



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:29 AM UTC

PDB ID : 3S9V / pdb_00003s9v
Title : abietadiene synthase from Abies grandis
Authors : Zhou, K.; Hoy, J.A.; Mann, F.M.; Honzatko, R.B.; Peters, R.J.
Deposited on : 2011-06-02
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

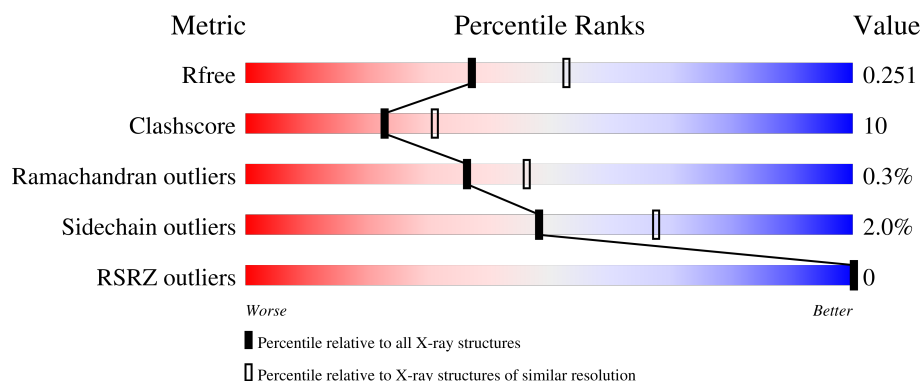
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	785	 73% 22% . .
1	B	785	 74% 22% . .
1	C	785	 76% 19% . .
1	D	785	 73% 22% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26081 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 Abietadiene synthase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	0	0
			6175	3954	1032	1158	31			
1	B	759	Total	C	N	O	S	0	0	0
			6202	3972	1036	1163	31			
1	C	759	Total	C	N	O	S	0	0	0
			6202	3972	1036	1163	31			
1	D	755	Total	C	N	O	S	0	0	0
			6175	3954	1032	1158	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	84	MET	-	expression tag	UNP Q38710
B	84	MET	-	expression tag	UNP Q38710
C	84	MET	-	expression tag	UNP Q38710
D	84	MET	-	expression tag	UNP Q38710

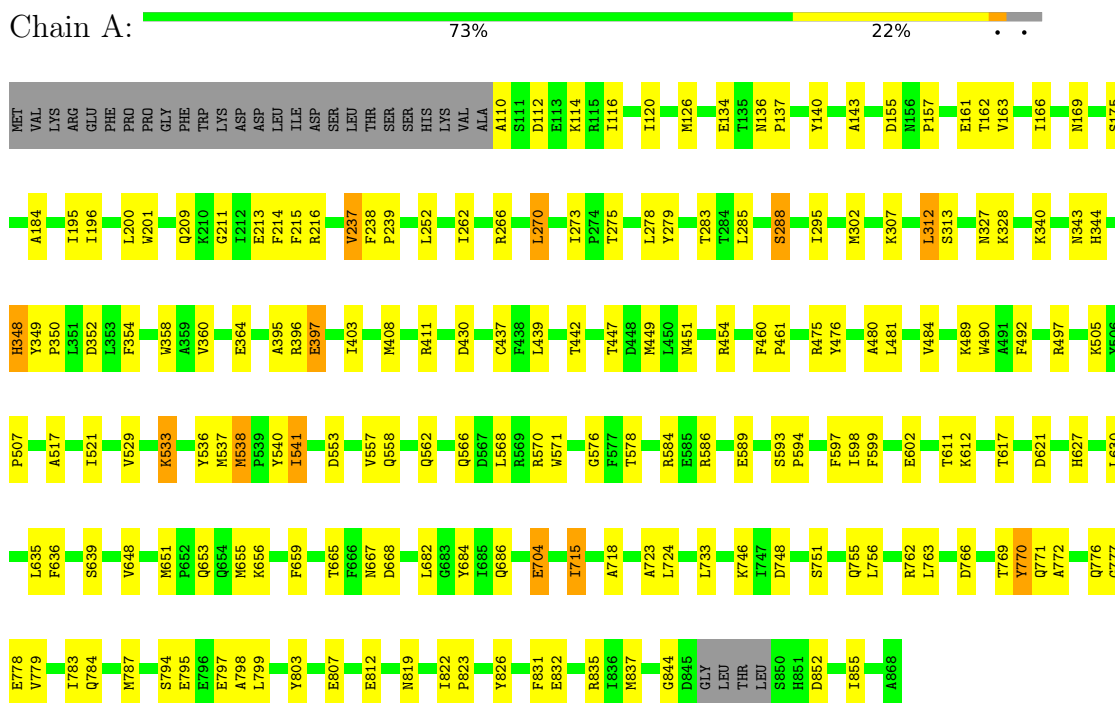
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	330	Total	O	0	0
			330	330		
2	B	323	Total	O	0	0
			323	323		
2	C	390	Total	O	0	0
			390	390		
2	D	284	Total	O	0	0
			284	284		

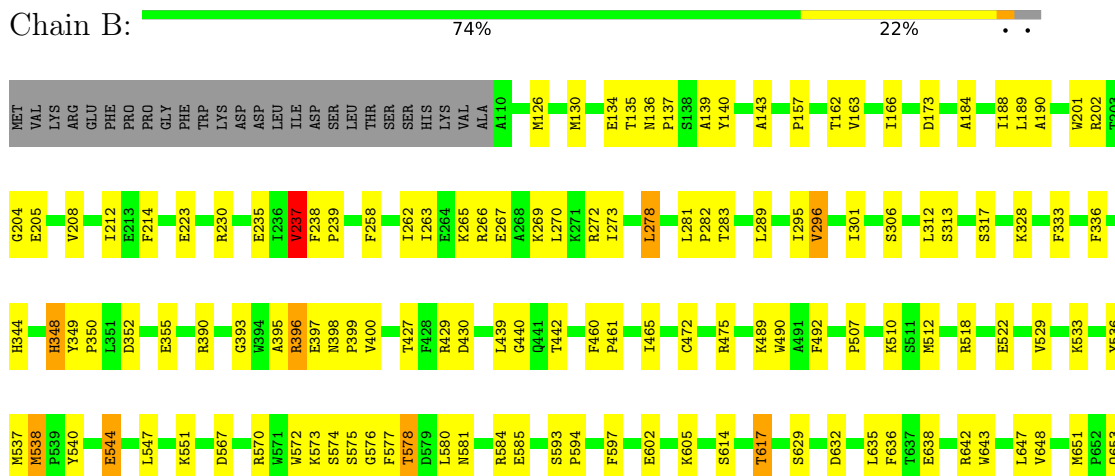
3 Residue-property plots

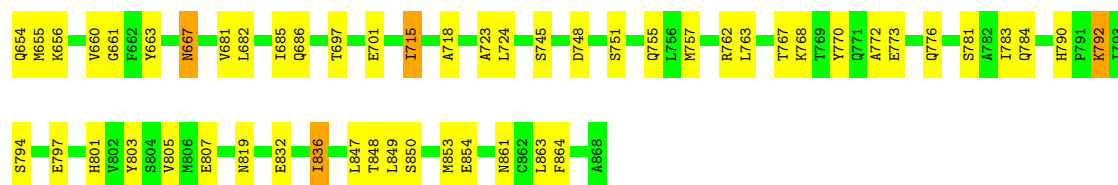
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Abietadiene synthase, chloroplastic



