



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:17 PM UTC

PDB ID : 4I3U / pdb_00004i3u
Title : Structure of phosphonoacetaldehyde dehydrogenase in complex with phosphonoacetaldehyde
Authors : Nair, S.K.; Agarwal, V.
Deposited on : 2012-11-26
Resolution : 2.10 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
Mogul : 2022.3.0, CSD as543be (2022)
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

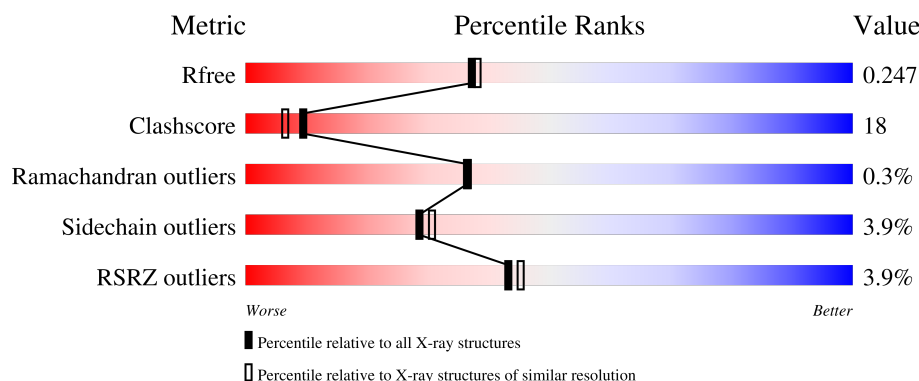
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	488	3% 73% 21% ...
1	B	488	4% 72% 23% ..
1	C	488	2% 74% 19% ..
1	D	488	5% 75% 18% ..
1	E	488	4% 73% 20% ...

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	488	
1	G	488	
1	H	488	

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
2	POA	B	500	-	X	-	-
2	POA	D	500	-	X	-	-
2	POA	E	500	-	X	-	-
2	POA	G	500	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 30980 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 Aldehyde dehydrogenase (NAD⁺).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	B	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	C	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	D	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	E	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	F	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	G	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			
1	H	473	Total	C	N	O	S	0	0	0
			3626	2294	630	683	19			

There are 24 discrepancies between the modelled and reference sequences:

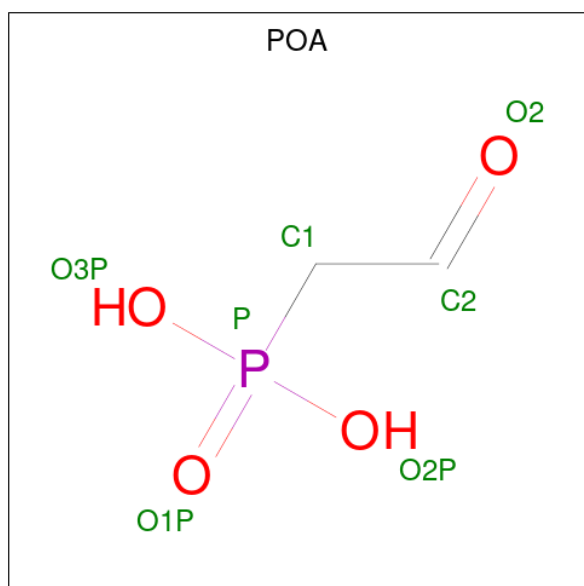
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q92UV7
A	-1	SER	-	expression tag	UNP Q92UV7
A	0	HIS	-	expression tag	UNP Q92UV7
B	-2	GLY	-	expression tag	UNP Q92UV7
B	-1	SER	-	expression tag	UNP Q92UV7
B	0	HIS	-	expression tag	UNP Q92UV7
C	-2	GLY	-	expression tag	UNP Q92UV7
C	-1	SER	-	expression tag	UNP Q92UV7
C	0	HIS	-	expression tag	UNP Q92UV7
D	-2	GLY	-	expression tag	UNP Q92UV7
D	-1	SER	-	expression tag	UNP Q92UV7
D	0	HIS	-	expression tag	UNP Q92UV7
E	-2	GLY	-	expression tag	UNP Q92UV7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q92UV7
E	0	HIS	-	expression tag	UNP Q92UV7
F	-2	GLY	-	expression tag	UNP Q92UV7
F	-1	SER	-	expression tag	UNP Q92UV7
F	0	HIS	-	expression tag	UNP Q92UV7
G	-2	GLY	-	expression tag	UNP Q92UV7
G	-1	SER	-	expression tag	UNP Q92UV7
G	0	HIS	-	expression tag	UNP Q92UV7
H	-2	GLY	-	expression tag	UNP Q92UV7
H	-1	SER	-	expression tag	UNP Q92UV7
H	0	HIS	-	expression tag	UNP Q92UV7

- Molecule 2 is PHOSPHONOACETALDEHYDE (CCD ID: POA) (formula: $C_2H_5O_4P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			7	2	4	1		
2	B	1	Total	C	O	P	0	0
			7	2	4	1		
2	C	1	Total	C	O	P	0	0
			7	2	4	1		
2	D	1	Total	C	O	P	0	0
			7	2	4	1		
2	E	1	Total	C	O	P	0	0
			7	2	4	1		
2	F	1	Total	C	O	P	0	0
			7	2	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	G	1	Total	C	O	P	0	0
			7	2	4	1		
2	H	1	Total	C	O	P	0	0
			7	2	4	1		

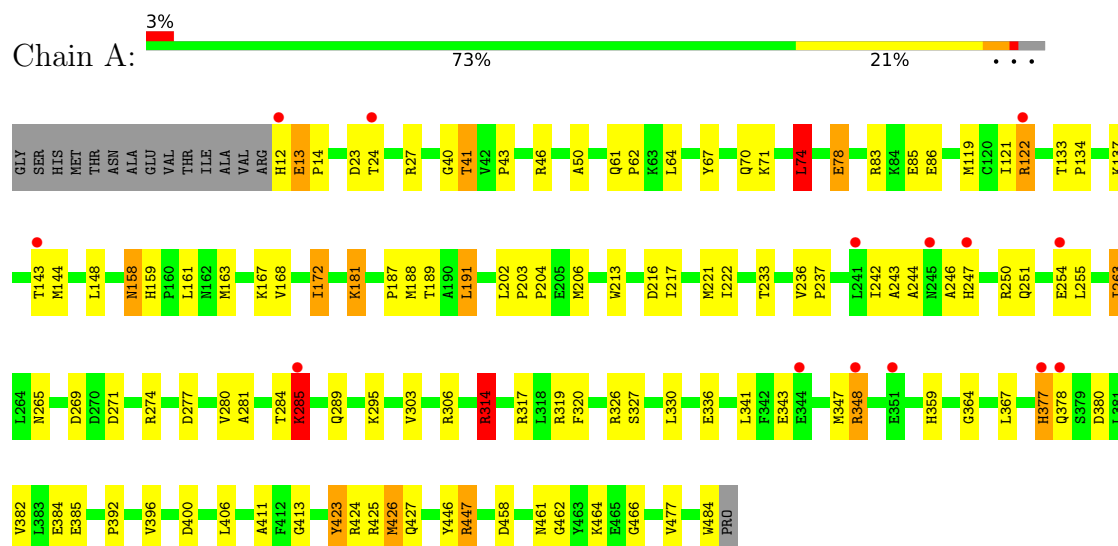
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	287	Total	O	0	0
			287	287		
3	B	233	Total	O	0	0
			233	233		
3	C	237	Total	O	0	0
			237	237		
3	D	258	Total	O	0	0
			258	258		
3	E	245	Total	O	0	0
			245	245		
3	F	225	Total	O	0	0
			225	225		
3	G	204	Total	O	0	0
			204	204		
3	H	227	Total	O	0	0
			227	227		

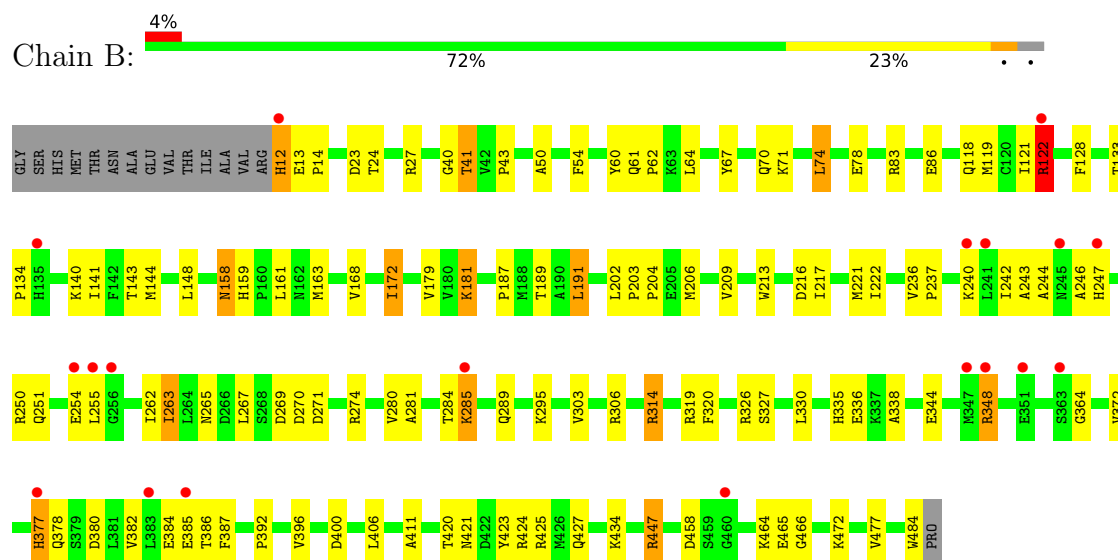
3 Residue-property plots

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.

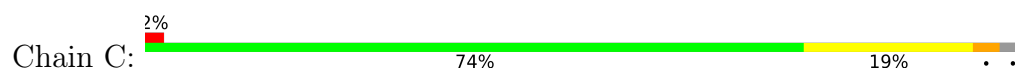
• Molecule 1: Aldehyde dehydrogenase (NAD⁺)

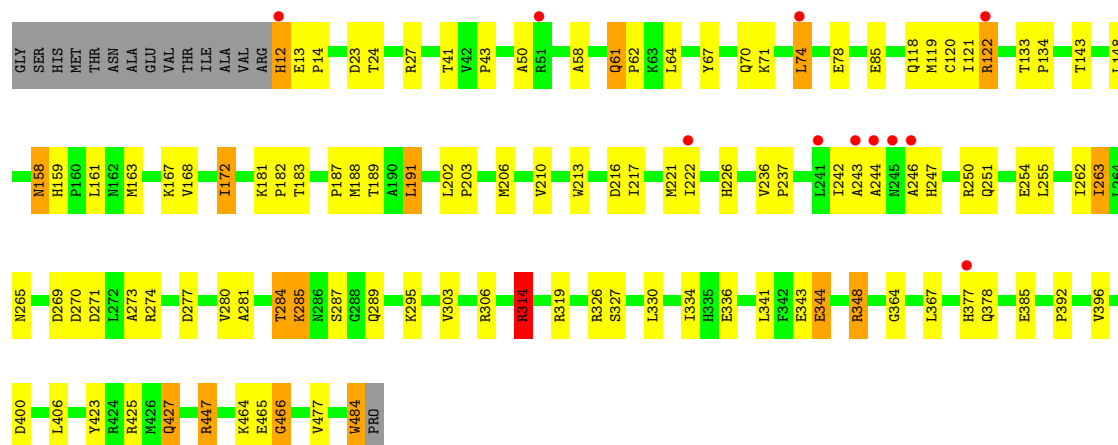


• Molecule 1: Aldehyde dehydrogenase (NAD⁺)

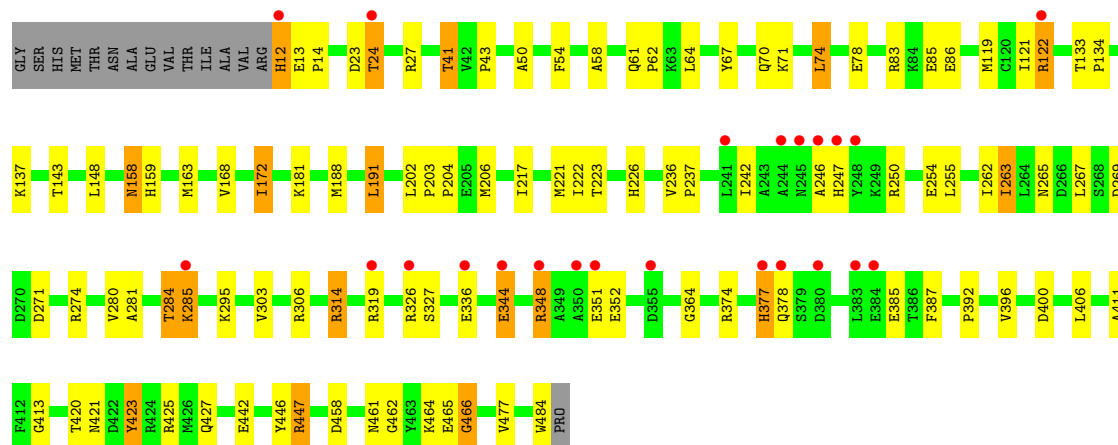
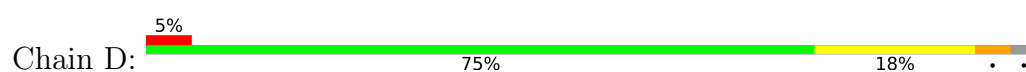


• Molecule 1: Aldehyde dehydrogenase (NAD⁺)

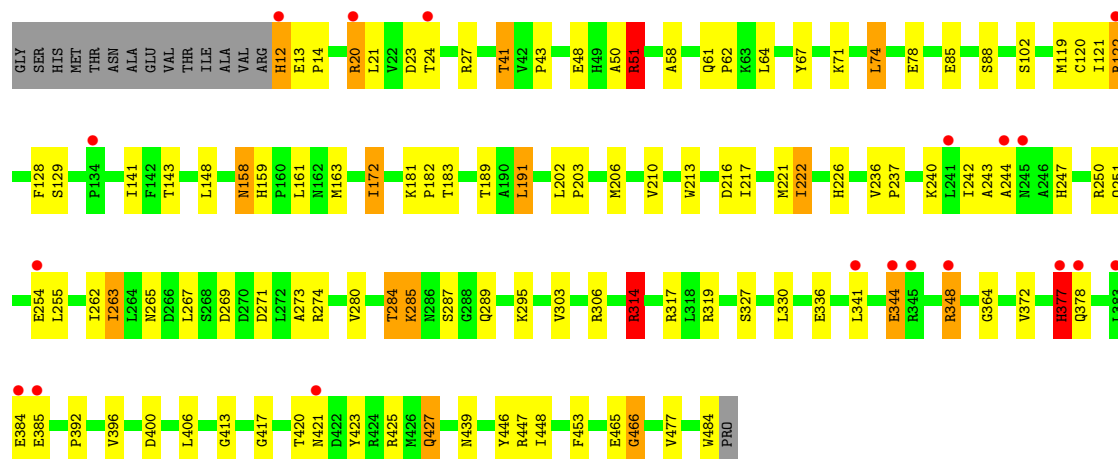
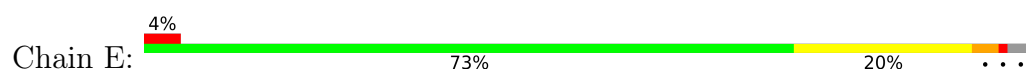




