2:B:725:LEU:CD1	2:B:745:PHE:HD1	2.32	0.41
2:B:773:ARG:HD2	4:B:951:HOH:O	2.19	0.41
1:A:121:ALA:HA	1:A:197:VAL:O	2.19	0.41
1:A:316:GLY:CA	3:A:351:DAH:CD2	2.98	0.41
2:B:231:GLN:HG2	2:B:241:PRO:CG	2.50	0.41
2:B:445:THR:HG21	4:B:965:HOH:O	2.18	0.41
2:B:723:GLU:HB3	2:B:724:SER:H	1.59	0.41
2:B:286:LEU:HD23	2:B:286:LEU:HA	1.80	0.41
2:B:498:LEU:HD22	4:B:1075:HOH:O	2.20	0.41
2:B:249:THR:O	2:B:252:VAL:O	2.37	0.41
2:B:652:LEU:HD12	2:B:653:GLY:H	1.85	0.41
1:A:118:GLY:O	1:A:195:ARG:HB2	2.21	0.41
2:B:159:GLU:O	2:B:159:GLU:HG3	2.20	0.41
2:B:161:THR:HA	2:B:162:PRO:HD3	1.89	0.41
2:B:16:GLU:O	2:B:17:SER:HB3	2.20	0.41
1:A:127:VAL:HG23	2:B:577:PHE:CE2	2.55	0.41
1:A:142:HIS:N	4:A:439:HOH:O	2.53	0.41
1:A:290:VAL:O	1:A:294:VAL:CG1	2.69	0.41
2:B:62:LYS:HZ3	2:B:62:LYS:HB2	1.84	0.41
1:A:348:GLY:O	1:A:349:VAL:C	2.58	0.41
2:B:175:ARG:O	2:B:178:HIS:HB3	2.21	0.41
2:B:231:GLN:HG2	2:B:241:PRO:CB	2.51	0.41
2:B:604:SER:HA	2:B:608:LEU:CD2	2.48	0.41
2:B:747:LEU:O	2:B:748:ARG:HG3	2.21	0.41
1:A:221:GLY:HA3	1:A:315:PHE:CZ	2.57	0.40
1:A:237:ILE:HG22	1:A:251:VAL:HG11	2.02	0.40
2:B:224:ALA:N	2:B:244:ASN:HD22	2.18	0.40
2:B:287:ASP:OD2	2:B:291:ARG:NH2	2.53	0.40
2:B:710:VAL:HB	4:B:1019:HOH:O	2.20	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ILE:HG22	2:B:109:GLN:HG2	2.04	0.40
2:B:294:HIS:ND1	2:B:296:GLU:HB2	2.37	0.40
2:B:403:ALA:HA	2:B:445:THR:HB	2.02	0.40
2:B:543:ALA:CB	4:B:843:HOH:O	2.69	0.40
2:B:728:PHE:CG	2:B:746:HIS:CE1	3.08	0.40
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.95	0.40
1:A:206:GLU:HG3	1:A:207:GLN:N	2.36	0.40
1:A:313:PHE:C	1:A:313:PHE:CD1	2.94	0.40
1:A:316:GLY:N	3:A:351:DAH:CD2	2.84	0.40
2:B:277:ALA:O	2:B:295:PRO:HA	2.21	0.40
2:B:434:ARG:O	2:B:444:VAL:HA	2.22	0.40
2:B:569:LEU:HD12	2:B:569:LEU:HA	1.94	0.40
1:A:234:LYS:HG2	1:A:253:PHE:CE1	2.55	0.40
1:A:288:PRO:HG2	2:B:457:GLU:HG3	2.02	0.40
1:A:322:LEU:HA	1:A:322:LEU:HD22	1.90	0.40
2:B:243:ASN:O	2:B:244:ASN:C	2.59	0.40
2:B:278:ARG:HD3	2:B:278:ARG:HA	1.91	0.40
2:B:502:LEU:HA	2:B:502:LEU:HD12	1.93	0.40
2:B:196:LEU:O	2:B:196:LEU:HD12	2.20	0.40
2:B:40:PRO:HD2	4:B:827:HOH:O	2.21	0.40
2:B:567:ARG:HH12	2:B:594:VAL:HG12	1.84	0.40
2:B:651:PHE:C	2:B:651:PHE:CD1	2.95	0.40
2:B:99:LEU:C	2:B:99:LEU:HD13	2.42	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PRO:O	4:B:884:HOH:O[5_665]	2.00	0.20
1:A:191:THR:OG1	4:B:884:HOH:O[5_665]	2.12	0.08
4:B:821:HOH:O	4:B:821:HOH:O[5_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	264/350 (75%)	240 (91%)	20 (8%)	4 (2%)	13	38
2	B	783/785 (100%)	706 (90%)	57 (7%)	20 (3%)	7	23
All	All	1047/1135 (92%)	946 (90%)	77 (7%)	24 (2%)	8	26

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	349	VAL
2	B	244	ASN
2	B	253	MET
2	B	738	GLU
2	B	99	LEU
2	B	449	HIS
2	B	545	ARG
2	B	737	PRO
2	B	754	ARG
1	A	337	GLY
2	B	357	SER
2	B	590	PHE
2	B	740	HIS
1	A	93	ALA
1	A	208	THR
2	B	770	GLU
2	B	243	ASN
2	B	741	LYS
2	B	534	LEU
2	B	100	GLY
2	B	687	PRO
2	B	632	PRO
2	B	752	PRO
2	B	535	ASN

5.3.2 Protein sidechains ⓘ

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	214/277 (77%)	181 (85%)	33 (15%)	3	9
2	B	630/630 (100%)	527 (84%)	103 (16%)	3	7
All	All	844/907 (93%)	708 (84%)	136 (16%)	3	7