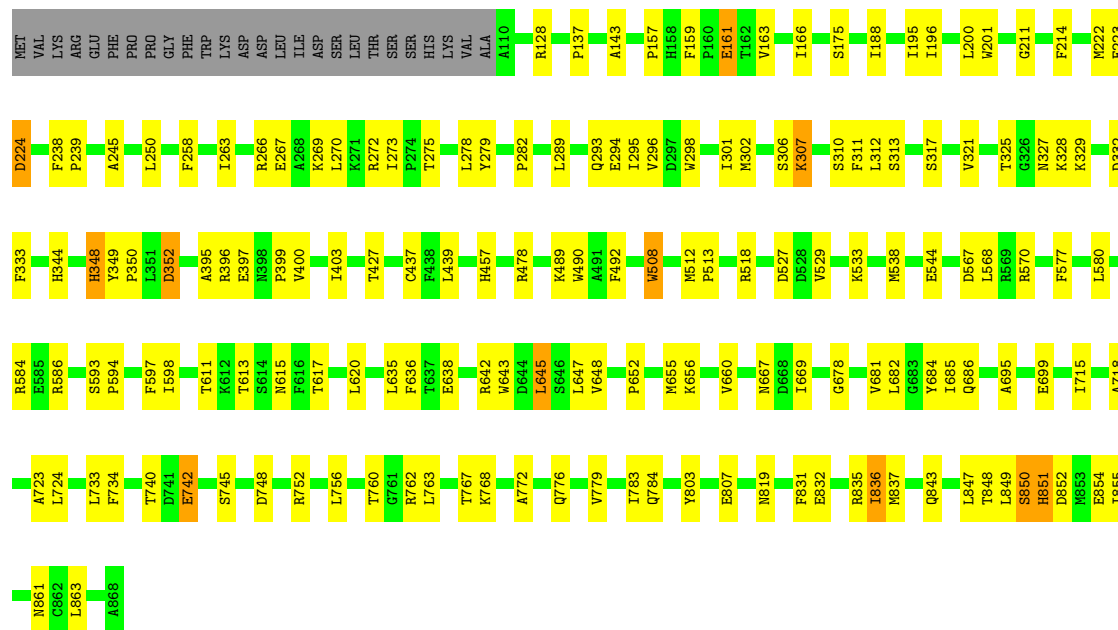
- Molecule 1: Abietadiene synthase, chloroplastic





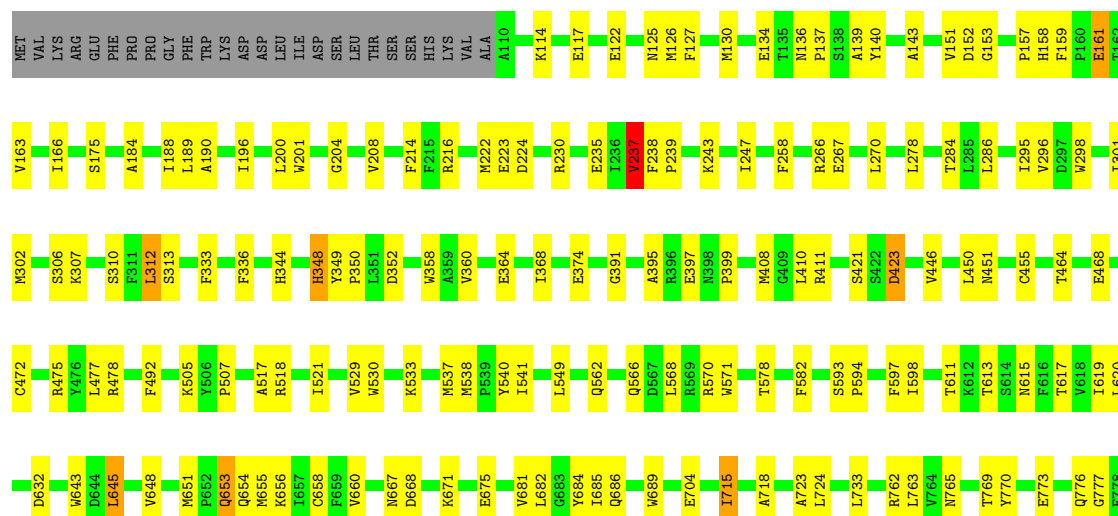
- Molecule 1: Abietadiene synthase, chloroplastic

Chain C: 76% 19% ..



- Molecule 1: Abietadiene synthase, chloroplastic

Chain D: 73% 22% ..





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.84Å 189.09Å 99.89Å 90.00° 91.45° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.30) 97.4 (50.00-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.251 0.197 , 0.251	Depositor DCC
R_{free} test set	14822 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtriage
Anisotropy	0.909	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.217 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26081	wwPDB-VP
Average B, all atoms (Å ²)	34.0	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 41.88 % 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 2.2119e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	1/6321 (0.0%)	0.86	13/8548 (0.2%)
1	B	0.40	1/6349 (0.0%)	0.86	14/8588 (0.2%)
1	C	0.41	0/6349	0.85	12/8588 (0.1%)
1	D	0.40	0/6321	0.85	17/8548 (0.2%)
All	All	0.40	2/25340 (0.0%)	0.85	56/34272 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	538	MET	SD-CE	-7.37	1.61	1.79
1	B	538	MET	SD-CE	-5.98	1.64	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	352	ASP	N-CA-C	7.75	120.62	111.71
1	B	863	LEU	N-CA-C	7.56	122.63	113.41
1	A	352	ASP	N-CA-C	7.52	119.48	111.28
1	A	533	LYS	N-CA-C	-7.08	103.56	111.71
1	D	159	PHE	CA-C-N	6.95	126.46	119.24
1	D	159	PHE	C-N-CA	6.95	126.46	119.24
1	D	790	HIS	CA-C-N	6.92	127.49	119.47
1	D	790	HIS	C-N-CA	6.92	127.49	119.47
1	A	667	ASN	N-CA-C	-6.66	104.10	111.82
1	C	224	ASP	N-CA-C	-6.60	104.40	114.16
1	D	667	ASN	N-CA-C	-6.37	104.20	112.23
1	A	538	MET	CA-C-N	6.35	126.83	119.47
1	A	538	MET	C-N-CA	6.35	126.83	119.47
1	A	237	VAL	N-CA-C	6.28	117.84	111.00
1	C	538	MET	CA-C-N	6.25	126.73	119.47
1	C	538	MET	C-N-CA	6.25	126.73	119.47
1	A	723	ALA	N-CA-C	6.24	122.23	113.56
1	C	819	ASN	N-CA-C	6.22	120.95	113.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	352	ASP	N-CA-C	6.16	118.79	111.71
1	C	863	LEU	N-CA-C	6.01	121.27	113.88
1	B	653	GLN	N-CA-C	5.88	117.38	110.97
1	D	538	MET	CA-C-N	5.86	126.26	119.47
1	D	538	MET	C-N-CA	5.86	126.26	119.47
1	C	667	ASN	N-CA-C	-5.85	104.99	111.36
1	A	819	ASN	N-CA-C	5.80	120.42	113.23
1	D	237	VAL	N-CA-C	5.78	116.56	110.72
1	B	723	ALA	N-CA-C	5.77	121.58	113.56
1	C	723	ALA	N-CA-C	5.77	121.58	113.56
1	D	819	ASN	N-CA-C	5.76	120.03	112.89
1	A	169	ASN	N-CA-C	5.67	119.87	111.87
1	C	352	ASP	N-CA-C	5.66	117.45	111.28
1	B	578	THR	N-CA-C	-5.66	105.87	112.89
1	C	159	PHE	CA-C-N	5.65	125.76	119.32
1	C	159	PHE	C-N-CA	5.65	125.76	119.32
1	B	819	ASN	N-CA-C	5.57	119.80	112.89
1	C	533	LYS	N-CA-C	-5.51	105.37	111.71
1	D	570	ARG	N-CA-C	-5.47	106.73	113.41
1	A	328	LYS	N-CA-C	5.39	118.07	111.82
1	B	667	ASN	N-CA-C	-5.37	105.08	111.69
1	B	237	VAL	N-CA-C	5.34	116.83	111.00
1	B	533	LYS	N-CA-C	-5.33	105.55	111.36
1	D	446	VAL	N-CA-C	5.33	115.54	110.42
1	D	541	ILE	N-CA-C	-5.32	107.42	111.62
1	A	273	ILE	N-CA-C	5.29	113.18	108.63
1	B	328	LYS	N-CA-C	5.29	117.05	111.28
1	D	818	VAL	N-CA-C	5.28	116.36	111.45
1	C	293	GLN	N-CA-C	5.25	118.46	111.75
1	D	723	ALA	N-CA-C	5.24	120.85	113.56
1	D	533	LYS	N-CA-C	-5.23	105.58	111.28
1	B	790	HIS	CA-C-N	5.19	126.33	119.84
1	B	790	HIS	C-N-CA	5.19	126.33	119.84
1	B	393	GLY	N-CA-C	-5.08	106.70	112.79
1	B	864	PHE	N-CA-C	5.06	119.66	112.93
1	D	391	GLY	N-CA-C	-5.02	106.92	112.04
1	A	541	ILE	N-CA-C	-5.01	107.91	112.12
1	A	599	PHE	N-CA-C	5.00	119.09	112.89

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	6175	0	6045	139	0
1	B	6202	0	6078	128	0
1	C	6202	0	6078	112	0
1	D	6175	0	6045	130	0
2	A	330	0	0	9	0
2	B	323	0	0	7	0
2	C	390	0	0	5	0
2	D	284	0	0	4	0
All	All	26081	0	24246	507	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 10.