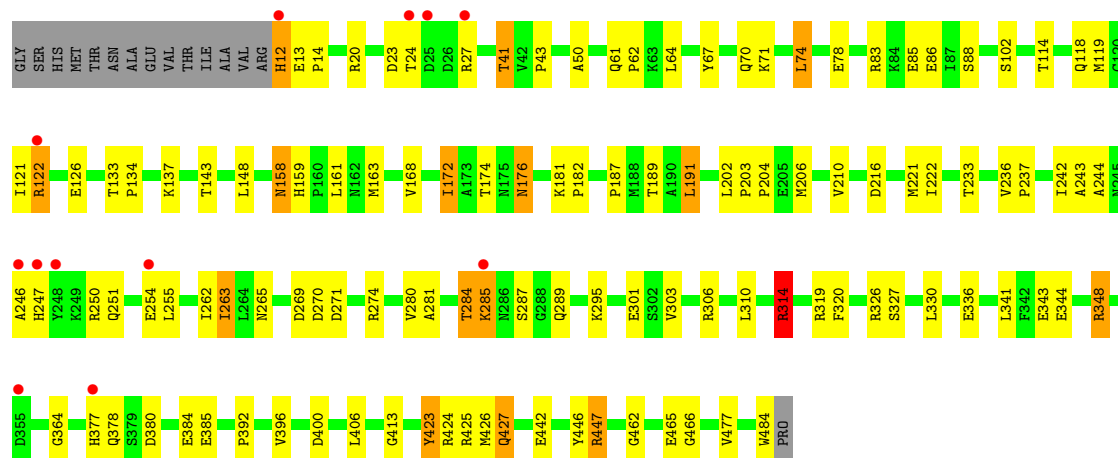
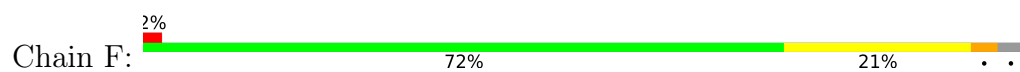
• Molecule 1: Aldehyde dehydrogenase (NAD⁺)



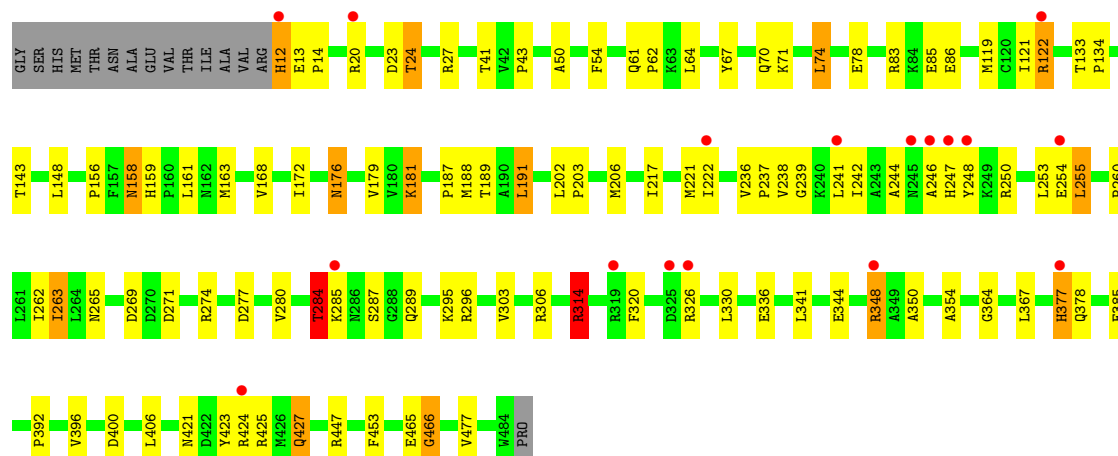
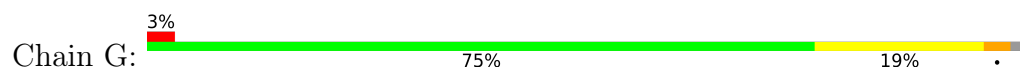
• Molecule 1: Aldehyde dehydrogenase (NAD⁺)



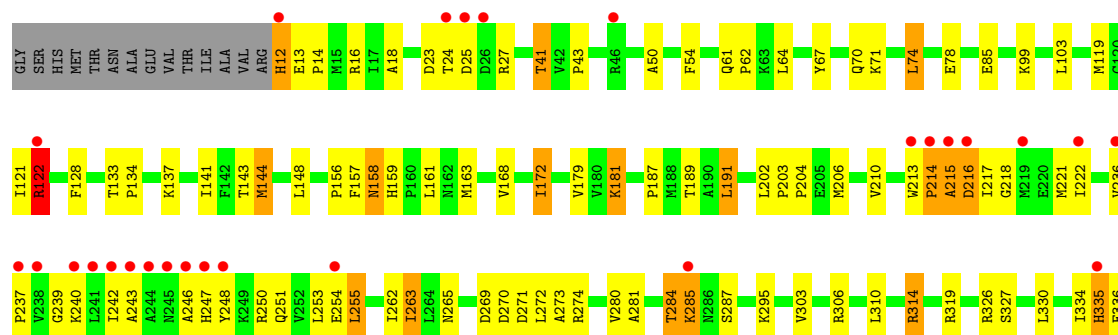
• Molecule 1: Aldehyde dehydrogenase (NAD⁺)



• Molecule 1: Aldehyde dehydrogenase (NAD⁺)



• Molecule 1: Aldehyde dehydrogenase (NAD⁺)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.35Å 172.88Å 138.97Å 90.00° 106.73° 90.00°	Depositor
Resolution (Å)	39.11 – 2.10 39.11 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.6 (39.11-2.10) 96.6 (39.11-2.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.7.1_743, REFMAC	Depositor
R, R_{free}	0.210 , 0.253 0.205 , 0.247	Depositor DCC
R_{free} test set	11837 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30980	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

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

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	0.82	6/3698 (0.2%)	1.00	11/5030 (0.2%)
1	B	0.77	5/3698 (0.1%)	0.96	6/5030 (0.1%)
1	C	0.82	5/3698 (0.1%)	1.00	12/5030 (0.2%)
1	D	0.89	8/3698 (0.2%)	1.01	14/5030 (0.3%)
1	E	0.86	8/3698 (0.2%)	1.02	11/5030 (0.2%)
1	F	0.82	8/3698 (0.2%)	0.97	10/5030 (0.2%)
1	G	0.79	6/3698 (0.2%)	0.99	12/5030 (0.2%)
1	H	0.84	5/3698 (0.1%)	1.04	13/5030 (0.3%)
All	All	0.83	51/29584 (0.2%)	1.00	89/40240 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	E	0	1
1	F	0	1
All	All	0	3

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	158	ASN	CG-OD1	-14.63	0.95	1.23
1	G	176	ASN	CG-ND2	-11.28	1.09	1.33
1	F	176	ASN	CG-ND2	-10.70	1.10	1.33
1	G	176	ASN	CG-OD1	-10.66	1.03	1.23
1	E	222	ILE	CA-CB	9.77	1.67	1.54
1	F	176	ASN	CG-OD1	-9.14	1.06	1.23
1	F	423	TYR	CG-CD1	-8.67	1.21	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	423	TYR	CG-CD2	-8.56	1.21	1.39
1	F	423	TYR	CE1-CZ	-8.53	1.17	1.38
1	F	423	TYR	CG-CD2	-8.41	1.21	1.39
1	A	423	TYR	CG-CD2	-8.33	1.21	1.39
1	D	423	TYR	CG-CD1	-7.97	1.22	1.39
1	D	423	TYR	CE2-CZ	-7.66	1.19	1.38
1	F	423	TYR	CE2-CZ	-7.54	1.20	1.38
1	A	423	TYR	CE1-CZ	-7.54	1.20	1.38
1	A	423	TYR	CG-CD1	-7.49	1.23	1.39
1	E	222	ILE	CB-CG2	-7.38	1.28	1.52
1	A	423	TYR	CE2-CZ	-7.30	1.20	1.38
1	D	284	THR	CB-CG2	-7.23	1.28	1.52
1	D	423	TYR	CE1-CZ	-7.20	1.21	1.38
1	E	377	HIS	CA-C	6.94	1.62	1.52
1	H	284	THR	CB-CG2	-6.82	1.30	1.52
1	H	270	ASP	C-O	-6.56	1.16	1.24
1	C	484	TRP	NE1-CE2	-6.40	1.30	1.37
1	D	284	THR	CB-OG1	-6.29	1.33	1.43
1	C	343	GLU	CD-OE2	-6.05	1.13	1.25
1	H	423	TYR	CE2-CZ	-6.00	1.23	1.38
1	G	423	TYR	CG-CD1	-5.85	1.27	1.39
1	C	343	GLU	CD-OE1	-5.72	1.14	1.25
1	G	284	THR	CB-CG2	-5.66	1.33	1.52
1	F	284	THR	CB-CG2	-5.60	1.34	1.52
1	E	284	THR	CB-CG2	-5.54	1.34	1.52
1	A	122	ARG	CB-CG	-5.49	1.35	1.52
1	E	51	ARG	CD-NE	-5.49	1.38	1.46
1	B	344	GLU	CB-CG	-5.45	1.36	1.52
1	B	122	ARG	CG-CD	-5.45	1.36	1.52
1	E	423	TYR	CG-CD1	-5.41	1.27	1.39
1	C	423	TYR	CG-CD1	-5.40	1.28	1.39
1	C	284	THR	CB-CG2	-5.36	1.34	1.52
1	F	343	GLU	CD-OE2	-5.32	1.15	1.25
1	E	314	ARG	CZ-NH2	-5.26	1.26	1.33
1	B	423	TYR	CE1-CZ	-5.25	1.25	1.38
1	D	122	ARG	CB-CG	-5.23	1.36	1.52
1	E	423	TYR	CG-CD2	-5.12	1.28	1.39
1	B	423	TYR	CE2-CZ	-5.12	1.25	1.38
1	H	272	LEU	C-O	-5.12	1.17	1.24
1	G	423	TYR	CG-CD2	-5.12	1.28	1.39
1	B	423	TYR	CG-CD1	-5.11	1.28	1.39
1	G	122	ARG	CB-CG	-5.09	1.37	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	122	ARG	CB-CG	-5.06	1.37	1.52
1	A	314	ARG	CZ-NH2	-5.03	1.26	1.33

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	158	ASN	N-CA-CB	-12.31	92.03	110.12
1	E	314	ARG	NE-CZ-NH2	10.52	128.67	119.20
1	H	214	PRO	CA-C-N	-10.45	104.59	122.56
1	H	214	PRO	C-N-CA	-10.45	104.59	122.56
1	A	314	ARG	NE-CZ-NH2	9.21	127.49	119.20
1	D	122	ARG	CB-CA-C	-9.04	94.97	109.80
1	C	314	ARG	NE-CZ-NH2	8.91	127.22	119.20
1	G	122	ARG	CB-CA-C	-8.59	95.70	109.80
1	G	314	ARG	NE-CZ-NH2	8.54	126.89	119.20
1	F	158	ASN	N-CA-CB	-8.45	96.22	110.49
1	A	122	ARG	CB-CA-C	-8.34	96.12	109.80
1	C	122	ARG	CB-CA-C	-7.92	96.81	109.80
1	E	74	LEU	CD1-CG-CD2	-7.87	93.48	110.80
1	A	158	ASN	N-CA-CB	-7.83	97.26	110.49
1	C	158	ASN	N-CA-CB	-7.81	97.30	110.49
1	B	158	ASN	N-CA-CB	-7.60	97.65	110.49
1	A	122	ARG	CG-CD-NE	-7.42	95.67	112.00
1	D	284	THR	OG1-CB-CG2	-7.36	94.58	109.30
1	E	158	ASN	N-CA-CB	-7.36	98.05	110.49
1	G	158	ASN	N-CA-CB	-7.33	98.10	110.49
1	D	122	ARG	CG-CD-NE	-7.15	96.26	112.00
1	A	466	GLY	N-CA-C	-7.14	103.69	112.68
1	H	314	ARG	CG-CD-NE	-7.09	96.40	112.00
1	H	157	PHE	CA-C-N	7.09	129.78	120.28
1	H	157	PHE	C-N-CA	7.09	129.78	120.28
1	F	314	ARG	CG-CD-NE	-7.08	96.42	112.00
1	B	466	GLY	N-CA-C	-6.91	103.97	112.68
1	H	284	THR	OG1-CB-CG2	-6.91	95.49	109.30
1	E	427	GLN	CA-CB-CG	6.80	127.69	114.10
1	G	122	ARG	CG-CD-NE	-6.72	97.22	112.00
1	G	284	THR	OG1-CB-CG2	-6.68	95.95	109.30
1	E	314	ARG	CD-NE-CZ	6.67	133.74	124.40
1	D	314	ARG	CG-CD-NE	-6.64	97.39	112.00
1	B	74	LEU	CD1-CG-CD2	-6.49	96.52	110.80
1	D	158	ASN	CB-CG-ND2	6.45	126.07	116.40
1	G	314	ARG	CD-NE-CZ	6.44	133.41	124.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	314	ARG	CG-CD-NE	-6.26	98.23	112.00
1	H	172	ILE	CB-CA-C	-6.19	104.04	111.97
1	D	466	GLY	N-CA-C	-6.18	104.89	112.68
1	G	314	ARG	NE-CZ-NH1	-6.16	115.34	121.50
1	H	466	GLY	N-CA-C	-6.14	104.94	112.68
1	C	314	ARG	CD-NE-CZ	6.06	132.89	124.40
1	H	284	THR	CB-CA-C	5.93	118.39	109.13
1	D	284	THR	CB-CA-C	5.89	118.32	109.13
1	D	158	ASN	N-CA-C	5.84	118.42	111.71
1	A	285	LYS	CG-CD-CE	-5.79	97.97	111.30
1	E	51	ARG	CG-CD-NE	5.79	124.74	112.00
1	G	255	LEU	CD1-CG-CD2	-5.77	98.11	110.80
1	F	314	ARG	CD-NE-CZ	5.76	132.47	124.40
1	C	343	GLU	OE1-CD-OE2	-5.76	109.07	122.90
1	C	74	LEU	CD1-CG-CD2	-5.75	98.16	110.80
1	B	172	ILE	CB-CA-C	-5.70	104.67	111.97
1	C	122	ARG	CG-CD-NE	-5.70	99.46	112.00
1	F	466	GLY	N-CA-C	-5.67	105.53	112.68
1	A	172	ILE	CB-CA-C	-5.66	104.73	111.97
1	E	285	LYS	CB-CG-CD	5.64	124.27	111.30
1	H	255	LEU	CD1-CG-CD2	-5.55	98.58	110.80
1	D	284	THR	N-CA-CB	-5.54	103.64	111.00
1	D	314	ARG	CD-NE-CZ	5.53	132.14	124.40
1	F	423	TYR	CE1-CZ-CE2	-5.52	109.25	120.30
1	F	172	ILE	CB-CA-C	-5.51	104.92	111.97
1	H	215	ALA	CA-C-O	-5.51	112.77	119.43
1	E	172	ILE	CB-CA-C	-5.47	104.97	111.97
1	A	314	ARG	CD-NE-CZ	5.40	131.96	124.40
1	D	285	LYS	CB-CA-C	-5.34	101.10	109.70
1	C	61	GLN	CB-CA-C	-5.34	105.63	110.44
1	C	120	CYS	N-CA-C	5.32	117.83	111.71
1	D	423	TYR	CE1-CZ-CE2	-5.28	109.74	120.30
1	G	285	LYS	CB-CA-C	-5.28	101.20	109.70
1	G	466	GLY	N-CA-C	-5.28	106.03	112.68
1	H	216	ASP	CB-CA-C	-5.25	102.20	110.86
1	C	466	GLY	N-CA-C	-5.24	106.08	112.68
1	F	423	TYR	CD1-CG-CD2	-5.22	110.27	118.10
1	C	172	ILE	CB-CA-C	-5.19	105.14	112.14
1	G	176	ASN	OD1-CG-ND2	-5.18	117.42	122.60
1	C	334	ILE	N-CA-C	5.16	115.88	110.62
1	E	466	GLY	N-CA-C	-5.15	106.20	112.68
1	E	120	CYS	N-CA-C	5.14	117.63	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	423	TYR	CD1-CG-CD2	-5.13	110.40	118.10
1	F	176	ASN	OD1-CG-ND2	-5.11	117.49	122.60
1	A	13	GLU	N-CA-C	5.11	117.57	109.40
1	D	172	ILE	CB-CA-C	-5.10	105.44	111.97
1	A	74	LEU	CD1-CG-CD2	-5.10	99.59	110.80
1	B	344	GLU	CB-CG-CD	5.09	121.26	112.60
1	F	343	GLU	OE1-CD-OE2	-5.08	110.70	122.90
1	E	284	THR	OG1-CB-CG2	-5.07	99.17	109.30
1	A	423	TYR	CE1-CZ-CE2	-5.06	110.18	120.30
1	F	174	THR	OG1-CB-CG2	5.05	119.41	109.30
1	G	427	GLN	CA-CB-CG	5.02	124.13	114.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	ARG	Sidechain
1	E	377	HIS	Sidechain
1	F	314	ARG	Sidechain