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	VAL
1	A	88	VAL
1	A	110	LEU
1	A	115	ARG
1	A	139	ILE
1	A	157	GLU
1	A	161	LEU
1	A	162	GLU
1	A	165	LEU
1	A	174	LEU
1	A	178	HIS
1	A	179	THR
1	A	185	ARG
1	A	191	THR
1	A	198	VAL
1	A	202	VAL
1	A	204	ARG
1	A	207	GLN
1	A	215	VAL
1	A	222	LEU
1	A	240	LEU
1	A	250	LYS
1	A	256	VAL
1	A	261	VAL
1	A	286	VAL
1	A	301	LEU
1	A	308	ARG
1	A	317	LEU
1	A	319	VAL
1	A	322	LEU
1	A	325	LEU
1	A	329	ILE
1	A	341	LYS
2	B	12	VAL
2	B	19	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	20	VAL
2	B	21	LEU
2	B	24	ARG
2	B	28	LEU
2	B	32	THR
2	B	38	VAL
2	B	60	ARG
2	B	70	ARG
2	B	80	ASN
2	B	83	LYS
2	B	99	LEU
2	B	111	VAL
2	B	112	ARG
2	B	132	LEU
2	B	133	LEU
2	B	134	GLU
2	B	138	ASP
2	B	140	LEU
2	B	144	THR
2	B	147	SER
2	B	154	VAL
2	B	155	VAL
2	B	157	ASP
2	B	173	LEU
2	B	184	LEU
2	B	196	LEU
2	B	204	VAL
2	B	222	ARG
2	B	228	LEU
2	B	240	ARG
2	B	253	MET
2	B	260	MET
2	B	274	VAL
2	B	276	ARG
2	B	282	ARG
2	B	313	LEU
2	B	329	GLU
2	B	333	LEU
2	B	359	ARG
2	B	362	ARG
2	B	374	ARG
2	B	375	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	377	LEU
2	B	379	LEU
2	B	388	VAL
2	B	393	LEU
2	B	428	LEU
2	B	435	VAL
2	B	438	GLU
2	B	441	THR
2	B	444	VAL
2	B	445	THR
2	B	449	HIS
2	B	451	LEU
2	B	463	VAL
2	B	467	GLN
2	B	470	GLU
2	B	493	ARG
2	B	497	ARG
2	B	498	LEU
2	B	503	SER
2	B	505	LEU
2	B	509	GLU
2	B	510	VAL
2	B	526	LEU
2	B	530	ARG
2	B	532	LEU
2	B	537	LEU
2	B	548	LEU
2	B	549	PHE
2	B	557	LYS
2	B	559	ASN
2	B	560	LEU
2	B	562	LEU
2	B	571	PHE
2	B	576	VAL
2	B	578	ARG
2	B	583	THR
2	B	600	LYS
2	B	601	GLU
2	B	609	LEU
2	B	619	ARG
2	B	622	LEU
2	B	626	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	642	VAL
2	B	647	GLU
2	B	661	GLN
2	B	665	LEU
2	B	670	LEU
2	B	675	LEU
2	B	694	PHE
2	B	695	ARG
2	B	697	LEU
2	B	727	LEU
2	B	730	LEU
2	B	732	GLN
2	B	740	HIS
2	B	754	ARG
2	B	756	LEU
2	B	767	ARG
2	B	780	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	HIS
1	A	207	GLN
1	A	218	GLN
2	B	80	ASN
2	B	101	GLN
2	B	178	HIS
2	B	212	HIS
2	B	244	ASN
2	B	261	HIS
2	B	350	HIS
2	B	369	GLN
2	B	381	GLN
2	B	467	GLN
2	B	732	GLN
2	B	751	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	DAH	A	351	-	11,14,14	0.86	0	14,19,19	0.45	0
3	DAH	B	786	-	11,14,14	0.86	0	14,19,19	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAH	A	351	-	-	0/4/8/8	0/1/1/1
3	DAH	B	786	-	-	0/4/8/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	351	DAH	9	0
3	B	786	DAH	14	0

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	265/350 (75%)	-0.19	5 (1%) 70 66	45, 60, 106, 148	0
2	B	779/785 (99%)	-0.12	25 (3%) 51 44	41, 63, 133, 173	0
All	All	1044/1135 (91%)	-0.14	30 (2%) 55 49	41, 62, 128, 173	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	738	GLU	4.7
2	B	736	LEU	3.9
2	B	732	GLN	3.8
2	B	733	GLY	3.5
2	B	756	LEU	3.4
2	B	689	ARG	3.3
2	B	773	ARG	3.2
2	B	739	GLY	3.0
2	B	704	PRO	2.7
1	A	271	TRP	2.7
1	A	276	LYS	2.7
2	B	34	ARG	2.7
2	B	694	PHE	2.7
2	B	98	GLY	2.7
2	B	697	LEU	2.6
2	B	778	GLY	2.6
2	B	753	LYS	2.6
2	B	731	TYR	2.5
1	A	205	PHE	2.4
2	B	779	LEU	2.4
2	B	537	LEU	2.3
2	B	741	LYS	2.2
2	B	734	PRO	2.2
2	B	777	PHE	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	207	GLN	2.0
2	B	679	ASP	2.0
1	A	273	GLU	2.0
2	B	101	GLN	2.0
2	B	682	LEU	2.0
2	B	730	LEU	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	DAH	B	786	14/14	0.78	0.35	3.44	20,20,20,20	0
3	DAH	A	351	14/14	0.83	0.25	1.29	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.