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)
1:A:718:ALA:HB1	1:A:762:ARG:HD3	1.26	1.16
1:B:718:ALA:HB1	1:B:762:ARG:HD3	1.30	1.11
1:C:718:ALA:HB1	1:C:762:ARG:HD3	1.25	1.08
1:A:354:PHE:HE2	1:A:538:MET:HE3	1.27	0.97
1:D:718:ALA:HB1	1:D:762:ARG:HD3	1.46	0.97
1:A:536:TYR:HE1	1:A:538:MET:HE1	1.34	0.93
1:A:648:VAL:HG13	1:A:656:LYS:HG3	1.53	0.91
1:A:354:PHE:CE2	1:A:538:MET:HE3	2.07	0.89
1:D:161:GLU:H	1:D:161:GLU:CD	1.82	0.88
1:A:536:TYR:CE1	1:A:538:MET:HE1	2.10	0.86
1:B:651:MET:HG2	1:B:655:MET:HE2	1.59	0.85
1:B:536:TYR:CD1	1:B:538:MET:HE3	2.12	0.84
1:D:230:ARG:NH2	1:D:235:GLU:HB2	1.93	0.82
1:A:566:GLN:HB3	1:A:570:ARG:HH12	1.42	0.82
1:B:718:ALA:CB	1:B:762:ARG:HD3	2.11	0.81
1:C:188:ILE:HD13	1:C:222:MET:HE2	1.64	0.80
1:A:137:PRO:HB3	1:A:344:HIS:CD2	2.16	0.80
1:C:307:LYS:HE3	1:C:307:LYS:O	1.81	0.80
1:B:648:VAL:HG12	1:B:656:LYS:HE3	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:TYR:HD1	1:B:538:MET:HE3	1.47	0.79
1:C:718:ALA:CB	1:C:762:ARG:HD3	2.11	0.79
1:D:648:VAL:HG12	1:D:656:LYS:HE3	1.65	0.78
1:A:651:MET:HG2	1:A:655:MET:HE2	1.66	0.78
1:B:137:PRO:HB3	1:B:344:HIS:CD2	2.19	0.78
1:C:635:LEU:HB2	1:C:655:MET:HE1	1.66	0.77
1:B:847:LEU:HB3	1:B:850:SER:OG	1.84	0.77
1:A:536:TYR:HE1	1:A:538:MET:CE	1.99	0.76
1:C:847:LEU:HB3	1:C:850:SER:HB2	1.68	0.76
1:C:161:GLU:CD	1:C:161:GLU:H	1.94	0.76
1:C:648:VAL:HG13	1:C:656:LYS:HG3	1.65	0.76
1:D:794:SER:HB3	1:D:797:GLU:HG3	1.67	0.76
1:D:653:GLN:HG3	1:D:654:GLN:N	1.99	0.75
1:C:645:LEU:HD23	1:C:645:LEU:N	2.03	0.74
1:D:239:PRO:HB2	1:D:266:ARG:HD3	1.70	0.74
1:C:137:PRO:HB3	1:C:344:HIS:CD2	2.23	0.72
1:D:651:MET:CB	1:D:655:MET:HE2	2.19	0.72
1:A:568:LEU:HD13	1:A:611:THR:HG21	1.71	0.72
1:D:651:MET:HB3	1:D:655:MET:HE2	1.70	0.72
1:C:684:TYR:CE2	1:C:733:LEU:HD11	2.25	0.72
1:B:794:SER:HB3	1:B:797:GLU:HG3	1.72	0.71
1:C:636:PHE:HB2	1:C:655:MET:HE3	1.72	0.71
1:D:137:PRO:HB3	1:D:344:HIS:CD2	2.25	0.71
1:D:793:ILE:HG23	1:D:797:GLU:HB2	1.73	0.71
1:D:803:TYR:O	1:D:807:GLU:HG2	1.92	0.70
1:C:772:ALA:O	1:C:776:GLN:HG3	1.91	0.70
1:A:278:LEU:HD23	1:A:285:LEU:HD13	1.72	0.69
1:A:684:TYR:CE2	1:A:733:LEU:HD11	2.28	0.69
1:A:787:MET:HE3	1:A:795:GLU:HA	1.73	0.69
1:A:766:ASP:O	1:A:770:TYR:HB3	1.92	0.69
1:A:718:ALA:CB	1:A:762:ARG:HD3	2.13	0.69
1:A:270:LEU:HG	1:A:295:ILE:HD13	1.76	0.68
1:C:742:GLU:H	1:C:742:GLU:CD	2.02	0.68
1:A:635:LEU:HB2	1:A:655:MET:HE1	1.74	0.67
1:B:651:MET:CG	1:B:655:MET:HE2	2.24	0.67
1:B:157:PRO:HG2	1:B:163:VAL:HG21	1.75	0.67
1:C:239:PRO:HB2	1:C:266:ARG:HD3	1.77	0.67
1:C:584:ARG:NH1	1:C:586:ARG:HD3	2.10	0.67
1:B:656:LYS:O	1:B:660:VAL:HG23	1.94	0.66
1:C:584:ARG:HH12	1:C:586:ARG:HD3	1.61	0.66
1:B:306:SER:OG	1:B:399:PRO:HG3	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:PRO:HG3	1:D:201:TRP:CE2	2.31	0.66
1:A:852:ASP:HA	1:A:855:ILE:HD13	1.79	0.65
1:A:275:THR:HG23	1:A:279:TYR:CE1	2.32	0.65
1:A:855:ILE:H	1:A:855:ILE:HD12	1.62	0.65
1:D:648:VAL:HG13	1:D:656:LYS:HG3	1.78	0.65
1:D:682:LEU:O	1:D:686:GLN:HG3	1.98	0.64
1:D:645:LEU:N	1:D:645:LEU:HD23	2.13	0.64
1:D:648:VAL:CG1	1:D:656:LYS:HG3	2.27	0.64
1:A:275:THR:HG23	1:A:279:TYR:HE1	1.61	0.64
1:D:472:CYS:HA	1:D:475:ARG:HH21	1.62	0.63
1:C:763:LEU:O	1:C:767:THR:HG23	1.97	0.63
1:B:442:THR:O	1:B:442:THR:HG22	1.98	0.63
1:B:239:PRO:HB2	1:B:266:ARG:HD3	1.81	0.62
1:D:645:LEU:HD23	1:D:645:LEU:H	1.63	0.62
1:C:294:GLU:HG2	2:C:1257:HOH:O	1.98	0.62
1:A:682:LEU:O	1:A:686:GLN:HG3	2.00	0.62
1:B:238:PHE:HB3	1:B:239:PRO:HD3	1.80	0.62
1:C:851:HIS:CE1	1:C:855:ILE:HD11	2.35	0.62
1:B:648:VAL:HG13	1:B:656:LYS:HG3	1.80	0.62
1:A:481:LEU:HB2	2:A:1088:HOH:O	1.99	0.62
1:C:512:MET:HE2	1:C:836:ILE:HG12	1.82	0.62
1:A:396:ARG:HD2	1:A:397:GLU:HG2	1.83	0.61
1:B:157:PRO:HG3	1:B:201:TRP:CE2	2.36	0.61
1:B:269:LYS:O	1:B:273:ILE:HG13	1.99	0.61
1:A:349:TYR:CG	1:A:350:PRO:HA	2.35	0.61
1:A:597:PHE:CD1	1:A:598:ILE:HG23	2.36	0.61
1:A:442:THR:HG22	1:A:442:THR:O	2.00	0.61
1:A:566:GLN:HB3	1:A:570:ARG:NH1	2.16	0.61
1:B:537:MET:O	1:B:538:MET:HE2	2.00	0.61
1:A:157:PRO:HG2	1:A:163:VAL:HG21	1.83	0.60
1:B:205:GLU:HG3	2:B:1099:HOH:O	2.01	0.60
1:D:143:ALA:HA	1:D:166:ILE:HD11	1.82	0.60
1:A:772:ALA:O	1:A:776:GLN:HG3	2.02	0.60
1:A:783:ILE:HD12	1:A:783:ILE:H	1.66	0.60
1:C:645:LEU:HD23	1:C:645:LEU:H	1.67	0.60
1:A:126:MET:HE3	1:A:540:TYR:CD1	2.36	0.60
1:A:209:GLN:O	1:A:213:GLU:HG3	2.01	0.60
1:A:636:PHE:HB2	1:A:655:MET:HE3	1.82	0.59
1:C:638:GLU:O	1:C:642:ARG:HG2	2.02	0.59
1:D:161:GLU:CD	1:D:161:GLU:N	2.59	0.59