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	3626	0	3654	164	1
1	B	3626	0	3654	141	1
1	C	3626	0	3654	131	1
1	D	3626	0	3654	137	8
1	E	3626	0	3654	134	0
1	F	3626	0	3654	141	0
1	G	3626	0	3654	128	0
1	H	3626	0	3654	153	8
2	A	7	0	2	2	0
2	B	7	0	2	2	0
2	C	7	0	2	2	0
2	D	7	0	2	2	0
2	E	7	0	2	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	7	0	2	2	0
2	G	7	0	2	3	0
2	H	7	0	2	1	0
3	A	287	0	0	32	0
3	B	233	0	0	34	0
3	C	237	0	0	19	0
3	D	258	0	0	22	1
3	E	245	0	0	23	0
3	F	225	0	0	32	0
3	G	204	0	0	35	1
3	H	227	0	0	31	1
All	All	30980	0	29248	1046	11

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 18.

All (1046) 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:12:HIS:CE1	1:C:85:GLU:HG3	1.47	1.45
1:A:359:HIS:O	1:G:326:ARG:CD	1.76	1.32
1:C:216:ASP:OD2	3:C:824:HOH:O	1.55	1.24
1:H:314:ARG:NH1	3:H:633:HOH:O	1.64	1.23
1:D:314:ARG:NH2	3:D:739:HOH:O	1.72	1.23
1:H:271:ASP:OD1	1:H:274:ARG:NH1	1.72	1.22
1:F:274:ARG:NH2	3:F:777:HOH:O	1.67	1.22
1:E:206:MET:SD	3:E:839:HOH:O	1.95	1.22
1:A:12:HIS:CE1	1:C:85:GLU:CG	2.22	1.21
1:B:285:LYS:HE3	3:B:809:HOH:O	1.40	1.20
1:A:12:HIS:CD2	1:C:85:GLU:HB2	1.76	1.20
1:B:274:ARG:NH2	3:B:734:HOH:O	1.73	1.19
1:D:319:ARG:HD2	3:D:849:HOH:O	1.42	1.19
1:E:216:ASP:OD2	3:E:820:HOH:O	1.59	1.19
1:A:221:MET:SD	3:A:879:HOH:O	1.97	1.19
1:A:85:GLU:OE2	3:A:613:HOH:O	1.60	1.17
1:A:71:LYS:HD2	3:A:883:HOH:O	1.43	1.16
1:D:24:THR:HG22	1:D:43:PRO:HB3	1.26	1.16
1:F:126:GLU:OE1	3:F:678:HOH:O	1.62	1.16
1:B:12:HIS:N	3:B:817:HOH:O	1.78	1.15
1:F:71:LYS:HD2	3:F:644:HOH:O	1.47	1.14
1:F:314:ARG:NH1	3:F:820:HOH:O	1.80	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:THR:HG22	1:G:43:PRO:HB3	1.21	1.14
1:A:24:THR:HG22	1:A:43:PRO:HB3	1.28	1.14
1:A:216:ASP:OD2	3:A:662:HOH:O	1.63	1.14
1:C:24:THR:HG22	1:C:43:PRO:HB3	1.27	1.13
1:H:24:THR:HG22	1:H:43:PRO:HB3	1.32	1.12
1:H:348:ARG:HH11	1:H:348:ARG:HG3	1.01	1.12
1:F:247:HIS:O	3:F:716:HOH:O	1.63	1.12
1:G:348:ARG:HG3	1:G:348:ARG:HH11	1.09	1.11
1:E:348:ARG:HG3	1:E:348:ARG:HH11	1.12	1.11
1:B:348:ARG:HG3	1:B:348:ARG:HH11	1.08	1.10
1:H:221:MET:SD	3:H:807:HOH:O	2.08	1.10
1:E:24:THR:HG22	1:E:43:PRO:HB3	1.22	1.10
1:A:12:HIS:HD2	3:C:615:HOH:O	1.37	1.07
1:A:12:HIS:N	3:A:880:HOH:O	1.85	1.07
1:G:62:PRO:HB3	1:G:206:MET:HE2	1.35	1.07
1:B:206:MET:SD	3:B:825:HOH:O	2.13	1.07
1:B:24:THR:HG22	1:B:43:PRO:HB3	1.32	1.07
1:H:236:VAL:HA	1:H:255:LEU:HD23	1.37	1.06
1:F:348:ARG:HG3	1:F:348:ARG:HH11	1.13	1.06
1:G:158:ASN:HB2	3:G:639:HOH:O	1.53	1.06
1:C:270:ASP:OD1	1:E:319:ARG:NH1	1.88	1.06
1:G:421:ASN:HB3	3:G:677:HOH:O	1.56	1.05
1:G:254:GLU:OE1	3:G:665:HOH:O	1.73	1.04
1:F:62:PRO:HB3	1:F:206:MET:HE2	1.37	1.04
1:A:359:HIS:O	1:G:326:ARG:HD2	0.87	1.03
1:F:24:THR:HG22	1:F:43:PRO:HB3	1.36	1.03
1:H:70:GLN:OE1	3:H:758:HOH:O	1.74	1.03
1:A:12:HIS:NE2	1:C:85:GLU:HB2	1.72	1.03
1:B:424:ARG:NH1	3:B:806:HOH:O	1.89	1.03
1:B:62:PRO:HB3	1:B:206:MET:HE2	1.39	1.02
1:E:62:PRO:HB3	1:E:206:MET:HE2	1.39	1.02
1:B:216:ASP:OD2	3:B:698:HOH:O	1.78	1.01
1:G:163:MET:HE3	3:G:659:HOH:O	1.61	1.01
1:A:384:GLU:OE2	3:A:722:HOH:O	1.78	1.01
1:G:206:MET:SD	3:G:756:HOH:O	2.20	1.00
1:E:58:ALA:CB	1:E:226:HIS:HD2	1.76	0.99
1:D:62:PRO:HB3	1:D:206:MET:HE2	1.44	0.99
1:H:280:VAL:O	1:H:284:THR:HG22	1.61	0.99
1:E:377:HIS:HD2	3:E:650:HOH:O	1.46	0.98
1:D:314:ARG:NH1	3:D:639:HOH:O	1.96	0.98
1:F:12:HIS:N	3:F:759:HOH:O	1.96	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HH11	1:A:348:ARG:HG3	1.30	0.97
1:B:472:LYS:NZ	3:B:821:HOH:O	1.95	0.97
1:G:280:VAL:O	1:G:284:THR:HG22	1.65	0.96
1:G:24:THR:CG2	1:G:43:PRO:HB3	1.95	0.96
1:E:271:ASP:OD1	1:E:274:ARG:NH1	1.97	0.96
1:D:377:HIS:HD2	1:D:406:LEU:HG	1.31	0.96
1:B:250:ARG:NH2	3:B:805:HOH:O	1.99	0.95
1:A:424:ARG:NH1	3:A:741:HOH:O	1.99	0.95
1:H:62:PRO:HB3	1:H:206:MET:HE2	1.48	0.95
1:A:12:HIS:NE2	1:C:85:GLU:CG	2.30	0.94
1:F:271:ASP:OD1	1:F:274:ARG:NH1	1.99	0.94
1:H:50:ALA:HB1	1:H:221:MET:HE2	1.48	0.94
1:G:236:VAL:HA	1:G:255:LEU:HD23	1.48	0.94
1:D:314:ARG:CZ	3:D:639:HOH:O	2.16	0.94
1:D:271:ASP:OD1	1:D:274:ARG:NH1	2.00	0.94
1:E:50:ALA:HB1	1:E:221:MET:HE2	1.48	0.94
1:C:62:PRO:HB3	1:C:206:MET:HE2	1.50	0.93
1:D:247:HIS:NE2	1:E:21:LEU:O	2.01	0.93
1:E:421:ASN:HB3	3:E:841:HOH:O	1.69	0.92
1:A:62:PRO:HB3	1:A:206:MET:HE2	1.48	0.92
1:C:12:HIS:ND1	1:C:41:THR:CG2	2.32	0.92
1:E:24:THR:CG2	1:E:43:PRO:HB3	2.00	0.91
1:D:348:ARG:HG3	1:D:348:ARG:HH11	1.36	0.91
1:G:280:VAL:O	1:G:284:THR:CG2	2.18	0.91
1:H:85:GLU:OE1	3:H:615:HOH:O	1.89	0.90
1:A:12:HIS:NE2	1:C:85:GLU:CB	2.34	0.90
1:D:24:THR:CG2	1:D:43:PRO:HB3	2.00	0.90
1:H:348:ARG:HG3	1:H:348:ARG:NH1	1.74	0.90
1:D:378:GLN:HG2	3:D:723:HOH:O	1.71	0.89
1:F:465:GLU:OE2	3:F:804:HOH:O	1.90	0.89
1:A:12:HIS:HE1	1:C:85:GLU:HG3	1.27	0.89
1:B:421:ASN:HB3	3:B:657:HOH:O	1.70	0.89
1:D:280:VAL:O	1:D:284:THR:HG22	1.73	0.89
1:F:62:PRO:CB	1:F:206:MET:HE2	2.03	0.88
1:C:213:TRP:HD1	3:C:824:HOH:O	1.56	0.88
1:F:67:TYR:CZ	1:F:71:LYS:HD3	2.09	0.88
1:B:348:ARG:HG3	1:B:348:ARG:NH1	1.83	0.87
1:E:348:ARG:HG3	1:E:348:ARG:NH1	1.86	0.87
1:C:24:THR:CG2	1:C:43:PRO:HB3	2.05	0.87
1:F:50:ALA:HB1	1:F:221:MET:HE2	1.57	0.86
1:A:447:ARG:HD3	3:A:601:HOH:O	1.73	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:THR:CG2	1:B:43:PRO:HB3	2.04	0.86
1:G:62:PRO:CB	1:G:206:MET:HE2	2.04	0.86
1:H:12:HIS:ND1	1:H:41:THR:HG22	1.90	0.85
1:B:62:PRO:CB	1:B:206:MET:HE2	2.04	0.85
1:H:24:THR:CG2	1:H:43:PRO:HB3	2.06	0.85
1:G:163:MET:HG3	3:G:804:HOH:O	1.75	0.85
1:D:421:ASN:HB3	3:H:620:HOH:O	1.74	0.85
1:G:348:ARG:HG3	1:G:348:ARG:NH1	1.81	0.84
1:E:62:PRO:CB	1:E:206:MET:HE2	2.06	0.84
1:F:24:THR:CG2	1:F:43:PRO:HB3	2.08	0.84
1:A:50:ALA:HB1	1:A:221:MET:HE2	1.59	0.84
1:A:12:HIS:ND1	1:A:41:THR:HG22	1.93	0.84
1:A:24:THR:CG2	1:A:43:PRO:HB3	2.08	0.84
1:E:448:ILE:HG23	3:E:840:HOH:O	1.75	0.84
1:G:50:ALA:HB1	1:G:221:MET:HE2	1.59	0.84
1:B:12:HIS:ND1	1:B:41:THR:CG2	2.41	0.84
1:F:148:LEU:H	1:F:176:ASN:HD21	1.26	0.84
1:H:348:ARG:HH11	1:H:348:ARG:CG	1.86	0.83
1:E:448:ILE:CG2	3:E:840:HOH:O	2.25	0.83
1:F:12:HIS:ND1	1:F:41:THR:CG2	2.42	0.83
1:D:62:PRO:CB	1:D:206:MET:HE2	2.09	0.82
1:H:67:TYR:CZ	1:H:71:LYS:HD3	2.14	0.82
1:B:67:TYR:CZ	1:B:71:LYS:HD3	2.14	0.82
1:B:12:HIS:ND1	1:B:41:THR:HG22	1.94	0.82
1:C:50:ALA:HB1	1:C:221:MET:HE2	1.62	0.82
1:E:484:TRP:C	3:E:705:HOH:O	2.23	0.82
1:H:447:ARG:HD3	3:H:612:HOH:O	1.78	0.82
1:A:121:ILE:HG23	3:A:851:HOH:O	1.78	0.81
1:G:447:ARG:HD3	3:G:746:HOH:O	1.79	0.81
1:F:62:PRO:HB3	1:F:206:MET:CE	2.10	0.81
1:B:280:VAL:O	1:B:284:THR:HG23	1.80	0.81
1:E:12:HIS:ND1	1:E:41:THR:HG22	1.95	0.81
1:D:377:HIS:CD2	1:D:406:LEU:HG	2.16	0.81
1:A:271:ASP:OD1	1:A:274:ARG:NH1	2.14	0.80
1:E:12:HIS:ND1	1:E:41:THR:CG2	2.44	0.80
1:H:12:HIS:ND1	1:H:41:THR:CG2	2.43	0.80
1:H:62:PRO:CB	1:H:206:MET:HE2	2.12	0.80
1:A:62:PRO:CB	1:A:206:MET:HE2	2.12	0.80
1:A:250:ARG:HH11	1:D:462:GLY:HA3	1.47	0.80
1:B:447:ARG:HD3	3:B:636:HOH:O	1.80	0.80
1:C:62:PRO:CB	1:C:206:MET:HE2	2.12	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:250:ARG:HH11	1:H:462:GLY:HA3	1.44	0.80
1:E:62:PRO:HB3	1:E:206:MET:CE	2.12	0.79
1:A:67:TYR:CZ	1:A:71:LYS:HD3	2.16	0.79
1:A:181:LYS:HE2	3:A:641:HOH:O	1.82	0.79
1:A:12:HIS:ND1	1:A:41:THR:CG2	2.45	0.79
1:F:447:ARG:HD3	3:F:640:HOH:O	1.81	0.79
1:C:67:TYR:CZ	1:C:71:LYS:HD3	2.18	0.78
1:A:12:HIS:NE2	3:A:745:HOH:O	2.12	0.78
1:D:12:HIS:ND1	1:D:41:THR:CG2	2.47	0.78
1:G:67:TYR:CZ	1:G:71:LYS:HD3	2.19	0.78
1:G:12:HIS:ND1	1:G:41:THR:HG23	1.98	0.77
1:D:447:ARG:HD3	3:D:668:HOH:O	1.83	0.77
1:E:67:TYR:CZ	1:E:71:LYS:HD3	2.19	0.77
1:A:137:LYS:HE3	1:D:442:GLU:OE2	1.84	0.77
1:F:12:HIS:ND1	1:F:41:THR:HG22	1.99	0.77
1:D:67:TYR:CZ	1:D:71:LYS:HD3	2.20	0.77
1:A:348:ARG:HG3	1:A:348:ARG:NH1	1.98	0.77
1:G:277:ASP:OD1	1:G:314:ARG:HD3	1.83	0.77
1:H:62:PRO:HB3	1:H:206:MET:CE	2.15	0.76
1:C:348:ARG:HG3	1:C:348:ARG:HH11	1.50	0.76
1:E:447:ARG:HD3	3:E:625:HOH:O	1.84	0.76
1:B:285:LYS:HG2	3:B:809:HOH:O	1.85	0.76
1:H:216:ASP:HB2	3:H:602:HOH:O	1.86	0.76
1:D:62:PRO:HB3	1:D:206:MET:CE	2.15	0.76
1:A:462:GLY:HA3	1:D:250:ARG:HH11	1.50	0.76
1:E:384:GLU:HG3	3:E:807:HOH:O	1.86	0.76
1:C:348:ARG:HG3	1:C:348:ARG:NH1	1.99	0.76
1:B:271:ASP:OD1	1:B:274:ARG:NH1	2.18	0.76
1:C:62:PRO:HB3	1:C:206:MET:CE	2.16	0.75
1:G:62:PRO:HB3	1:G:206:MET:CE	2.14	0.75
1:E:317:ARG:NH1	3:E:833:HOH:O	2.17	0.75
1:B:119:MET:HE1	1:B:122:ARG:HH21	1.51	0.75
1:G:303:VAL:HG12	1:G:306:ARG:NH2	2.02	0.75
1:H:378:GLN:HA	1:H:378:GLN:OE1	1.86	0.75
1:F:348:ARG:HG3	1:F:348:ARG:NH1	1.85	0.75
1:D:12:HIS:ND1	1:D:41:THR:HG22	2.02	0.75
1:B:50:ALA:HB1	1:B:221:MET:HE2	1.67	0.75
1:G:348:ARG:HD3	3:G:674:HOH:O	1.87	0.74
1:B:484:TRP:C	3:C:831:HOH:O	2.30	0.74
1:H:158:ASN:HB2	3:H:808:HOH:O	1.88	0.74
1:F:280:VAL:O	1:F:284:THR:HG23	1.88	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:HIS:ND1	1:D:377:HIS:C	2.46	0.73
1:F:424:ARG:HB2	3:F:703:HOH:O	1.87	0.73
1:H:181:LYS:HE2	3:H:627:HOH:O	1.86	0.73
1:C:378:GLN:HG2	3:C:661:HOH:O	1.87	0.73
1:C:447:ARG:HD3	3:C:604:HOH:O	1.87	0.73
1:D:378:GLN:OE1	1:D:378:GLN:HA	1.89	0.73
1:H:334:ILE:HG23	1:H:335:HIS:ND1	2.03	0.73
1:F:41:THR:HB	3:F:738:HOH:O	1.88	0.73
1:F:50:ALA:HB1	1:F:221:MET:CE	2.19	0.73
1:A:62:PRO:HB3	1:A:206:MET:CE	2.18	0.73
1:G:85:GLU:OE2	3:G:759:HOH:O	2.08	0.72
1:A:12:HIS:CE1	1:C:85:GLU:CB	2.71	0.72
1:B:274:ARG:CZ	3:B:734:HOH:O	2.26	0.71
1:H:50:ALA:HB1	1:H:221:MET:CE	2.20	0.71
1:D:54:PHE:CE2	1:D:221:MET:HE2	2.25	0.71
1:C:280:VAL:O	1:C:284:THR:HG23	1.89	0.71
1:E:50:ALA:HB1	1:E:221:MET:CE	2.20	0.71
1:C:27:ARG:HH21	1:C:41:THR:HG23	1.54	0.71
1:C:303:VAL:HG12	1:C:306:ARG:NH2	2.04	0.71
1:D:336:GLU:OE2	3:D:775:HOH:O	2.07	0.70
1:G:67:TYR:O	1:G:71:LYS:HG2	1.91	0.70
1:A:341:LEU:HD12	3:A:760:HOH:O	1.91	0.70
1:E:172:ILE:HD12	1:E:202:LEU:CD1	2.22	0.70
1:D:54:PHE:HE2	1:D:221:MET:HE2	1.57	0.70
1:G:447:ARG:NH1	1:G:453:PHE:CD2	2.60	0.70
1:H:12:HIS:N	3:H:687:HOH:O	2.23	0.69
1:F:12:HIS:CE1	1:F:27:ARG:NH2	2.60	0.69
1:H:159:HIS:HB2	1:H:163:MET:HG2	1.74	0.69
1:F:216:ASP:OD2	3:F:756:HOH:O	2.10	0.69
1:E:447:ARG:NH1	1:E:453:PHE:CD2	2.60	0.69
1:G:248:TYR:CD1	3:G:637:HOH:O	2.45	0.69
1:A:13:GLU:O	1:A:43:PRO:HD3	1.92	0.69
1:G:119:MET:HE1	1:G:122:ARG:HH21	1.56	0.69
1:G:271:ASP:OD1	1:G:274:ARG:NH1	2.24	0.69
1:D:423:TYR:C	1:D:423:TYR:CD2	2.70	0.69
1:E:119:MET:O	1:E:122:ARG:HB2	1.93	0.69
1:B:62:PRO:HB3	1:B:206:MET:CE	2.19	0.69
1:B:172:ILE:HD12	1:B:202:LEU:CD1	2.22	0.69
1:F:172:ILE:HD12	1:F:202:LEU:CD1	2.23	0.69
1:F:462:GLY:HA3	1:H:250:ARG:HH11	1.58	0.69
1:B:303:VAL:HG12	1:B:306:ARG:NH2	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:ALA:CB	1:E:226:HIS:CD2	2.67	0.68
1:F:119:MET:HE1	1:F:122:ARG:HH21	1.58	0.68
1:C:159:HIS:HB2	1:C:163:MET:HG2	1.75	0.68
1:F:310:LEU:O	3:F:820:HOH:O	2.10	0.68
1:E:163:MET:CE	2:E:500:POA:H11	2.23	0.68
1:G:163:MET:CG	3:G:804:HOH:O	2.38	0.68
1:H:255:LEU:HD12	1:H:255:LEU:N	2.09	0.68
1:H:50:ALA:CB	1:H:221:MET:HE2	2.23	0.68
1:A:50:ALA:HB1	1:A:221:MET:CE	2.23	0.68
1:B:158:ASN:HB2	3:B:827:HOH:O	1.94	0.68
1:F:12:HIS:CE1	3:F:721:HOH:O	2.45	0.68
1:A:159:HIS:HB2	1:A:163:MET:HG2	1.76	0.68
1:H:13:GLU:O	1:H:43:PRO:HD3	1.93	0.68
1:C:12:HIS:ND1	1:C:41:THR:HG22	2.08	0.68
1:G:239:GLY:HA3	1:G:255:LEU:HD21	1.75	0.68
1:C:213:TRP:CD1	3:C:824:HOH:O	2.38	0.68
1:G:172:ILE:HD12	1:G:202:LEU:CD1	2.24	0.67
1:D:172:ILE:HD12	1:D:202:LEU:CD1	2.25	0.67
1:A:348:ARG:HD3	3:A:790:HOH:O	1.94	0.67
1:D:159:HIS:HB2	1:D:163:MET:HG2	1.76	0.67
1:H:239:GLY:HA3	1:H:255:LEU:HD21	1.75	0.67
1:B:40:GLY:HA2	3:B:817:HOH:O	1.95	0.67
1:E:159:HIS:HB2	1:E:163:MET:HG2	1.77	0.67
1:B:159:HIS:HB2	1:B:163:MET:HG2	1.75	0.66
1:F:427:GLN:HG3	3:F:621:HOH:O	1.95	0.66
1:A:213:TRP:HD1	3:A:662:HOH:O	1.78	0.66
1:D:12:HIS:CE1	3:D:789:HOH:O	2.48	0.66
1:D:326:ARG:HG2	1:D:326:ARG:HH11	1.59	0.66
1:C:172:ILE:HD12	1:C:202:LEU:CD1	2.25	0.66
1:D:377:HIS:HD2	1:D:406:LEU:CG	2.08	0.66
1:E:213:TRP:HD1	3:E:820:HOH:O	1.76	0.66
1:D:172:ILE:HD12	1:D:202:LEU:HD13	1.78	0.66
1:F:378:GLN:OE1	1:F:378:GLN:HA	1.96	0.66
1:G:378:GLN:OE1	1:G:378:GLN:HA	1.94	0.66
1:H:119:MET:HE1	1:H:122:ARG:HH21	1.60	0.66
1:A:27:ARG:HH21	1:A:41:THR:HG23	1.60	0.66
1:C:271:ASP:OD1	1:C:274:ARG:NH1	2.29	0.66
1:B:67:TYR:O	1:B:71:LYS:HG2	1.94	0.66
1:D:58:ALA:CB	1:D:226:HIS:CD2	2.79	0.66
1:E:378:GLN:HA	1:E:378:GLN:OE1	1.96	0.66
1:G:295:LYS:HE2	1:G:385:GLU:HG3	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:ARG:NE	3:H:723:HOH:O	2.22	0.66
1:B:13:GLU:O	1:B:43:PRO:HD3	1.96	0.66
1:C:336:GLU:CD	3:C:817:HOH:O	2.39	0.66
1:F:181:LYS:HE2	3:F:632:HOH:O	1.97	0.65
1:A:384:GLU:OE1	3:A:831:HOH:O	2.13	0.65
1:H:484:TRP:C	3:H:823:HOH:O	2.39	0.65
1:D:303:VAL:HG12	1:D:306:ARG:NH2	2.11	0.65
1:E:213:TRP:CD1	3:E:820:HOH:O	2.47	0.65
1:F:67:TYR:O	1:F:71:LYS:HG2	1.96	0.65
1:G:241:LEU:HD23	3:G:758:HOH:O	1.95	0.65
1:A:119:MET:HE1	1:A:122:ARG:HH21	1.61	0.65
1:E:447:ARG:NH1	1:E:453:PHE:CG	2.64	0.65
3:F:679:HOH:O	1:H:247:HIS:HB3	1.96	0.65
1:H:280:VAL:O	1:H:284:THR:CG2	2.41	0.65
1:F:23:ASP:OD1	1:F:27:ARG:NH1	2.30	0.65
1:F:484:TRP:C	3:F:691:HOH:O	2.39	0.65
1:A:280:VAL:O	1:A:284:THR:HG23	1.96	0.65
1:B:122:ARG:NH1	1:C:122:ARG:NH1	2.44	0.65
1:C:23:ASP:OD1	1:C:27:ARG:NH1	2.29	0.65
1:F:250:ARG:NH1	1:H:462:GLY:HA3	2.12	0.65
1:G:156:PRO:HG2	3:G:804:HOH:O	1.96	0.65
1:G:12:HIS:ND1	1:G:41:THR:CG2	2.61	0.64
1:E:23:ASP:OD1	1:E:27:ARG:NH1	2.30	0.64
1:G:23:ASP:OD1	1:G:27:ARG:NH1	2.30	0.64
1:B:23:ASP:OD1	1:B:27:ARG:NH1	2.30	0.64
1:B:319:ARG:HD2	3:B:760:HOH:O	1.95	0.64
1:A:423:TYR:C	1:A:423:TYR:CD2	2.75	0.64
1:E:348:ARG:HD3	3:E:702:HOH:O	1.96	0.64
1:G:119:MET:O	1:G:122:ARG:HB2	1.98	0.64
1:G:172:ILE:HD12	1:G:202:LEU:HD13	1.80	0.64
1:C:172:ILE:HD12	1:C:202:LEU:HD13	1.78	0.64
1:D:27:ARG:HH21	1:D:41:THR:HG23	1.62	0.64
1:C:378:GLN:HA	1:C:378:GLN:OE1	1.97	0.64
1:B:172:ILE:HD12	1:B:202:LEU:HD13	1.79	0.64
1:G:255:LEU:N	1:G:255:LEU:HD12	2.12	0.64
1:B:121:ILE:HD11	1:C:119:MET:CE	2.28	0.64
1:B:163:MET:CE	2:B:500:POA:H11	2.28	0.64
1:F:159:HIS:HB2	1:F:163:MET:HG2	1.79	0.63
1:H:303:VAL:HG12	1:H:306:ARG:NH2	2.13	0.63
1:H:456:ILE:HB	3:H:690:HOH:O	1.97	0.63
1:A:163:MET:CE	2:A:500:POA:H11	2.28	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:ALA:HB1	1:D:221:MET:CE	2.27	0.63
1:D:461:ASN:HB2	3:D:803:HOH:O	1.98	0.63
1:G:50:ALA:HB1	1:G:221:MET:CE	2.27	0.63
1:D:247:HIS:CE1	1:E:21:LEU:O	2.52	0.63
1:E:119:MET:HE1	1:E:122:ARG:HH21	1.63	0.63
1:D:50:ALA:HB1	1:D:221:MET:HE3	1.79	0.63
1:G:241:LEU:CD2	3:G:758:HOH:O	2.47	0.63
1:A:172:ILE:HD12	1:A:202:LEU:CD1	2.28	0.63
1:D:377:HIS:CD2	1:D:406:LEU:CG	2.82	0.63
1:F:303:VAL:HG12	1:F:306:ARG:NH2	2.14	0.63
1:B:27:ARG:HH21	1:B:41:THR:HG23	1.63	0.63
1:G:159:HIS:HB2	1:G:163:MET:HG2	1.80	0.63
1:H:50:ALA:CB	1:H:221:MET:CE	2.77	0.63
1:C:13:GLU:O	1:C:43:PRO:HD3	1.98	0.63
1:F:41:THR:CB	3:F:738:HOH:O	2.45	0.63
1:F:172:ILE:HD12	1:F:202:LEU:HD13	1.79	0.63
1:A:378:GLN:OE1	1:A:378:GLN:HA	1.99	0.62
1:D:119:MET:HE1	1:D:122:ARG:HH21	1.64	0.62
1:E:303:VAL:HG12	1:E:306:ARG:NH2	2.14	0.62
1:D:67:TYR:O	1:D:71:LYS:HG2	1.99	0.62
1:A:121:ILE:HD11	1:H:119:MET:HE2	1.80	0.62
1:D:50:ALA:CB	1:D:221:MET:HE3	2.30	0.62
1:B:386:THR:HA	3:B:683:HOH:O	1.98	0.62
1:G:248:TYR:CG	3:G:637:HOH:O	2.52	0.62
1:H:248:TYR:HA	3:H:767:HOH:O	1.99	0.62
1:C:427:GLN:HG3	3:C:669:HOH:O	1.99	0.62
1:D:23:ASP:OD1	1:D:27:ARG:NH1	2.33	0.62
1:H:23:ASP:OD1	1:H:27:ARG:NH1	2.32	0.62
1:C:119:MET:O	1:C:122:ARG:HB2	2.00	0.62
1:D:13:GLU:O	1:D:43:PRO:HD3	1.99	0.62
1:G:13:GLU:O	1:G:43:PRO:HD3	2.00	0.62
1:B:122:ARG:CZ	1:C:122:ARG:CZ	2.78	0.62
1:B:163:MET:HE1	2:B:500:POA:H11	1.82	0.61
1:B:250:ARG:CZ	3:B:805:HOH:O	2.43	0.61