1:D:718:ALA:CB	1:D:762:ARG:HD3	2.27	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASN:HB3	1:A:537:MET:HE2	1.85	0.59
1:C:648:VAL:CG1	1:C:656:LYS:HG3	2.33	0.59
1:A:350:PRO:HG2	1:A:395:ALA:HB1	1.84	0.58
1:B:350:PRO:HG2	1:B:395:ALA:HB1	1.85	0.58
1:B:648:VAL:CG1	1:B:656:LYS:HG3	2.33	0.58
1:C:681:VAL:O	1:C:685:ILE:HG12	2.02	0.58
1:B:235:GLU:OE2	1:B:262:ILE:HG13	2.03	0.58
1:C:783:ILE:HD12	1:C:783:ILE:N	2.19	0.58
1:A:783:ILE:HD12	1:A:783:ILE:N	2.19	0.58
1:A:239:PRO:HB2	1:A:266:ARG:CD	2.34	0.58
1:A:408:MET:HE2	2:A:1019:HOH:O	2.04	0.58
1:A:216:ARG:HD3	2:A:1015:HOH:O	2.03	0.58
1:C:143:ALA:HA	1:C:166:ILE:HD11	1.84	0.58
1:D:408:MET:HE3	1:D:451:ASN:CG	2.29	0.58
1:A:536:TYR:CE1	1:A:538:MET:CE	2.80	0.57
1:A:140:TYR:OH	1:A:237:VAL:HG11	2.04	0.57
1:D:307:LYS:HD3	1:D:397:GLU:HB3	1.86	0.57
1:B:135:THR:HB	1:B:538:MET:HE1	1.85	0.57
1:D:350:PRO:HG2	1:D:395:ALA:HB1	1.86	0.57
1:D:239:PRO:HB2	1:D:266:ARG:CD	2.33	0.57
1:C:306:SER:OG	1:C:399:PRO:HG3	2.05	0.56
1:D:298:TRP:O	1:D:302:MET:HG2	2.05	0.56
1:A:358:TRP:CH2	1:A:408:MET:HG3	2.41	0.56
1:B:638:GLU:HG3	1:B:647:LEU:HD11	1.86	0.56
1:B:390:ARG:HG3	1:B:390:ARG:HH11	1.70	0.56
1:B:130:MET:HE2	1:B:355:GLU:HG2	1.86	0.56
1:D:222:MET:HG3	1:D:258:PHE:CE2	2.41	0.56
1:D:831:PHE:CE2	1:D:835:ARG:HD2	2.40	0.56
1:A:239:PRO:HB2	1:A:266:ARG:HD3	1.87	0.56
1:A:794:SER:OG	1:A:797:GLU:HB2	2.05	0.56
1:A:751:SER:O	1:A:755:GLN:HG3	2.06	0.56
1:D:715:ILE:HD11	1:D:763:LEU:HD21	1.87	0.56
1:C:349:TYR:CG	1:C:350:PRO:HA	2.41	0.55
1:D:114:LYS:HA	1:D:117:GLU:HG2	1.89	0.55
1:B:681:VAL:O	1:B:685:ILE:HG12	2.06	0.55
1:C:269:LYS:O	1:C:273:ILE:HG13	2.06	0.55
1:D:243:LYS:O	1:D:247:ILE:HG12	2.06	0.55
1:A:779:VAL:HA	1:A:784:GLN:HE22	1.70	0.55
1:C:295:ILE:O	1:C:295:ILE:HG22	2.06	0.55
1:B:349:TYR:CG	1:B:350:PRO:HA	2.42	0.55
1:C:779:VAL:HA	1:C:784:GLN:NE2	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:ILE:C	1:D:295:ILE:HD12	2.32	0.55
1:D:408:MET:HE3	1:D:451:ASN:OD1	2.07	0.55
1:A:112:ASP:O	1:A:116:ILE:HG13	2.07	0.55
1:A:538:MET:HG3	2:A:1006:HOH:O	2.05	0.55
1:D:216:ARG:HD3	2:D:1006:HOH:O	2.06	0.55
1:A:517:ALA:O	1:A:521:ILE:HG13	2.07	0.54
1:B:763:LEU:O	1:B:767:THR:HG23	2.08	0.54
1:B:518:ARG:HD2	1:B:861:ASN:O	2.08	0.54
1:B:581:ASN:CG	1:B:654:GLN:HE22	2.15	0.54
1:D:648:VAL:CG1	1:D:656:LYS:HE3	2.37	0.54
1:B:130:MET:CE	1:B:355:GLU:HG2	2.38	0.54
1:C:852:ASP:HA	1:C:855:ILE:HD12	1.89	0.54
1:D:306:SER:OG	1:D:399:PRO:HG3	2.07	0.54
1:A:803:TYR:O	1:A:807:GLU:HG2	2.07	0.54
1:A:161:GLU:HG3	1:A:343:ASN:HA	1.88	0.54
1:B:439:LEU:HD23	1:B:440:GLY:N	2.23	0.54
1:B:783:ILE:HD12	1:B:783:ILE:N	2.23	0.54
1:A:184:ALA:HB3	2:A:1008:HOH:O	2.09	0.53
1:D:518:ARG:HD2	1:D:861:ASN:O	2.09	0.53
1:D:184:ALA:HB3	2:D:1017:HOH:O	2.09	0.53
1:D:582:PHE:HZ	1:D:658:CYS:SG	2.32	0.53
1:A:403:ILE:HG22	1:A:437:CYS:HA	1.90	0.53
1:B:573:LYS:C	1:B:575:SER:H	2.16	0.53
1:B:751:SER:O	1:B:755:GLN:HG3	2.09	0.53
1:D:134:GLU:HG3	1:D:540:TYR:CE2	2.44	0.53
1:B:427:THR:HG22	1:B:439:LEU:HD12	1.91	0.53
1:B:792:LYS:NZ	1:B:792:LYS:HB3	2.24	0.53
1:B:848:THR:CG2	1:C:678:GLY:HA3	2.38	0.53
1:A:630:LEU:HD11	1:A:704:GLU:HG2	1.91	0.52
1:B:184:ALA:HB3	2:B:1034:HOH:O	2.08	0.52
1:C:613:THR:O	1:C:617:THR:HG23	2.09	0.52
1:B:772:ALA:O	1:B:776:GLN:HG3	2.09	0.52
1:D:223:GLU:CD	1:D:223:GLU:H	2.17	0.52
1:D:349:TYR:CG	1:D:350:PRO:HA	2.44	0.52
1:B:134:GLU:HG3	1:B:540:TYR:CZ	2.44	0.52
1:B:235:GLU:OE2	1:B:265:LYS:HD3	2.08	0.52
1:B:803:TYR:O	1:B:807:GLU:HG2	2.10	0.52
1:D:139:ALA:HB3	1:D:190:ALA:HB1	1.91	0.52
1:B:439:LEU:HD23	1:B:439:LEU:C	2.35	0.52
1:D:296:VAL:HG11	1:D:301:ILE:HG13	1.91	0.52
1:D:643:TRP:HB2	1:D:686:GLN:HE21	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:597:PHE:HD1	1:A:598:ILE:HG23	1.74	0.52
1:A:408:MET:HE3	1:A:451:ASN:OD1	2.10	0.52
1:A:288:SER:HB3	1:A:533:LYS:HE2	1.91	0.52
1:A:746:LYS:HD3	1:A:822:ILE:HG12	1.91	0.52
1:C:567:ASP:HA	1:C:570:ARG:HH11	1.74	0.52
1:B:278:LEU:HD23	1:B:278:LEU:O	2.10	0.52
1:D:850:SER:O	1:D:854:GLU:HG2	2.10	0.52
1:C:745:SER:HA	1:C:748:ASP:OD2	2.10	0.51
1:D:684:TYR:CE2	1:D:733:LEU:HD11	2.46	0.51
1:C:128:ARG:HD2	2:C:1305:HOH:O	2.10	0.51
1:D:238:PHE:HB3	1:D:239:PRO:HD3	1.92	0.51
1:D:781:SER:HB2	2:D:1215:HOH:O	2.11	0.51
1:B:643:TRP:CD1	1:B:682:LEU:HD21	2.46	0.51
1:B:576:GLY:C	1:B:578:THR:H	2.19	0.51
1:B:636:PHE:HB2	1:B:655:MET:HE3	1.93	0.51
1:D:157:PRO:HG2	1:D:163:VAL:HG21	1.91	0.51
1:A:215:PHE:CD1	1:A:252:LEU:HD22	2.46	0.51
1:B:492:PHE:CD2	1:B:529:VAL:HG23	2.46	0.51