1:A:27:ARG:HE	1:A:41:THR:HG23	1.64	0.61
1:B:86:GLU:OE1	3:B:702:HOH:O	2.16	0.61
1:D:484:TRP:C	3:D:698:HOH:O	2.43	0.61
1:F:187:PRO:O	1:F:191:LEU:HD23	2.00	0.61
1:H:27:ARG:HH21	1:H:41:THR:HG23	1.63	0.61
1:A:188:MET:HE3	3:A:744:HOH:O	1.99	0.61
1:A:167:LYS:NZ	3:A:654:HOH:O	2.33	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:HD11	1:C:119:MET:HE2	1.83	0.61
1:C:167:LYS:NZ	3:C:684:HOH:O	2.33	0.61
1:B:50:ALA:HB1	1:B:221:MET:CE	2.30	0.61
1:D:247:HIS:CE1	1:E:21:LEU:HB2	2.36	0.61
1:C:67:TYR:O	1:C:71:LYS:HG2	2.00	0.61
1:G:12:HIS:CE1	1:G:27:ARG:NH2	2.69	0.61
1:C:50:ALA:HB1	1:C:221:MET:CE	2.31	0.60
1:E:269:ASP:OD1	1:E:306:ARG:HD2	2.01	0.60
1:B:244:ALA:O	1:B:247:HIS:CE1	2.54	0.60
1:D:280:VAL:O	1:D:284:THR:CG2	2.49	0.60
1:H:336:GLU:HG3	1:H:364:GLY:HA2	1.84	0.60
1:A:67:TYR:O	1:A:71:LYS:HG2	2.00	0.60
1:C:24:THR:HG22	1:C:43:PRO:CB	2.18	0.60
1:E:12:HIS:CE1	1:E:27:ARG:NH2	2.70	0.60
1:B:378:GLN:OE1	1:B:378:GLN:HA	2.01	0.60
1:C:319:ARG:NH2	1:C:327:SER:OG	2.34	0.60
1:A:250:ARG:NH1	1:D:462:GLY:HA3	2.15	0.60
3:A:835:HOH:O	1:D:247:HIS:HB3	2.01	0.60
1:F:12:HIS:CE1	1:F:41:THR:CG2	2.85	0.60
1:H:27:ARG:HE	1:H:41:THR:HG23	1.66	0.60
1:B:119:MET:CE	1:C:121:ILE:HD11	2.31	0.60
1:G:12:HIS:N	3:G:630:HOH:O	2.35	0.60
1:H:396:VAL:HG12	1:H:406:LEU:HD23	1.82	0.60
1:A:23:ASP:OD1	1:A:27:ARG:NH1	2.35	0.60
1:A:122:ARG:CZ	1:H:122:ARG:CZ	2.80	0.60
1:H:310:LEU:HD22	3:H:633:HOH:O	2.00	0.60
3:D:677:HOH:O	1:E:20:ARG:HD2	2.01	0.59
1:E:172:ILE:HD12	1:E:202:LEU:HD11	1.85	0.59
1:A:484:TRP:C	3:H:800:HOH:O	2.46	0.59
1:F:400:ASP:OD2	1:F:425:ARG:HD2	2.01	0.59
1:H:271:ASP:OD1	1:H:274:ARG:CZ	2.49	0.59
1:H:273:ALA:CB	3:H:633:HOH:O	2.51	0.59
1:B:244:ALA:O	1:B:247:HIS:HE1	1.84	0.59
1:A:119:MET:CE	1:H:121:ILE:HD11	2.33	0.59
1:A:122:ARG:NH2	1:H:122:ARG:HD2	2.17	0.59
1:A:163:MET:HE1	2:A:500:POA:H11	1.85	0.59
1:A:295:LYS:HE2	1:A:385:GLU:HG3	1.85	0.59
1:C:464:LYS:HE2	3:C:646:HOH:O	2.03	0.59
1:E:14:PRO:O	1:E:191:LEU:CD1	2.51	0.59
1:A:462:GLY:HA3	1:D:250:ARG:NH1	2.16	0.59
1:C:203:PRO:HG2	1:C:206:MET:HE3	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:MET:CE	1:F:121:ILE:HD11	2.33	0.59
1:B:187:PRO:O	1:B:191:LEU:HD23	2.02	0.58
1:C:163:MET:CE	2:C:500:POA:H11	2.33	0.58
1:C:400:ASP:OD2	1:C:425:ARG:HD2	2.03	0.58
1:G:27:ARG:HB3	1:G:41:THR:OG1	2.03	0.58
1:A:244:ALA:HB1	1:E:21:LEU:HD12	1.84	0.58
1:A:187:PRO:O	1:A:191:LEU:HD23	2.03	0.58
1:A:384:GLU:CD	3:A:722:HOH:O	2.38	0.58
1:E:172:ILE:HD12	1:E:202:LEU:HD13	1.84	0.58
1:F:423:TYR:C	1:F:423:TYR:CD2	2.81	0.58
1:F:442:GLU:OE2	1:H:137:LYS:HE3	2.03	0.58
1:C:148:LEU:HD21	1:C:250:ARG:NH2	2.18	0.58
1:D:400:ASP:OD2	1:D:425:ARG:HD2	2.03	0.58
1:E:163:MET:HE1	2:E:500:POA:H11	1.86	0.58
1:E:13:GLU:O	1:E:43:PRO:HD3	2.03	0.58
1:A:70:GLN:HG3	1:A:74:LEU:CD2	2.34	0.58
1:D:134:PRO:HD3	1:H:67:TYR:CE1	2.39	0.58
1:E:50:ALA:CB	1:E:221:MET:CE	2.82	0.58
1:A:27:ARG:HG3	1:C:85:GLU:OE2	2.04	0.58
1:C:67:TYR:CE1	1:C:71:LYS:HD3	2.39	0.58
1:D:148:LEU:HD21	1:D:250:ARG:NH2	2.19	0.58
1:E:122:ARG:NH2	3:E:810:HOH:O	2.34	0.58
1:F:50:ALA:CB	1:F:221:MET:CE	2.82	0.58
1:H:400:ASP:OD2	1:H:425:ARG:HD2	2.04	0.58
1:F:148:LEU:H	1:F:176:ASN:ND2	1.98	0.58
1:H:187:PRO:O	1:H:191:LEU:HD23	2.04	0.58
1:E:67:TYR:O	1:E:71:LYS:HG2	2.03	0.57
1:F:250:ARG:HH11	1:H:462:GLY:CA	2.16	0.57
1:G:163:MET:CE	2:G:500:POA:H11	2.34	0.57
1:B:67:TYR:CE1	1:B:71:LYS:HD3	2.38	0.57
1:D:336:GLU:HG3	1:D:364:GLY:HA2	1.86	0.57
1:F:400:ASP:OD2	1:F:425:ARG:CD	2.52	0.57
1:G:163:MET:SD	3:G:804:HOH:O	2.57	0.57
1:H:24:THR:HG22	1:H:43:PRO:CB	2.22	0.57
1:A:172:ILE:HD12	1:A:202:LEU:HD13	1.86	0.57
1:A:12:HIS:CD2	3:A:745:HOH:O	2.55	0.57
1:D:377:HIS:NE2	1:D:406:LEU:HD11	2.19	0.57
1:H:12:HIS:CE1	1:H:41:THR:CG2	2.87	0.57
1:E:12:HIS:CE1	1:E:41:THR:CG2	2.87	0.57
1:E:58:ALA:HB3	1:E:226:HIS:HD2	1.64	0.57
1:A:122:ARG:HD3	1:H:122:ARG:NH2	2.20	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:ASN:ND2	3:G:659:HOH:O	2.38	0.57
1:D:247:HIS:HE1	1:E:21:LEU:HB2	1.69	0.56
1:F:13:GLU:O	1:F:43:PRO:HD3	2.04	0.56
1:F:27:ARG:HH21	1:F:41:THR:HG23	1.69	0.56
1:G:396:VAL:HG12	1:G:406:LEU:HD23	1.87	0.56
1:A:50:ALA:CB	1:A:221:MET:CE	2.83	0.56
1:B:400:ASP:OD2	1:B:425:ARG:CD	2.54	0.56
1:C:143:THR:HG21	3:C:662:HOH:O	2.05	0.56
1:D:148:LEU:CD2	1:D:250:ARG:NH2	2.68	0.56
1:D:158:ASN:HD22	1:D:387:PHE:HZ	1.53	0.56
1:D:377:HIS:CD2	1:D:406:LEU:HD11	2.41	0.56
1:E:250:ARG:HD2	3:E:658:HOH:O	2.04	0.56
1:E:280:VAL:O	1:E:284:THR:HG23	2.04	0.56
1:H:222:ILE:HD12	1:H:242:ILE:HG23	1.87	0.56
1:F:163:MET:CE	2:F:500:POA:H11	2.35	0.56
1:A:121:ILE:HD11	1:H:119:MET:CE	2.36	0.56
1:A:122:ARG:NH2	1:H:122:ARG:CD	2.68	0.56
1:G:163:MET:CE	3:G:659:HOH:O	2.34	0.56
1:A:247:HIS:HB3	3:D:748:HOH:O	2.05	0.56
1:C:12:HIS:CE1	1:C:41:THR:CG2	2.88	0.56
1:E:158:ASN:OD1	1:E:289:GLN:O	2.23	0.56
1:H:348:ARG:NH1	1:H:348:ARG:CG	2.53	0.56
1:B:254:GLU:HG2	3:B:742:HOH:O	2.06	0.56
1:C:119:MET:HE1	1:C:122:ARG:HH21	1.71	0.56
1:F:172:ILE:HD13	3:F:652:HOH:O	2.06	0.56
1:F:269:ASP:OD1	1:F:306:ARG:HD2	2.05	0.56
1:A:336:GLU:HG3	1:A:364:GLY:HA2	1.87	0.56
1:B:12:HIS:CE1	1:B:41:THR:CG2	2.89	0.56
1:D:12:HIS:CE1	1:D:27:ARG:NH2	2.73	0.56
1:F:378:GLN:HB2	3:F:677:HOH:O	2.05	0.56
1:A:137:LYS:HD2	1:D:446:TYR:CE1	2.41	0.56
1:B:119:MET:HE2	1:C:121:ILE:HD11	1.88	0.56
1:G:269:ASP:OD1	1:G:306:ARG:HD2	2.06	0.56
1:B:213:TRP:HD1	3:B:698:HOH:O	1.89	0.56
1:D:71:LYS:NZ	3:D:779:HOH:O	2.13	0.55
1:B:140:LYS:HE3	3:B:829:HOH:O	2.05	0.55
1:D:12:HIS:CE1	1:D:41:THR:CG2	2.90	0.55
1:D:377:HIS:CD2	1:D:406:LEU:CD1	2.89	0.55
1:E:67:TYR:CE1	1:E:71:LYS:HD3	2.41	0.55
1:H:133:THR:HB	1:H:134:PRO:HD2	1.87	0.55
1:D:400:ASP:OD2	1:D:425:ARG:CD	2.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:THR:HG21	1:E:20:ARG:NH2	2.22	0.55
1:F:24:THR:HG22	1:F:43:PRO:CB	2.25	0.55
1:H:85:GLU:CD	3:H:615:HOH:O	2.43	0.55
1:A:213:TRP:CD1	3:A:662:HOH:O	2.58	0.55
1:A:347:MET:HE1	3:G:771:HOH:O	2.07	0.55
1:B:396:VAL:HG12	1:B:406:LEU:HD23	1.87	0.55
1:D:396:VAL:HG12	1:D:406:LEU:HD23	1.88	0.55
1:G:447:ARG:NH1	1:G:453:PHE:CG	2.74	0.55
1:A:254:GLU:C	1:A:255:LEU:HD12	2.32	0.55
1:A:378:GLN:HG2	3:A:651:HOH:O	2.05	0.55
1:C:12:HIS:CE1	1:C:27:ARG:NH2	2.75	0.55
1:D:269:ASP:OD1	1:D:306:ARG:HD2	2.07	0.55
1:H:243:ALA:HA	1:H:251:GLN:OE1	2.07	0.55
1:C:148:LEU:CD2	1:C:250:ARG:NH2	2.70	0.55
1:A:119:MET:HE2	1:H:121:ILE:HD11	1.89	0.55
1:C:400:ASP:OD2	1:C:425:ARG:CD	2.55	0.55
1:F:14:PRO:O	1:F:191:LEU:HD12	2.07	0.55
1:A:46:ARG:NH1	3:A:797:HOH:O	2.29	0.55
1:G:14:PRO:O	1:G:191:LEU:HD12	2.07	0.55
1:F:70:GLN:HG3	1:F:74:LEU:CD2	2.37	0.54
1:G:158:ASN:OD1	1:G:289:GLN:O	2.24	0.54
1:A:24:THR:HG22	1:A:43:PRO:CB	2.19	0.54
1:G:156:PRO:HB2	3:G:639:HOH:O	2.05	0.54
1:G:336:GLU:HG3	1:G:364:GLY:HA2	1.89	0.54
1:H:172:ILE:HD12	1:H:202:LEU:CD1	2.37	0.54
1:H:326:ARG:NH1	3:H:615:HOH:O	1.92	0.54
1:D:58:ALA:CB	1:D:226:HIS:HD2	2.17	0.54
1:C:14:PRO:O	1:C:191:LEU:HD12	2.07	0.54
1:G:377:HIS:HD2	3:G:699:HOH:O	1.90	0.54
1:B:70:GLN:O	1:B:74:LEU:HD23	2.08	0.54
1:B:434:LYS:HG2	3:B:819:HOH:O	2.06	0.54
1:G:163:MET:HE1	2:G:500:POA:H11	1.90	0.54
1:F:396:VAL:HG12	1:F:406:LEU:HD23	1.88	0.54
1:G:248:TYR:CE1	3:G:637:HOH:O	2.61	0.54
1:A:12:HIS:CE1	1:A:27:ARG:NH2	2.75	0.54
1:B:400:ASP:OD2	1:B:425:ARG:HD2	2.07	0.54
1:D:222:ILE:HD12	1:D:242:ILE:HG23	1.90	0.54
1:E:24:THR:HG22	1:E:43:PRO:CB	2.16	0.54
1:E:273:ALA:HB1	1:E:314:ARG:NH1	2.22	0.54
1:G:241:LEU:HB3	3:G:758:HOH:O	2.07	0.54
1:G:400:ASP:OD2	1:G:425:ARG:CD	2.56	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:OD1	1:A:306:ARG:HD2	2.07	0.54
1:C:396:VAL:HG12	1:C:406:LEU:HD23	1.89	0.54
1:A:12:HIS:CE1	1:C:85:GLU:HB2	2.38	0.54
1:G:326:ARG:HG2	1:G:326:ARG:HH11	1.74	0.53
1:H:148:LEU:HD21	1:H:250:ARG:NH2	2.23	0.53
1:A:396:VAL:HG12	1:A:406:LEU:HD23	1.90	0.53
1:B:122:ARG:NH2	1:C:122:ARG:HD3	2.23	0.53
1:D:122:ARG:NH1	1:F:122:ARG:NH1	2.55	0.53
1:B:236:VAL:HB	1:B:237:PRO:HD3	1.90	0.53
1:C:336:GLU:HG3	1:C:364:GLY:HA2	1.91	0.53
1:E:27:ARG:HE	1:E:41:THR:HG23	1.73	0.53
1:E:50:ALA:CB	1:E:221:MET:HE2	2.29	0.53
1:G:70:GLN:HG3	1:G:74:LEU:CD2	2.39	0.53
1:D:133:THR:HB	1:D:134:PRO:HD2	1.90	0.53
1:F:222:ILE:HD12	1:F:242:ILE:HG23	1.89	0.53
1:G:67:TYR:CE1	1:G:71:LYS:HD3	2.42	0.53
1:A:12:HIS:CD2	3:C:615:HOH:O	2.26	0.53
1:A:281:ALA:O	1:A:285:LYS:HB2	2.08	0.53
1:B:254:GLU:C	1:B:255:LEU:HD12	2.33	0.53
1:D:12:HIS:HE1	3:D:789:HOH:O	1.85	0.53
1:F:250:ARG:HD2	3:F:667:HOH:O	2.08	0.53
1:F:319:ARG:NH2	1:F:327:SER:OG	2.42	0.53
1:H:148:LEU:CD2	1:H:250:ARG:NH2	2.72	0.53
1:H:400:ASP:OD2	1:H:425:ARG:CD	2.55	0.53
1:G:148:LEU:CD2	1:G:250:ARG:NH2	2.71	0.53
1:G:148:LEU:HD21	1:G:250:ARG:NH2	2.24	0.53
1:G:188:MET:HE3	3:G:628:HOH:O	2.09	0.53
1:A:464:LYS:HE2	3:A:856:HOH:O	2.08	0.53
1:C:269:ASP:OD1	1:C:306:ARG:HD2	2.09	0.53
1:E:396:VAL:HG12	1:E:406:LEU:HD23	1.91	0.53
1:G:236:VAL:HB	1:G:237:PRO:HD3	1.90	0.53
1:H:12:HIS:CE1	1:H:27:ARG:NH2	2.77	0.53
1:A:244:ALA:HA	1:D:247:HIS:ND1	2.23	0.53
1:G:64:LEU:HG	1:G:206:MET:HE1	1.91	0.53
1:H:222:ILE:HG23	1:H:246:ALA:HB2	1.91	0.53
1:B:269:ASP:OD1	1:B:306:ARG:HD2	2.09	0.53
1:B:270:ASP:HB3	3:B:734:HOH:O	2.09	0.53
1:B:336:GLU:HG3	1:B:364:GLY:HA2	1.90	0.53
1:D:119:MET:O	1:D:122:ARG:HB2	2.09	0.53
1:E:203:PRO:HG2	1:E:206:MET:HE3	1.90	0.53
1:A:14:PRO:O	1:A:191:LEU:HD12	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LYS:HE2	3:D:625:HOH:O	2.09	0.52
1:E:295:LYS:HE2	1:E:385:GLU:HG3	1.91	0.52
1:F:12:HIS:CE1	1:F:41:THR:HG21	2.44	0.52
1:F:85:GLU:OE1	1:F:85:GLU:HA	2.09	0.52
1:G:50:ALA:CB	1:G:221:MET:CE	2.87	0.52
1:E:336:GLU:HG3	1:E:364:GLY:HA2	1.92	0.52
1:H:476:ASN:HB3	3:H:818:HOH:O	2.08	0.52
1:A:78:GLU:OE2	3:A:837:HOH:O	2.19	0.52
1:H:67:TYR:O	1:H:71:LYS:HG2	2.10	0.52
1:A:12:HIS:NE2	1:C:85:GLU:HG2	2.20	0.52
1:C:265:ASN:OD1	1:C:425:ARG:NH2	2.39	0.52
1:F:67:TYR:CE1	1:F:71:LYS:HD3	2.45	0.52
1:F:243:ALA:HA	1:F:251:GLN:OE1	2.09	0.52
1:D:236:VAL:HB	1:D:237:PRO:HD3	1.92	0.52
1:E:254:GLU:HB3	3:E:740:HOH:O	2.10	0.52
1:G:158:ASN:HB3	3:G:804:HOH:O	2.09	0.52
1:B:27:ARG:HE	1:B:41:THR:HG23	1.74	0.52
1:E:181:LYS:HE2	3:E:714:HOH:O	2.09	0.52
1:F:148:LEU:CD2	1:F:250:ARG:NH2	2.73	0.52
1:F:222:ILE:HG23	1:F:246:ALA:HB2	1.90	0.52
1:A:400:ASP:OD2	1:A:425:ARG:HD2	2.10	0.52
1:D:27:ARG:HE	1:D:41:THR:HG23	1.75	0.52
2:G:500:POA:C2	3:G:659:HOH:O	2.56	0.52
1:F:12:HIS:CE1	1:F:27:ARG:HH21	2.26	0.52
1:G:222:ILE:HG23	1:G:246:ALA:HB2	1.91	0.52
1:H:236:VAL:HB	1:H:237:PRO:HD3	1.92	0.52
1:A:326:ARG:HG2	1:A:326:ARG:HH11	1.76	0.51
1:A:461:ASN:OD1	3:A:865:HOH:O	2.19	0.51
1:B:119:MET:O	1:B:122:ARG:HB2	2.10	0.51
1:B:172:ILE:HD12	1:B:202:LEU:HD11	1.92	0.51
1:B:319:ARG:NH2	1:B:327:SER:OG	2.43	0.51
1:D:134:PRO:HG3	1:H:67:TYR:CZ	2.45	0.51
1:G:348:ARG:HH11	1:G:348:ARG:CG	1.98	0.51
1:C:50:ALA:CB	1:C:221:MET:CE	2.88	0.51
1:D:188:MET:HE3	3:D:752:HOH:O	2.09	0.51
1:E:58:ALA:HB2	1:E:226:HIS:CD2	2.43	0.51
1:E:148:LEU:CD2	1:E:250:ARG:NH2	2.73	0.51
1:C:270:ASP:CG	1:E:319:ARG:HH12	2.18	0.51
1:E:254:GLU:C	1:E:255:LEU:HD12	2.35	0.51
1:F:301:GLU:HG3	3:F:799:HOH:O	2.09	0.51
1:G:187:PRO:O	1:G:191:LEU:HD23	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:CD2	1:B:250:ARG:NH2	2.74	0.51
1:C:247:HIS:N	3:C:737:HOH:O	2.43	0.51
1:E:244:ALA:O	1:E:247:HIS:CE1	2.63	0.51
1:G:163:MET:HE3	3:G:804:HOH:O	2.10	0.51
1:E:121:ILE:HD11	1:G:119:MET:CE	2.40	0.51
1:H:269:ASP:OD1	1:H:306:ARG:HD2	2.10	0.51
1:E:319:ARG:NH2	1:E:327:SER:OG	2.44	0.51
1:A:168:VAL:O	1:A:172:ILE:HG12	2.11	0.51
1:A:400:ASP:OD2	1:A:425:ARG:CD	2.59	0.51
1:B:24:THR:HG22	1:B:43:PRO:CB	2.23	0.51
1:D:119:MET:HE2	1:F:121:ILE:HD11	1.93	0.51
1:D:377:HIS:NE2	1:D:406:LEU:CD1	2.74	0.51
1:H:133:THR:HB	1:H:134:PRO:CD	2.40	0.51
1:A:244:ALA:CB	1:E:21:LEU:HD12	2.40	0.51
1:B:12:HIS:CE1	1:B:27:ARG:NH2	2.79	0.51
1:B:122:ARG:HD2	1:C:122:ARG:NH2	2.25	0.51
1:B:148:LEU:HD21	1:B:250:ARG:NH2	2.26	0.51
1:B:378:GLN:HB2	3:B:726:HOH:O	2.11	0.51
3:B:654:HOH:O	1:C:484:TRP:C	2.53	0.51
1:F:158:ASN:OD1	1:F:289:GLN:O	2.29	0.51
1:C:341:LEU:O	1:C:344:GLU:HB2	2.10	0.51
1:E:148:LEU:HD21	1:E:250:ARG:NH2	2.26	0.51
1:G:24:THR:CG2	1:G:43:PRO:CB	2.81	0.51
1:A:27:ARG:HH21	1:A:41:THR:CG2	2.22	0.50
1:B:14:PRO:O	1:B:191:LEU:HD12	2.11	0.50
1:B:222:ILE:HD12	1:B:242:ILE:HG23	1.93	0.50
1:C:222:ILE:HG23	1:C:246:ALA:HB2	1.93	0.50
1:C:222:ILE:HD12	1:C:242:ILE:HG23	1.92	0.50
1:F:336:GLU:HG3	1:F:364:GLY:HA2	1.92	0.50
1:H:14:PRO:O	1:H:191:LEU:HD12	2.12	0.50
1:H:156:PRO:HB2	3:H:808:HOH:O	2.11	0.50
1:C:58:ALA:CB	1:C:226:HIS:CD2	2.95	0.50
1:D:67:TYR:CE1	1:D:71:LYS:HD3	2.46	0.50
1:E:341:LEU:O	1:E:344:GLU:HB2	2.11	0.50
1:F:462:GLY:HA3	1:H:250:ARG:NH1	2.24	0.50
1:G:400:ASP:OD2	1:G:425:ARG:HD2	2.12	0.50
1:A:67:TYR:CE1	1:A:71:LYS:HD3	2.45	0.50
1:B:222:ILE:CD1	1:B:242:ILE:HG12	2.42	0.50
1:C:12:HIS:CE1	1:C:41:THR:HG21	2.46	0.50
1:E:400:ASP:OD2	1:E:425:ARG:HD2	2.11	0.50
1:F:236:VAL:HB	1:F:237:PRO:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:465:GLU:HG3	3:B:742:HOH:O	2.12	0.50
1:F:119:MET:O	1:F:122:ARG:HB2	2.11	0.50
1:B:50:ALA:CB	1:B:221:MET:CE	2.89	0.50
1:D:70:GLN:HG3	1:D:74:LEU:CD2	2.41	0.50
1:G:143:THR:HG21	3:G:707:HOH:O	2.12	0.50
1:A:148:LEU:HD21	1:A:250:ARG:NH2	2.26	0.50
1:A:317:ARG:NH1	3:A:747:HOH:O	2.42	0.50
1:C:187:PRO:O	1:C:191:LEU:HD23	2.11	0.50
1:C:188:MET:HE3	3:C:685:HOH:O	2.11	0.50
1:C:427:GLN:NE2	3:C:758:HOH:O	2.45	0.50
1:D:12:HIS:CE1	1:D:41:THR:HG21	2.47	0.50
1:F:281:ALA:O	1:F:285:LYS:HB2	2.12	0.50
1:G:148:LEU:H	1:G:176:ASN:HD21	1.58	0.50
1:G:222:ILE:HD12	1:G:242:ILE:HG23	1.93	0.50
1:E:172:ILE:HD13	3:E:626:HOH:O	2.10	0.50
1:H:172:ILE:HD13	3:H:665:HOH:O	2.12	0.50
1:B:12:HIS:CE1	1:B:41:THR:HG21	2.47	0.49
1:C:244:ALA:O	1:C:247:HIS:CE1	2.65	0.49
1:H:163:MET:CE	2:H:500:POA:H11	2.42	0.49
1:A:12:HIS:CE1	1:A:41:THR:CG2	2.95	0.49
1:B:421:ASN:HB3	3:B:830:HOH:O	2.12	0.49
1:E:12:HIS:CE1	1:E:41:THR:HG21	2.47	0.49
1:E:236:VAL:HB	1:E:237:PRO:HD3	1.93	0.49
1:E:265:ASN:OD1	1:E:425:ARG:NH2	2.42	0.49
1:A:314:ARG:HH21	1:A:314:ARG:HG3	1.77	0.49
1:E:48:GLU:HA	1:E:51:ARG:NH1	2.28	0.49
1:E:182:PRO:HD2	1:E:210:VAL:O	2.13	0.49
1:H:273:ALA:HB1	3:H:633:HOH:O	2.10	0.49
1:B:122:ARG:NH2	1:C:122:ARG:CD	2.76	0.49
1:C:14:PRO:O	1:C:191:LEU:CD1	2.60	0.49
1:G:269:ASP:HB2	3:G:782:HOH:O	2.11	0.49
1:G:424:ARG:NH1	3:G:700:HOH:O	2.22	0.49
1:B:161:LEU:HB2	1:B:189:THR:HG21	1.93	0.49
1:B:265:ASN:OD1	1:B:425:ARG:NH2	2.41	0.49
1:D:285:LYS:HG3	3:D:840:HOH:O	2.12	0.49
3:D:644:HOH:O	1:H:421:ASN:HB3	2.11	0.49
1:F:172:ILE:HD12	1:F:202:LEU:HD11	1.92	0.49
1:A:133:THR:HB	1:A:134:PRO:HD2	1.93	0.49
1:B:158:ASN:OD1	1:B:289:GLN:O	2.30	0.49
1:H:464:LYS:HE2	3:H:686:HOH:O	2.11	0.49
1:A:148:LEU:CD2	1:A:250:ARG:NH2	2.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ASN:OD1	1:A:425:ARG:NH2	2.43	0.49
1:C:163:MET:HE1	2:C:500:POA:H11	1.94	0.49
1:D:203:PRO:HG2	1:D:206:MET:HE3	1.93	0.49
1:B:144:MET:HE1	3:B:713:HOH:O	2.13	0.49
1:D:222:ILE:HG23	1:D:246:ALA:HB2	1.94	0.49
1:E:27:ARG:HH21	1:E:41:THR:HG23	1.78	0.49
1:F:378:GLN:HG2	3:F:677:HOH:O	2.13	0.49
1:H:281:ALA:O	1:H:285:LYS:HB2	2.13	0.49
1:D:122:ARG:CZ	1:F:122:ARG:CZ	2.91	0.49
1:A:244:ALA:O	1:A:247:HIS:CE1	2.66	0.49
1:C:12:HIS:ND1	1:C:41:THR:HG21	2.26	0.49
1:E:263:ILE:N	1:E:263:ILE:CD1	2.75	0.49
1:F:133:THR:HB	1:F:134:PRO:CD	2.43	0.49
1:H:319:ARG:NH2	1:H:327:SER:OG	2.46	0.49
1:F:348:ARG:HH11	1:F:348:ARG:CG	2.01	0.48
1:F:168:VAL:O	1:F:172:ILE:HG12	2.14	0.48
1:F:348:ARG:NH1	1:F:348:ARG:CG	2.65	0.48
1:H:67:TYR:CE1	1:H:71:LYS:HD3	2.48	0.48
1:H:326:ARG:HH11	1:H:326:ARG:HG2	1.78	0.48
1:D:265:ASN:OD1	1:D:425:ARG:NH2	2.42	0.48
1:G:172:ILE:HD12	1:G:202:LEU:HD11	1.92	0.48