1:C:275:THR:HG23	1:C:279:TYR:CE1	2.46	0.51
1:C:593:SER:HB2	1:C:594:PRO:CD	2.40	0.51
1:D:421:SER:OG	1:D:423:ASP:HB2	2.11	0.51
1:D:568:LEU:HD13	1:D:611:THR:HG21	1.93	0.51
1:C:740:THR:OG1	1:C:742:GLU:HG2	2.11	0.51
1:D:859:VAL:HG13	1:D:863:LEU:HD12	1.92	0.51
1:B:682:LEU:O	1:B:686:GLN:HG3	2.11	0.51
1:B:847:LEU:HG	1:B:849:LEU:H	1.75	0.51
1:C:289:LEU:HB2	1:C:317:SER:OG	2.10	0.51
1:A:196:ILE:O	1:A:200:LEU:HG	2.11	0.51
1:A:283:THR:O	1:A:312:LEU:HD13	2.11	0.51
1:A:558:GLN:O	1:A:562:GLN:HG3	2.11	0.51
1:A:855:ILE:HD12	1:A:855:ILE:N	2.26	0.51
1:C:157:PRO:HG3	1:C:201:TRP:CE2	2.45	0.51
1:C:222:MET:C	1:C:224:ASP:H	2.18	0.51
1:D:597:PHE:HD1	1:D:598:ILE:HG23	1.76	0.51
1:A:238:PHE:HB3	1:A:239:PRO:HD3	1.93	0.50
1:A:492:PHE:CD2	1:A:529:VAL:HG23	2.45	0.50
1:A:505:LYS:C	1:A:507:PRO:HD3	2.36	0.50
1:A:724:LEU:HD11	1:A:837:MET:HG3	1.93	0.50
1:A:553:ASP:O	1:A:557:VAL:HG23	2.12	0.50
1:B:848:THR:HG23	1:C:678:GLY:HA3	1.94	0.50
1:C:310:SER:HB3	1:C:333:PHE:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HG2	1:C:163:VAL:HG21	1.94	0.50
1:D:648:VAL:HA	1:D:651:MET:HE3	1.94	0.50
1:A:779:VAL:HG12	1:A:779:VAL:O	2.10	0.50
1:D:152:ASP:OD2	1:D:153:GLY:N	2.45	0.50
1:D:286:LEU:HB2	1:D:312:LEU:HD13	1.94	0.50
1:D:781:SER:OG	1:D:784:GLN:HB2	2.12	0.50
1:A:408:MET:CE	1:A:411:ARG:HH11	2.24	0.49
1:C:643:TRP:CD1	1:C:682:LEU:HD21	2.47	0.49
1:C:682:LEU:O	1:C:686:GLN:HG3	2.12	0.49
1:B:584:ARG:HG3	2:B:1244:HOH:O	2.11	0.49
1:B:850:SER:O	1:B:854:GLU:HG2	2.12	0.49
1:D:358:TRP:CH2	1:D:408:MET:HG3	2.47	0.49
1:A:360:VAL:O	1:A:364:GLU:HG3	2.12	0.49
1:B:269:LYS:HA	1:B:272:ARG:HE	1.76	0.49
1:B:567:ASP:HA	1:B:570:ARG:NH1	2.26	0.49
1:A:278:LEU:HD23	1:A:285:LEU:CD1	2.41	0.49
1:A:589:GLU:HB2	2:A:1329:HOH:O	2.13	0.49
1:C:803:TYR:O	1:C:807:GLU:HG2	2.12	0.49
1:A:110:ALA:HB1	1:A:114:LYS:HD3	1.94	0.49
1:A:715:ILE:HD11	1:A:763:LEU:HD21	1.95	0.49
1:B:239:PRO:HB3	1:B:263:ILE:HA	1.94	0.49
1:B:572:TRP:NE1	1:B:585:GLU:HG3	2.28	0.49
1:B:635:LEU:HB2	1:B:655:MET:HE1	1.95	0.49
1:A:408:MET:HE1	1:A:454:ARG:NH1	2.28	0.48
1:C:724:LEU:HD11	1:C:837:MET:HG3	1.95	0.48
1:B:230:ARG:NH1	1:B:235:GLU:OE1	2.46	0.48
1:C:492:PHE:CD2	1:C:529:VAL:HG23	2.49	0.48
1:D:472:CYS:HA	1:D:475:ARG:NH2	2.27	0.48
1:B:333:PHE:O	1:B:336:PHE:HB3	2.14	0.48
1:B:794:SER:HB3	1:B:797:GLU:CG	2.39	0.48
1:A:795:GLU:CD	1:A:795:GLU:C	2.80	0.48
1:B:507:PRO:HD2	1:B:510:LYS:HE3	1.96	0.48
1:C:478:ARG:HG2	1:C:478:ARG:HH11	1.79	0.48
1:D:175:SER:HB3	1:D:214:PHE:CD2	2.49	0.48
1:A:313:SER:O	1:A:348:HIS:HA	2.13	0.48
1:A:408:MET:HE1	1:A:411:ARG:HH11	1.78	0.48
1:A:639:SER:HB3	1:A:659:PHE:CZ	2.48	0.48
1:B:697:THR:O	1:B:701:GLU:HG3	2.14	0.48
1:C:577:PHE:CD1	1:C:580:LEU:HD11	2.49	0.48
1:C:847:LEU:O	1:C:850:SER:HB3	2.14	0.48
1:A:489:LYS:HE3	1:A:490:TRP:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HD2	1:B:396:ARG:O	2.13	0.48
1:B:629:SER:HB3	1:B:632:ASP:OD2	2.13	0.48
1:B:643:TRP:CE2	1:B:682:LEU:HD11	2.49	0.48
1:B:745:SER:HA	1:B:748:ASP:OD2	2.13	0.48
1:D:136:ASN:HB2	1:D:137:PRO:HD2	1.95	0.48
1:D:296:VAL:CG1	1:D:301:ILE:HG13	2.43	0.48
1:D:831:PHE:CD2	1:D:835:ARG:HD2	2.49	0.48
1:A:617:THR:O	1:A:621:ASP:HB2	2.13	0.48
1:D:505:LYS:C	1:D:507:PRO:HD3	2.39	0.48
1:B:223:GLU:OE2	1:B:258:PHE:HB2	2.13	0.48
1:D:196:ILE:O	1:D:200:LEU:HG	2.14	0.48
1:D:360:VAL:O	1:D:364:GLU:HG3	2.14	0.48
1:A:143:ALA:HA	1:A:166:ILE:HD11	1.95	0.47
1:B:398:ASN:CG	1:B:399:PRO:HD2	2.39	0.47
1:C:783:ILE:HD12	1:C:783:ILE:H	1.78	0.47
1:D:668:ASP:OD2	1:D:668:ASP:C	2.57	0.47
1:C:742:GLU:CD	1:C:742:GLU:N	2.71	0.47
1:C:239:PRO:HB3	1:C:263:ILE:HA	1.96	0.47
1:C:298:TRP:O	1:C:302:MET:HG2	2.13	0.47
1:D:134:GLU:HG3	1:D:540:TYR:CZ	2.49	0.47
1:D:230:ARG:HH22	1:D:235:GLU:HB2	1.75	0.47
1:D:368:ILE:HD12	1:D:549:LEU:HD23	1.96	0.47
1:D:776:GLN:HB3	1:D:779:VAL:HG21	1.95	0.47
1:C:439:LEU:C	1:C:439:LEU:HD23	2.40	0.47
1:C:756:LEU:O	1:C:760:THR:HG23	2.15	0.47
1:D:140:TYR:OH	1:D:237:VAL:CG1	2.62	0.47
1:D:464:THR:O	1:D:468:GLU:HG3	2.14	0.47
1:A:651:MET:CG	1:A:655:MET:HE2	2.40	0.47
1:B:306:SER:OG	1:B:399:PRO:CG	2.61	0.47
1:B:518:ARG:HG2	1:B:518:ARG:HH21	1.80	0.47
1:B:801:HIS:O	1:B:805:VAL:HG23	2.14	0.47
1:C:222:MET:C	1:C:224:ASP:N	2.73	0.47
1:C:849:LEU:O	1:C:850:SER:C	2.58	0.47
1:A:449:MET:HE2	1:A:449:MET:HA	1.97	0.47
1:C:329:LYS:HA	1:C:332:ASP:OD2	2.15	0.47
1:A:340:LYS:HD3	1:A:340:LYS:O	2.15	0.47
1:A:566:GLN:CB	1:A:570:ARG:HH12	2.22	0.47
1:C:222:MET:HG3	1:C:258:PHE:CE2	2.50	0.47
1:C:223:GLU:HB2	2:C:1254:HOH:O	2.14	0.47
1:D:267:GLU:OE1	1:D:267:GLU:HA	2.15	0.47
1:D:492:PHE:CD2	1:D:529:VAL:HG23	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:MET:HE3	1:A:451:ASN:CG	2.40	0.47
1:C:267:GLU:OE1	1:C:267:GLU:HA	2.15	0.47
1:C:396:ARG:HD2	1:C:396:ARG:O	2.15	0.47
1:C:350:PRO:HG2	1:C:395:ALA:HB1	1.98	0.46
1:D:562:GLN:O	1:D:566:GLN:HG2	2.15	0.46
1:A:783:ILE:H	1:A:783:ILE:CD1	2.28	0.46
1:A:831:PHE:O	1:A:835:ARG:HG3	2.15	0.46
1:D:597:PHE:CD1	1:D:598:ILE:HG23	2.49	0.46
1:B:544:GLU:HG3	2:B:1172:HOH:O	2.14	0.46
1:C:222:MET:O	1:C:224:ASP:N	2.42	0.46
1:D:651:MET:HB2	1:D:655:MET:HE2	1.97	0.46
1:B:208:VAL:O	1:B:212:ILE:HG13	2.16	0.46
1:C:518:ARG:HD3	1:C:861:ASN:HB3	1.97	0.46
1:D:204:GLY:O	1:D:208:VAL:HG23	2.16	0.46
1:D:724:LEU:HD11	1:D:837:MET:HG3	1.98	0.46
1:B:140:TYR:OH	1:B:237:VAL:HG11	2.15	0.46
1:C:597:PHE:CD1	1:C:598:ILE:HG23	2.51	0.46
1:C:718:ALA:O	1:C:762:ARG:HD2	2.15	0.46
1:A:140:TYR:OH	1:A:237:VAL:CG1	2.63	0.46
1:A:195:ILE:HD11	1:A:211:GLY:C	2.40	0.46
1:B:281:LEU:O	1:B:283:THR:HG23	2.16	0.46
1:B:605:LYS:HD2	1:B:605:LYS:HA	1.78	0.46
1:D:653:GLN:HG3	1:D:654:GLN:H	1.77	0.46
1:A:538:MET:HG2	1:A:541:ILE:HD12	1.98	0.46
1:B:313:SER:O	1:B:348:HIS:HA	2.16	0.46
1:C:768:LYS:HZ1	1:C:843:GLN:HB2	1.80	0.46
1:D:783:ILE:N	1:D:783:ILE:HD12	2.31	0.46
1:A:449:MET:HG3	1:A:476:TYR:CD1	2.51	0.46
1:A:756:LEU:HD11	1:A:812:GLU:HG2	1.98	0.46
1:B:295:ILE:C	1:B:295:ILE:HD12	2.41	0.46
1:A:798:ALA:O	1:A:799:LEU:C	2.60	0.45
1:B:289:LEU:HB2	1:B:317:SER:OG	2.16	0.45
1:A:480:ALA:O	1:A:484:VAL:HG23	2.16	0.45
1:A:823:PRO:HB2	1:A:826:TYR:HD1	1.80	0.45
1:D:127:PHE:HA	1:D:130:MET:HE3	1.97	0.45
1:D:593:SER:HB2	1:D:594:PRO:CD	2.46	0.45
1:A:439:LEU:C	1:A:439:LEU:HD23	2.42	0.45
1:B:140:TYR:OH	1:B:237:VAL:CG1	2.65	0.45
1:C:196:ILE:O	1:C:200:LEU:HG	2.17	0.45
1:D:681:VAL:O	1:D:685:ILE:HG12	2.17	0.45
1:B:306:SER:CB	1:B:399:PRO:HG3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:PHE:CG	1:B:832:GLU:HB3	2.50	0.45
1:B:651:MET:SD	1:B:655:MET:HE2	2.57	0.45
1:D:175:SER:HB3	1:D:214:PHE:CG	2.51	0.45
1:D:671:LYS:O	1:D:675:GLU:HG3	2.16	0.45
1:A:116:ILE:O	1:A:120:ILE:HG13	2.15	0.45
1:B:512:MET:HE2	1:B:836:ILE:HG12	1.98	0.45
1:B:593:SER:HB2	1:B:594:PRO:CD	2.47	0.45
1:C:195:ILE:HD11	1:C:211:GLY:C	2.42	0.45
1:C:282:PRO:HB2	1:C:400:VAL:CG1	2.46	0.45
1:B:135:THR:CB	1:B:538:MET:HE1	2.47	0.45
1:D:284:THR:HA	1:D:312:LEU:HD22	1.98	0.45
1:D:518:ARG:NH1	1:D:865:GLN:HG3	2.32	0.45
1:A:403:ILE:CG2	1:A:437:CYS:HA	2.46	0.45
1:B:614:SER:O	1:B:617:THR:HB	2.17	0.45
1:B:781:SER:OG	1:B:784:GLN:HG3	2.17	0.45
1:C:313:SER:O	1:C:348:HIS:HA	2.17	0.45
1:B:518:ARG:NH2	1:B:522:GLU:OE2	2.49	0.45
1:B:536:TYR:CE1	1:B:538:MET:HE3	2.51	0.45
1:B:768:LYS:HE2	2:B:1216:HOH:O	2.17	0.45
1:A:823:PRO:HB2	1:A:826:TYR:CD1	2.52	0.44
1:C:752:ARG:NH1	2:C:1173:HOH:O	2.48	0.44
1:D:472:CYS:CA	1:D:475:ARG:HH21	2.28	0.44
1:B:724:LEU:HB2	1:B:757:MET:HE3	2.00	0.44
1:D:122:GLU:O	1:D:125:ASN:HB3	2.18	0.44
1:D:517:ALA:O	1:D:521:ILE:HG13	2.17	0.44
1:A:239:PRO:HG3	1:A:262:ILE:HG23	2.00	0.44
1:B:162:THR:O	1:B:166:ILE:HG13	2.18	0.44
1:B:460:PHE:HB3	1:B:461:PRO:HD2	1.99	0.44
1:B:235:GLU:CD	1:B:265:LYS:HD3	2.43	0.44
1:B:748:ASP:HB2	2:B:1238:HOH:O	2.18	0.44
1:C:245:ALA:HB1	1:C:250:LEU:HD12	2.00	0.44
1:A:126:MET:HE3	1:A:540:TYR:HA	1.99	0.44
1:A:653:GLN:HA	1:A:653:GLN:HE21	1.83	0.44
1:C:328:LYS:H	1:C:328:LYS:HD2	1.83	0.44
1:C:642:ARG:NH1	1:C:647:LEU:HD21	2.32	0.44
1:D:793:ILE:HG23	1:D:797:GLU:CB	2.46	0.44
1:C:188:ILE:CD1	1:C:222:MET:HE2	2.43	0.44
1:D:645:LEU:HB2	1:D:648:VAL:HG21	1.99	0.44
1:D:613:THR:O	1:D:617:THR:HG23	2.18	0.43
1:A:475:ARG:HB2	1:A:475:ARG:NH1	2.32	0.43
1:B:188:ILE:HG13	1:B:189:LEU:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:ILE:HD13	1:B:715:ILE:HA	1.77	0.43
1:B:849:LEU:HG	1:B:853:MET:HE2	1.99	0.43
1:D:157:PRO:HG3	1:D:201:TRP:CD2	2.54	0.43
1:A:136:ASN:HB2	1:A:137:PRO:HD2	2.01	0.43
1:A:239:PRO:HB2	1:A:266:ARG:HD2	1.98	0.43
1:B:136:ASN:HB2	1:B:137:PRO:HD2	2.00	0.43
1:D:645:LEU:N	1:D:645:LEU:CD2	2.81	0.43
1:C:831:PHE:CE2	1:C:835:ARG:HD2	2.53	0.43
1:D:410:LEU:HD23	1:D:455:CYS:SG	2.59	0.43
1:A:157:PRO:HG3	1:A:201:TRP:CE2	2.53	0.43
1:A:460:PHE:HB3	1:A:461:PRO:HD2	2.01	0.43
1:C:306:SER:OG	1:C:399:PRO:CG	2.66	0.43
1:D:126:MET:CE	1:D:540:TYR:HA	2.48	0.43
1:D:615:ASN:O	1:D:619:ILE:HG13	2.19	0.43
1:D:770:TYR:HE2	1:D:784:GLN:HG2	1.83	0.43
1:A:748:ASP:HB2	2:A:1250:HOH:O	2.18	0.43
1:C:296:VAL:HG21	1:C:301:ILE:HG13	2.00	0.43