1:H:210:VAL:HG21	1:H:221:MET:HE3	1.96	0.48
1:A:158:ASN:OD1	1:A:289:GLN:O	2.31	0.48
1:C:348:ARG:HH11	1:C:348:ARG:CG	2.23	0.48
1:B:295:LYS:HE2	1:B:385:GLU:HG3	1.95	0.48
1:G:14:PRO:O	1:G:191:LEU:CD1	2.61	0.48
1:G:250:ARG:HD2	3:G:683:HOH:O	2.13	0.48
1:H:378:GLN:OE1	1:H:378:GLN:CA	2.56	0.48
1:C:64:LEU:HG	1:C:206:MET:HE1	1.96	0.48
1:D:163:MET:CE	2:D:500:POA:H11	2.43	0.48
1:D:262:ILE:C	1:D:263:ILE:HD12	2.39	0.48
1:A:27:ARG:HE	1:A:41:THR:CG2	2.27	0.48
1:C:70:GLN:O	1:C:74:LEU:HD23	2.14	0.48
1:F:262:ILE:C	1:F:263:ILE:HD12	2.38	0.48
1:F:270:ASP:HB3	3:F:707:HOH:O	2.13	0.48
1:H:161:LEU:HB2	1:H:189:THR:HG21	1.95	0.48
1:H:427:GLN:HG3	3:H:606:HOH:O	2.14	0.48
1:B:281:ALA:O	1:B:285:LYS:HB2	2.13	0.48
1:D:172:ILE:HD12	1:D:202:LEU:HD11	1.96	0.48
1:E:243:ALA:HA	1:E:251:GLN:OE1	2.14	0.48
1:B:222:ILE:HG23	1:B:246:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:MET:HE1	2:F:500:POA:H11	1.94	0.48
1:F:244:ALA:O	1:F:247:HIS:CE1	2.66	0.48
1:A:172:ILE:HD12	1:A:202:LEU:HD11	1.94	0.47
1:D:14:PRO:O	1:D:191:LEU:HD12	2.14	0.47
1:H:465:GLU:HB3	1:H:466:GLY:H	1.57	0.47
1:A:122:ARG:NH1	1:H:122:ARG:NH1	2.62	0.47
1:B:83:ARG:HD2	1:B:86:GLU:OE1	2.14	0.47
1:B:122:ARG:CZ	1:C:122:ARG:NE	2.78	0.47
1:F:12:HIS:HE1	3:F:721:HOH:O	1.90	0.47
1:G:238:VAL:HG13	3:G:758:HOH:O	2.13	0.47
1:A:319:ARG:NH2	1:A:327:SER:OG	2.46	0.47
1:C:161:LEU:HB2	1:C:189:THR:HG21	1.96	0.47
1:E:119:MET:O	1:E:122:ARG:CB	2.62	0.47
1:E:287:SER:HA	1:E:330:LEU:CD1	2.44	0.47
1:F:295:LYS:HE2	1:F:385:GLU:HG3	1.96	0.47
1:A:161:LEU:HB2	1:A:189:THR:HG21	1.96	0.47
1:A:163:MET:SD	1:A:233:THR:HG21	2.54	0.47
1:C:172:ILE:HD12	1:C:202:LEU:HD11	1.97	0.47
1:C:50:ALA:CB	1:C:221:MET:HE2	2.38	0.47
1:C:71:LYS:HE3	1:C:71:LYS:HB3	1.75	0.47
1:G:244:ALA:O	1:G:247:HIS:CE1	2.68	0.47
1:H:247:HIS:N	3:H:731:HOH:O	2.48	0.47
1:B:262:ILE:C	1:B:263:ILE:HD12	2.40	0.47
1:D:64:LEU:HG	1:D:206:MET:HE1	1.96	0.47
1:D:85:GLU:OE1	1:D:85:GLU:HA	2.15	0.47
1:D:133:THR:HB	1:D:134:PRO:CD	2.45	0.47
1:E:122:ARG:CZ	1:G:122:ARG:CZ	2.93	0.47
1:F:12:HIS:CE1	1:F:27:ARG:CZ	2.97	0.47
1:F:148:LEU:HD21	1:F:250:ARG:NH2	2.30	0.47
1:H:172:ILE:HD12	1:H:202:LEU:HD13	1.95	0.47
1:H:265:ASN:OD1	1:H:425:ARG:NH2	2.44	0.47
1:E:14:PRO:O	1:E:191:LEU:HD12	2.14	0.47
1:D:254:GLU:C	1:D:255:LEU:HD12	2.39	0.47
1:F:12:HIS:ND1	1:F:27:ARG:NH2	2.62	0.47
1:F:133:THR:HB	1:F:134:PRO:HD2	1.97	0.47
1:A:222:ILE:HD12	1:A:242:ILE:HG23	1.97	0.46
1:A:348:ARG:HH11	1:A:348:ARG:CG	2.09	0.46
1:B:64:LEU:HG	1:B:206:MET:HE1	1.98	0.46
1:C:12:HIS:ND1	1:C:41:THR:HG23	2.26	0.46
1:G:447:ARG:NH1	1:G:453:PHE:CE2	2.82	0.46
1:D:58:ALA:HB1	1:D:226:HIS:HD2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:MET:CE	1:G:121:ILE:HD11	2.46	0.46
1:F:27:ARG:HE	1:F:41:THR:HG23	1.81	0.46
1:G:254:GLU:C	1:G:255:LEU:HD12	2.40	0.46
1:H:85:GLU:OE1	1:H:85:GLU:HA	2.15	0.46
1:E:348:ARG:HH11	1:E:348:ARG:CG	2.01	0.46
1:B:118:GLN:HE22	1:C:70:GLN:CD	2.23	0.46
1:E:122:ARG:NH1	1:G:122:ARG:NH1	2.63	0.46
1:F:247:HIS:CD2	3:F:815:HOH:O	2.67	0.46
1:H:295:LYS:HE2	1:H:385:GLU:HG3	1.96	0.46
1:C:168:VAL:O	1:C:172:ILE:HG12	2.16	0.46
1:D:464:LYS:NZ	3:D:690:HOH:O	2.30	0.46
1:A:247:HIS:HA	3:A:711:HOH:O	2.16	0.46
1:C:236:VAL:HB	1:C:237:PRO:HD3	1.97	0.46
1:E:85:GLU:HA	1:E:85:GLU:OE1	2.15	0.46
1:H:203:PRO:HG2	1:H:206:MET:HE3	1.96	0.46
1:H:262:ILE:C	1:H:263:ILE:HD12	2.41	0.46
1:E:285:LYS:HG3	3:E:746:HOH:O	2.16	0.46
1:H:287:SER:HA	1:H:330:LEU:CD1	2.45	0.46
1:A:40:GLY:HA2	3:A:880:HOH:O	2.16	0.46
1:B:319:ARG:HD3	3:B:781:HOH:O	2.15	0.46
1:D:24:THR:CG2	1:D:43:PRO:CB	2.86	0.46
1:E:64:LEU:HG	1:E:206:MET:HE1	1.97	0.46
1:E:400:ASP:OD2	1:E:425:ARG:CD	2.64	0.46
1:E:448:ILE:HG22	3:E:840:HOH:O	2.03	0.45
1:F:83:ARG:HD2	1:F:86:GLU:OE1	2.17	0.45
1:A:71:LYS:HE3	1:A:71:LYS:HB3	1.72	0.45
1:A:172:ILE:HD13	3:A:661:HOH:O	2.16	0.45
1:B:133:THR:HB	1:B:134:PRO:HD2	1.98	0.45
1:E:58:ALA:HB3	1:E:226:HIS:CD2	2.46	0.45
1:C:158:ASN:OD1	1:C:289:GLN:O	2.34	0.45
1:D:295:LYS:HE2	1:D:385:GLU:HG3	1.97	0.45
1:G:253:LEU:HB3	1:G:255:LEU:HD11	1.97	0.45
1:H:70:GLN:HG3	1:H:74:LEU:CD2	2.46	0.45
1:H:143:THR:CG2	1:H:477:VAL:HG13	2.46	0.45
1:D:374:ARG:NE	3:D:837:HOH:O	2.28	0.45
1:G:400:ASP:OD2	1:G:425:ARG:HD3	2.16	0.45
1:D:14:PRO:O	1:D:191:LEU:CD1	2.65	0.45
1:G:262:ILE:C	1:G:263:ILE:HD12	2.42	0.45
1:E:210:VAL:HG21	1:E:221:MET:HE3	1.99	0.45
1:F:143:THR:CG2	1:F:477:VAL:HG13	2.47	0.45
1:H:253:LEU:HB3	1:H:255:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:HIS:HB2	1:B:163:MET:CG	2.43	0.45
1:B:168:VAL:O	1:B:172:ILE:HG12	2.15	0.45
1:B:255:LEU:N	1:B:255:LEU:CD1	2.79	0.45
1:G:158:ASN:ND2	3:G:639:HOH:O	2.50	0.45
1:A:27:ARG:NE	1:A:41:THR:HG23	2.32	0.45
1:A:222:ILE:CD1	1:A:242:ILE:HG12	2.47	0.45
1:E:129:SER:N	3:E:750:HOH:O	2.40	0.45
1:F:64:LEU:HG	1:F:206:MET:HE1	1.99	0.45
1:G:133:THR:HB	1:G:134:PRO:HD2	1.98	0.45
1:A:144:MET:HE1	3:F:627:HOH:O	2.17	0.45
1:B:222:ILE:HD12	1:B:242:ILE:HG12	1.99	0.45
1:B:243:ALA:HA	1:B:251:GLN:OE1	2.17	0.45
1:B:263:ILE:CD1	1:B:263:ILE:N	2.80	0.45
1:D:148:LEU:CD2	1:D:250:ARG:HH22	2.30	0.45
1:A:50:ALA:CB	1:A:221:MET:HE2	2.39	0.45
1:A:133:THR:HB	1:A:134:PRO:CD	2.47	0.45
1:C:143:THR:CG2	1:C:477:VAL:HG13	2.47	0.45
1:D:143:THR:CG2	1:D:477:VAL:HG13	2.47	0.45
1:F:263:ILE:HD12	1:F:263:ILE:N	2.32	0.45
1:F:326:ARG:HG2	1:F:326:ARG:HH11	1.82	0.45
1:A:423:TYR:HB3	1:F:426:MET:HE1	1.99	0.44
1:B:387:PHE:N	3:B:683:HOH:O	2.43	0.44
1:D:319:ARG:NH2	1:D:327:SER:OG	2.50	0.44
1:F:14:PRO:O	1:F:191:LEU:CD1	2.65	0.44
1:H:12:HIS:CE1	1:H:41:THR:HG21	2.51	0.44
1:H:25:ASP:OD2	3:H:769:HOH:O	2.21	0.44
1:C:243:ALA:HA	1:C:251:GLN:OE1	2.16	0.44
1:C:254:GLU:C	1:C:255:LEU:HD12	2.41	0.44
1:F:71:LYS:HE3	1:F:71:LYS:HB3	1.67	0.44
1:F:88:SER:HB2	1:F:102:SER:OG	2.18	0.44
1:F:161:LEU:HB2	1:F:189:THR:HG21	2.00	0.44
1:F:254:GLU:C	1:F:255:LEU:HD12	2.43	0.44
1:H:263:ILE:HD12	1:H:263:ILE:N	2.32	0.44
1:B:377:HIS:HA	1:B:382:VAL:HG21	2.00	0.44
1:B:406:LEU:HD12	1:B:406:LEU:HA	1.78	0.44
1:C:13:GLU:HA	1:C:14:PRO:HD3	1.91	0.44
1:H:143:THR:HG22	1:H:144:MET:N	2.33	0.44
1:B:400:ASP:OD2	1:B:425:ARG:HD3	2.15	0.44
1:C:182:PRO:HD2	1:C:210:VAL:O	2.18	0.44
1:C:465:GLU:HB3	1:C:466:GLY:H	1.60	0.44
1:D:348:ARG:HG3	1:D:348:ARG:NH1	2.13	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:254:GLU:C	1:H:255:LEU:HD12	2.42	0.44
1:A:64:LEU:HG	1:A:206:MET:HE1	2.00	0.44
1:A:423:TYR:OH	1:H:482:LEU:HB3	2.18	0.44
1:D:377:HIS:HE2	1:D:406:LEU:CD1	2.30	0.44
1:E:24:THR:CG2	1:E:43:PRO:CB	2.85	0.44
1:G:83:ARG:HD2	1:G:86:GLU:OE1	2.18	0.44
1:A:143:THR:CG2	1:A:477:VAL:HG13	2.48	0.44
1:B:181:LYS:HD2	1:B:217:ILE:HG23	2.00	0.44
1:B:380:ASP:O	1:B:384:GLU:HB2	2.18	0.44
1:C:287:SER:HA	1:C:330:LEU:CD1	2.47	0.44
1:H:203:PRO:HA	1:H:204:PRO:HD3	1.89	0.44
1:G:85:GLU:HA	1:G:85:GLU:OE1	2.18	0.44
1:G:341:LEU:O	1:G:344:GLU:HB2	2.18	0.44
1:H:27:ARG:HH21	1:H:41:THR:CG2	2.30	0.44
1:H:263:ILE:N	1:H:263:ILE:CD1	2.81	0.44
1:B:464:LYS:HE2	3:B:798:HOH:O	2.18	0.44
1:C:277:ASP:OD1	1:C:314:ARG:HD3	2.17	0.44
1:G:50:ALA:CB	1:G:221:MET:HE2	2.38	0.44
1:D:121:ILE:HD11	1:F:119:MET:CE	2.48	0.43
1:D:203:PRO:HA	1:D:204:PRO:HD3	1.85	0.43
2:D:500:POA:O1P	2:D:500:POA:O2	2.35	0.43
1:E:417:GLY:HA2	1:E:439:ASN:O	2.18	0.43
1:G:465:GLU:HB3	1:G:466:GLY:H	1.70	0.43
1:H:119:MET:O	1:H:122:ARG:HB2	2.17	0.43
1:A:27:ARG:NH2	1:A:41:THR:HG23	2.28	0.43
1:D:168:VAL:O	1:D:172:ILE:HG12	2.17	0.43
1:G:12:HIS:CE1	1:G:27:ARG:CZ	3.01	0.43
1:A:263:ILE:N	1:A:263:ILE:CD1	2.81	0.43
1:B:122:ARG:NE	1:C:122:ARG:CZ	2.81	0.43
1:F:62:PRO:CG	1:F:206:MET:HE2	2.46	0.43
1:G:168:VAL:O	1:G:172:ILE:HG12	2.17	0.43
1:G:350:ALA:HA	1:G:354:ALA:HB3	2.00	0.43
1:H:99:LYS:CE	3:H:615:HOH:O	2.66	0.43
1:H:446:TYR:CD2	1:H:446:TYR:C	2.96	0.43
1:A:12:HIS:HE2	1:C:85:GLU:CG	2.28	0.43
1:B:122:ARG:CD	1:C:122:ARG:NH2	2.81	0.43
1:F:424:ARG:HD3	3:F:703:HOH:O	2.19	0.43