1:C:307:LYS:HE3	1:C:307:LYS:C	2.43	0.43
1:C:620:LEU:HD21	1:C:636:PHE:CZ	2.54	0.43
1:D:765:ASN:O	1:D:769:THR:HG23	2.18	0.43
1:C:311:PHE:CE2	1:C:321:VAL:HG11	2.54	0.43
1:B:642:ARG:HD3	2:B:1200:HOH:O	2.17	0.43
1:B:663:TYR:O	1:B:667:ASN:ND2	2.51	0.43
1:D:126:MET:HE3	1:D:540:TYR:CD1	2.53	0.43
1:D:313:SER:O	1:D:348:HIS:HA	2.19	0.43
1:A:175:SER:HB3	1:A:214:PHE:CD2	2.54	0.43
1:B:239:PRO:HB2	1:B:266:ARG:CD	2.47	0.43
1:B:489:LYS:HE3	1:B:490:TRP:NE1	2.33	0.43
1:C:850:SER:O	1:C:854:GLU:HG2	2.19	0.43
1:A:430:ASP:OD1	1:A:430:ASP:C	2.61	0.43
1:A:653:GLN:HA	1:A:653:GLN:NE2	2.34	0.42
1:B:282:PRO:HB2	1:B:400:VAL:CG1	2.48	0.42
1:C:325:THR:HG22	1:C:327:ASN:H	1.84	0.42
1:A:161:GLU:HG2	1:A:162:THR:N	2.34	0.42
1:B:126:MET:HE3	1:B:540:TYR:CD1	2.54	0.42
1:D:530:TRP:CD1	1:D:530:TRP:N	2.88	0.42
1:D:598:ILE:HG13	1:D:598:ILE:O	2.18	0.42
1:A:593:SER:HB2	1:A:594:PRO:CD	2.50	0.42
1:A:597:PHE:CG	1:A:832:GLU:HB3	2.54	0.42
1:D:350:PRO:O	1:D:395:ALA:HB2	2.18	0.42
1:A:665:THR:O	1:A:668:ASP:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:695:ALA:O	1:C:699:GLU:HG3	2.20	0.42
1:D:653:GLN:HE21	1:D:653:GLN:HB2	1.56	0.42
1:A:447:THR:HG22	2:A:1334:HOH:O	2.19	0.42
1:A:492:PHE:HD2	1:A:529:VAL:HG23	1.85	0.42
1:C:352:ASP:OD2	1:C:352:ASP:N	2.52	0.42
1:C:427:THR:HG23	1:C:439:LEU:HD12	2.01	0.42
1:B:773:GLU:HG2	1:B:776:GLN:NE2	2.34	0.42
1:C:489:LYS:HE3	1:C:490:TRP:CE2	2.54	0.42
1:D:656:LYS:O	1:D:660:VAL:HG23	2.19	0.42
1:B:442:THR:O	1:B:442:THR:CG2	2.67	0.42
1:D:188:ILE:HG13	1:D:189:LEU:N	2.33	0.42
1:D:478:ARG:NH1	1:D:478:ARG:HG2	2.35	0.42
1:A:571:TRP:CG	1:A:612:LYS:HE2	2.54	0.42
1:B:430:ASP:C	1:B:430:ASP:OD1	2.62	0.42
1:C:568:LEU:HD13	1:C:611:THR:HG21	2.02	0.42
1:C:652:PRO:HD2	1:C:655:MET:HB3	2.01	0.42
1:D:408:MET:HE1	1:D:411:ARG:HH11	1.85	0.42
1:B:139:ALA:HB3	1:B:190:ALA:HB1	2.02	0.42
1:A:779:VAL:HA	1:A:784:GLN:NE2	2.34	0.42
1:D:478:ARG:HG2	1:D:478:ARG:HH11	1.84	0.42
1:B:580:LEU:HA	1:B:654:GLN:OE1	2.20	0.41
1:C:294:GLU:O	1:C:295:ILE:HD13	2.20	0.41
1:D:333:PHE:O	1:D:336:PHE:HB3	2.19	0.41
1:D:786:TYR:CZ	1:D:801:HIS:ND1	2.88	0.41
1:A:715:ILE:HD11	1:A:763:LEU:CD2	2.50	0.41
1:B:269:LYS:HB2	1:B:272:ARG:HH21	1.86	0.41
1:B:577:PHE:CE1	1:B:661:GLY:HA3	2.55	0.41
1:C:593:SER:HB2	1:C:594:PRO:HD3	2.02	0.41
1:D:643:TRP:HB2	1:D:686:GLN:NE2	2.33	0.41
1:A:134:GLU:HG3	1:A:540:TYR:CE2	2.55	0.41
1:B:204:GLY:O	1:B:208:VAL:HG23	2.20	0.41
1:B:547:LEU:HG	1:B:551:LYS:HE3	2.02	0.41
1:D:151:VAL:HG23	1:D:158:HIS:CE1	2.56	0.41
1:A:627:HIS:HA	2:A:1226:HOH:O	2.20	0.41
1:C:161:GLU:CD	1:C:161:GLU:N	2.71	0.41
1:C:403:ILE:HG22	1:C:437:CYS:HA	2.02	0.41
1:C:567:ASP:HA	1:C:570:ARG:NH1	2.35	0.41
1:D:136:ASN:HB3	1:D:537:MET:HE2	2.03	0.41
1:D:450:LEU:HA	1:D:477:LEU:HD11	2.03	0.41
1:A:307:LYS:NZ	1:A:307:LYS:HB3	2.36	0.41
1:A:484:VAL:O	1:A:497:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ALA:HA	1:B:166:ILE:HD11	2.02	0.41
1:B:632:ASP:O	1:B:655:MET:HE1	2.21	0.41
1:C:175:SER:HB3	1:C:214:PHE:CD2	2.56	0.41
1:C:238:PHE:HB3	1:C:239:PRO:HD3	2.02	0.41
1:C:597:PHE:CG	1:C:832:GLU:HB3	2.56	0.41
1:C:768:LYS:NZ	1:C:843:GLN:HB2	2.36	0.41
1:A:302:MET:HE2	1:A:327:ASN:ND2	2.35	0.41
1:A:358:TRP:CZ3	1:A:408:MET:HG3	2.56	0.41
1:A:576:GLY:C	1:A:578:THR:H	2.27	0.41
1:D:632:ASP:O	1:D:655:MET:HE1	2.21	0.41
1:A:584:ARG:HH21	1:A:586:ARG:HB3	1.86	0.41
1:A:777:GLY:O	1:A:778:GLU:C	2.63	0.41
1:B:239:PRO:HG3	1:B:262:ILE:HG23	2.03	0.41
1:C:269:LYS:HG3	1:C:272:ARG:HH21	1.86	0.41
1:C:645:LEU:HA	2:C:1161:HOH:O	2.21	0.41
1:A:155:ASP:O	1:A:155:ASP:CG	2.64	0.41
1:C:669:ILE:HG23	1:C:734:PHE:CZ	2.56	0.41
1:D:620:LEU:HD12	1:D:689:TRP:CZ3	2.56	0.41
1:A:396:ARG:C	1:A:397:GLU:HG2	2.46	0.40
1:A:855:ILE:H	1:A:855:ILE:CD1	2.30	0.40
1:B:429:ARG:HD2	1:B:465:ILE:CD1	2.51	0.40
1:C:457:HIS:HB3	1:C:508:TRP:HB3	2.03	0.40
1:D:374:GLU:HG3	2:D:1247:HOH:O	2.21	0.40
1:B:173:ASP:O	1:B:214:PHE:HB2	2.21	0.40
1:C:656:LYS:O	1:C:660:VAL:HG23	2.21	0.40
1:D:408:MET:CE	1:D:411:ARG:HH11	2.34	0.40
1:D:568:LEU:O	1:D:571:TRP:HB3	2.21	0.40
1:D:578:THR:O	1:D:578:THR:HG22	2.20	0.40
1:A:769:THR:C	1:A:771:GLN:N	2.77	0.40
1:B:472:CYS:HA	1:B:475:ARG:NH2	2.36	0.40
1:D:222:MET:C	1:D:224:ASP:H	2.29	0.40
1:A:110:ALA:CB	1:A:114:LYS:HD3	2.51	0.40
1:C:478:ARG:HG2	1:C:478:ARG:NH1	2.36	0.40
1:D:310:SER:HB3	1:D:333:PHE:CD2	2.56	0.40
1:B:157:PRO:HG3	1:B:201:TRP:NE1	2.37	0.40
1:B:296:VAL:HG13	1:B:301:ILE:HG13	2.03	0.40
1:D:864:PHE:O	1:D:866:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

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	751/785 (96%)	724 (96%)	26 (4%)	1 (0%)	48	60
1	B	757/785 (96%)	722 (95%)	34 (4%)	1 (0%)	48	60
1	C	757/785 (96%)	732 (97%)	21 (3%)	4 (0%)	24	31
1	D	751/785 (96%)	719 (96%)	30 (4%)	2 (0%)	36	46
All	All	3016/3140 (96%)	2897 (96%)	111 (4%)	8 (0%)	36	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	848	THR
1	C	508	TRP
1	B	574	SER
1	C	850	SER
1	D	851	HIS
1	C	851	HIS
1	D	777	GLY
1	A	844	GLY

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	671/698 (96%)	662 (99%)	9 (1%)	61	77
1	B	674/698 (97%)	657 (98%)	17 (2%)	42	60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	674/698 (97%)	659 (98%)	15 (2%)	45	65
1	D	671/698 (96%)	657 (98%)	14 (2%)	47	66
All	All	2690/2792 (96%)	2635 (98%)	55 (2%)	48	67

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	LEU
1	A	288	SER
1	A	312	LEU
1	A	348	HIS
1	A	397	GLU
1	A	602	GLU
1	A	704	GLU
1	A	715	ILE
1	A	770	TYR
1	B	202	ARG
1	B	237	VAL
1	B	267	GLU
1	B	270	LEU
1	B	278	LEU
1	B	296	VAL
1	B	312	LEU
1	B	348	HIS
1	B	396	ARG
1	B	397	GLU
1	B	544	GLU
1	B	602	GLU
1	B	617	THR
1	B	715	ILE
1	B	770	TYR
1	B	792	LYS
1	B	836	ILE
1	C	161	GLU
1	C	270	LEU
1	C	278	LEU
1	C	307	LYS
1	C	312	LEU
1	C	348	HIS
1	C	397	GLU
1	C	513	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	527	ASP
1	C	544	GLU
1	C	615	ASN
1	C	645	LEU
1	C	715	ILE
1	C	742	GLU
1	C	836	ILE
1	D	161	GLU
1	D	237	VAL
1	D	270	LEU
1	D	278	LEU
1	D	312	LEU
1	D	348	HIS
1	D	423	ASP
1	D	645	LEU
1	D	653	GLN
1	D	704	GLU
1	D	715	ILE
1	D	773	GLU
1	D	784	GLN
1	D	836	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	371	HIS
1	A	432	ASN
1	A	479	ASN
1	A	615	ASN
1	A	653	GLN
1	A	776	GLN
1	A	784	GLN
1	A	865	GLN
1	B	168	GLN
1	B	169	ASN
1	B	348	HIS
1	B	776	GLN
1	C	125	ASN
1	C	169	ASN
1	C	293	GLN
1	C	335	ASN
1	C	348	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	371	HIS
1	C	386	HIS
1	C	441	GLN
1	C	687	ASN
1	C	776	GLN
1	D	229	HIS
1	D	293	GLN
1	D	348	HIS
1	D	371	HIS
1	D	441	GLN
1	D	615	ASN
1	D	627	HIS
1	D	687	ASN
1	D	819	ASN
1	D	838	GLN

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 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 [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	755/785 (96%)	-1.47	0 100 100	14, 29, 63, 115	1 (0%)
1	B	759/785 (96%)	-1.45	0 100 100	10, 31, 66, 98	1 (0%)
1	C	759/785 (96%)	-1.51	0 100 100	13, 28, 61, 102	1 (0%)
1	D	755/785 (96%)	-1.44	0 100 100	15, 33, 66, 103	1 (0%)
All	All	3028/3140 (96%)	-1.47	0 100 100	10, 30, 65, 115	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.