1:G:287:SER:HA	1:G:330:LEU:CD1	2.49	0.43
1:A:143:THR:HG22	1:A:477:VAL:HG13	2.00	0.43
1:A:236:VAL:HB	1:A:237:PRO:HD3	2.00	0.43
1:A:343:GLU:OE2	3:A:863:HOH:O	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:ILE:C	1:C:263:ILE:HD12	2.43	0.43
1:H:181:LYS:HD2	1:H:217:ILE:HG23	2.01	0.43
1:A:377:HIS:HA	1:A:382:VAL:HG21	2.01	0.43
1:B:421:ASN:CB	3:B:657:HOH:O	2.46	0.43
1:C:181:LYS:HE2	3:C:624:HOH:O	2.18	0.43
1:E:128:PHE:HB2	1:E:141:ILE:HB	2.01	0.43
1:E:267:LEU:HD21	1:E:420:THR:HA	2.00	0.43
1:A:244:ALA:HB1	1:E:21:LEU:HB2	2.01	0.43
1:B:54:PHE:CE1	1:B:179:VAL:HB	2.54	0.43
1:G:161:LEU:HB2	1:G:189:THR:HG21	1.99	0.43
1:F:114:THR:O	1:F:118:GLN:HG3	2.19	0.43
1:F:148:LEU:HD22	1:F:250:ARG:NH2	2.34	0.43
1:F:263:ILE:N	1:F:263:ILE:CD1	2.81	0.43
1:G:54:PHE:CE1	1:G:179:VAL:HB	2.54	0.43
1:A:14:PRO:O	1:A:191:LEU:CD1	2.67	0.43
1:C:148:LEU:CD2	1:C:250:ARG:HH22	2.31	0.43
1:F:287:SER:HA	1:F:330:LEU:CD1	2.49	0.43
1:G:265:ASN:OD1	1:G:425:ARG:NH2	2.43	0.43
1:A:181:LYS:HD2	1:A:217:ILE:HG23	2.00	0.43
1:A:243:ALA:HA	1:A:251:GLN:OE1	2.19	0.43
1:B:62:PRO:CG	1:B:206:MET:HE2	2.48	0.43
1:B:70:GLN:HG3	1:B:74:LEU:HD23	2.01	0.43
1:B:320:PHE:HA	1:B:330:LEU:O	2.18	0.43
1:C:378:GLN:OE1	1:C:378:GLN:CA	2.66	0.43
1:E:12:HIS:CE1	1:E:27:ARG:HH21	2.35	0.43
1:E:88:SER:HB2	1:E:102:SER:OG	2.19	0.43
1:F:400:ASP:OD2	1:F:425:ARG:HD3	2.17	0.43
1:G:260:PRO:HA	1:G:296:ARG:O	2.19	0.43
1:C:181:LYS:HD2	1:C:217:ILE:HG23	2.01	0.42
1:E:181:LYS:HD2	1:E:217:ILE:HG23	2.00	0.42
1:F:320:PHE:HA	1:F:330:LEU:O	2.19	0.42
1:B:203:PRO:HA	1:B:204:PRO:HD3	1.85	0.42
1:D:326:ARG:HG2	1:D:326:ARG:NH1	2.30	0.42
1:D:406:LEU:HA	1:D:406:LEU:HD12	1.80	0.42
1:F:265:ASN:OD1	1:F:425:ARG:NH2	2.48	0.42
1:F:406:LEU:HA	1:F:406:LEU:HD12	1.76	0.42
1:H:27:ARG:NH2	1:H:41:THR:HG23	2.32	0.42
1:H:64:LEU:HG	1:H:206:MET:HE1	2.02	0.42
1:H:255:LEU:N	1:H:255:LEU:CD1	2.81	0.42
1:B:24:THR:CG2	1:B:43:PRO:CB	2.89	0.42
1:D:281:ALA:O	1:D:285:LYS:HG2	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:ILE:HD12	1:E:242:ILE:HG23	2.00	0.42
1:E:236:VAL:HG13	1:E:240:LYS:HE3	2.02	0.42
1:E:465:GLU:HB3	1:E:466:GLY:H	1.68	0.42
1:G:181:LYS:HD2	1:G:217:ILE:HG23	2.01	0.42
1:A:222:ILE:HG23	1:A:246:ALA:HB2	2.01	0.42
1:B:191:LEU:HD22	1:B:209:VAL:HG11	2.01	0.42
1:B:348:ARG:HH11	1:B:348:ARG:CG	1.98	0.42
1:C:263:ILE:HD12	1:C:263:ILE:N	2.33	0.42
1:D:465:GLU:HB3	1:D:466:GLY:H	1.64	0.42
1:E:384:GLU:CG	3:E:807:HOH:O	2.55	0.42
1:A:277:ASP:OD1	1:A:314:ARG:HD3	2.19	0.42
1:E:447:ARG:NH1	1:E:453:PHE:CE2	2.87	0.42
1:H:236:VAL:N	1:H:237:PRO:CD	2.83	0.42
1:A:12:HIS:CE1	1:A:41:THR:HG21	2.53	0.42
1:A:303:VAL:HG12	1:A:306:ARG:NH2	2.35	0.42
1:A:484:TRP:C	3:A:855:HOH:O	2.62	0.42
1:B:263:ILE:HD12	1:B:263:ILE:N	2.35	0.42
1:B:411:ALA:O	1:B:458:ASP:HB2	2.18	0.42
1:D:223:THR:CG2	1:E:20:ARG:NH2	2.82	0.42
1:D:263:ILE:N	1:D:263:ILE:CD1	2.83	0.42
1:B:70:GLN:CD	1:C:118:GLN:HE22	2.28	0.42
1:C:85:GLU:CD	1:C:326:ARG:HH22	2.27	0.42
3:D:664:HOH:O	1:H:144:MET:HE1	2.19	0.42
1:D:411:ALA:O	1:D:458:ASP:HB2	2.20	0.42
1:H:246:ALA:C	3:H:731:HOH:O	2.62	0.42
1:B:27:ARG:NH2	1:B:41:THR:HG23	2.32	0.42
1:B:143:THR:CG2	1:B:477:VAL:HG13	2.50	0.42
1:A:203:PRO:HA	1:A:204:PRO:HD3	1.86	0.42
1:A:295:LYS:CE	1:A:385:GLU:HG3	2.49	0.42
1:A:411:ALA:O	1:A:458:ASP:HB2	2.20	0.42
1:E:273:ALA:HB1	1:E:314:ARG:HH11	1.85	0.42
1:G:406:LEU:HD12	1:G:406:LEU:HA	1.83	0.42
1:A:423:TYR:HE1	1:H:482:LEU:HD13	1.85	0.41
1:D:148:LEU:HD22	1:D:250:ARG:NH2	2.35	0.41
1:E:446:TYR:OH	3:E:840:HOH:O	1.62	0.41
1:F:244:ALA:HA	1:H:247:HIS:ND1	2.35	0.41
1:H:236:VAL:HG13	1:H:240:LYS:HE3	2.01	0.41
1:A:12:HIS:HE2	1:C:85:GLU:HG2	1.83	0.41
1:B:119:MET:HE3	1:C:121:ILE:CD1	2.49	0.41
1:F:182:PRO:HD2	1:F:210:VAL:O	2.20	0.41
1:F:310:LEU:CA	3:F:820:HOH:O	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:214:PRO:O	1:H:218:GLY:HA3	2.20	0.41
1:H:380:ASP:O	1:H:384:GLU:HB2	2.20	0.41
1:B:60:TYR:HE2	1:B:206:MET:HE3	1.85	0.41
1:B:348:ARG:HD3	3:B:776:HOH:O	2.19	0.41
1:C:133:THR:HB	1:C:134:PRO:HD2	2.02	0.41
1:C:336:GLU:OE1	3:C:817:HOH:O	2.22	0.41
1:F:137:LYS:HD2	1:H:446:TYR:CE1	2.55	0.41
1:G:143:THR:CG2	1:G:477:VAL:HG13	2.50	0.41
1:H:103:LEU:HD11	3:H:615:HOH:O	2.20	0.41
1:A:423:TYR:CB	1:F:426:MET:HE1	2.50	0.41
1:C:295:LYS:HE2	1:C:385:GLU:HG3	2.02	0.41
1:E:377:HIS:CE1	1:E:406:LEU:HD11	2.55	0.41
1:F:446:TYR:CD2	1:F:446:TYR:C	2.97	0.41
1:H:172:ILE:HD12	1:H:202:LEU:HD11	2.02	0.41
1:A:446:TYR:CE1	1:D:137:LYS:HD2	2.56	0.41
1:D:121:ILE:HD11	1:F:119:MET:HE2	2.02	0.41
1:D:267:LEU:HD21	1:D:420:THR:HA	2.02	0.41
1:E:159:HIS:HB2	1:E:163:MET:CG	2.49	0.41
1:F:203:PRO:HA	1:F:204:PRO:HD3	1.84	0.41
1:G:320:PHE:HA	1:G:330:LEU:O	2.19	0.41
1:H:54:PHE:CE1	1:H:179:VAL:HB	2.56	0.41
1:H:71:LYS:HE3	1:H:71:LYS:HB3	1.65	0.41
1:F:12:HIS:HE1	1:F:27:ARG:NE	2.19	0.41
1:F:380:ASP:O	1:F:384:GLU:HB2	2.20	0.41
1:A:426:MET:HE1	1:F:423:TYR:CB	2.50	0.41
1:E:148:LEU:CD2	1:E:250:ARG:HH22	2.33	0.41
1:G:378:GLN:OE1	1:G:378:GLN:CA	2.66	0.41
1:H:336:GLU:HG3	1:H:364:GLY:CA	2.51	0.41
1:B:128:PHE:HB2	1:B:141:ILE:HB	2.03	0.41
1:D:83:ARG:HD2	1:D:86:GLU:OE1	2.20	0.41
1:E:161:LEU:HB2	1:E:189:THR:HG21	2.03	0.41
1:E:446:TYR:CD2	1:E:446:TYR:C	2.98	0.41
1:G:203:PRO:HG2	1:G:206:MET:HE3	2.02	0.41
1:A:83:ARG:HD2	1:A:86:GLU:OE1	2.21	0.41
1:A:320:PHE:HA	1:A:330:LEU:O	2.21	0.41
1:A:380:ASP:O	1:A:384:GLU:HB2	2.21	0.41
1:B:236:VAL:HG13	1:B:240:LYS:HE3	2.03	0.41
1:B:267:LEU:HD21	1:B:420:THR:HA	2.02	0.41
1:C:172:ILE:HD13	3:C:636:HOH:O	2.20	0.41
1:C:263:ILE:N	1:C:263:ILE:CD1	2.84	0.41
1:D:12:HIS:ND1	1:D:27:ARG:NH2	2.68	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:MET:O	1:F:122:ARG:CB	2.69	0.41
1:F:341:LEU:O	1:F:344:GLU:HB2	2.21	0.41
1:F:424:ARG:CB	3:F:703:HOH:O	2.60	0.41
1:G:133:THR:HB	1:G:134:PRO:CD	2.51	0.41
1:G:159:HIS:HB2	1:G:163:MET:CG	2.47	0.41
1:H:18:ALA:HA	1:H:204:PRO:O	2.21	0.41
1:D:421:ASN:CB	3:H:620:HOH:O	2.51	0.41
1:E:143:THR:CG2	1:E:477:VAL:HG13	2.51	0.41
1:F:310:LEU:HA	3:F:820:HOH:O	2.20	0.41
1:H:168:VAL:O	1:H:172:ILE:HG12	2.21	0.41
1:A:12:HIS:CG	1:C:85:GLU:HB2	2.42	0.40
1:B:335:HIS:CE1	1:B:338:ALA:HB2	2.56	0.40
1:C:273:ALA:HB1	1:C:314:ARG:NH1	2.36	0.40
1:D:159:HIS:HB2	1:D:163:MET:CG	2.48	0.40
1:D:172:ILE:HD13	3:D:613:HOH:O	2.22	0.40
1:E:12:HIS:CE1	1:E:27:ARG:CZ	3.04	0.40
1:E:255:LEU:N	1:E:255:LEU:CD1	2.84	0.40
1:F:378:GLN:CG	3:F:677:HOH:O	2.68	0.40
1:H:335:HIS:ND1	1:H:335:HIS:N	2.68	0.40
1:H:390:ILE:O	1:H:392:PRO:HD3	2.21	0.40
1:D:27:ARG:HH21	1:D:41:THR:CG2	2.31	0.40
1:E:203:PRO:HG2	1:E:206:MET:CE	2.52	0.40
1:B:14:PRO:O	1:B:191:LEU:CD1	2.70	0.40
1:D:12:HIS:CE1	1:D:27:ARG:CZ	3.04	0.40
1:D:181:LYS:HD2	1:D:217:ILE:HG23	2.02	0.40
1:F:163:MET:SD	1:F:233:THR:HG21	2.61	0.40
1:G:148:LEU:HD22	1:G:250:ARG:NH2	2.36	0.40
1:H:128:PHE:HB2	1:H:141:ILE:HB	2.03	0.40
1:B:27:ARG:NH2	3:B:658:HOH:O	2.53	0.40
1:C:281:ALA:O	1:C:285:LYS:HB2	2.22	0.40
1:E:254:GLU:HG3	1:E:465:GLU:OE1	2.21	0.40
1:G:13:GLU:HA	1:G:14:PRO:HD3	1.95	0.40
1:H:16:ARG:HH11	1:H:191:LEU:HD12	1.86	0.40
1:H:159:HIS:HB2	1:H:163:MET:CG	2.46	0.40
1:A:122:ARG:CD	1:H:122:ARG:NH2	2.85	0.40
1:B:326:ARG:HG2	1:B:326:ARG:HH11	1.86	0.40
1:C:24:THR:CG2	1:C:43:PRO:CB	2.90	0.40
1:E:262:ILE:C	1:E:263:ILE:HD12	2.46	0.40
1:G:248:TYR:CD2	3:G:637:HOH:O	2.74	0.40
1:H:400:ASP:OD2	1:H:425:ARG:HD3	2.22	0.40

All (11) 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:D:348:ARG:NH1	1:H:216:ASP:OD2[1_655]	1.18	1.02
1:D:348:ARG:NH1	1:H:216:ASP:CG[1_655]	1.59	0.61
1:A:269:ASP:OD2	1:C:226:HIS:CE1[2_444]	1.98	0.22
1:D:348:ARG:CG	1:H:216:ASP:OD2[1_655]	1.98	0.22
1:D:348:ARG:NH1	1:H:216:ASP:CB[1_655]	2.01	0.19
1:D:352:GLU:OE2	3:H:650:HOH:O[1_655]	2.06	0.14
1:D:344:GLU:OE2	1:H:216:ASP:O[1_655]	2.08	0.12
1:D:348:ARG:CZ	1:H:216:ASP:OD2[1_655]	2.12	0.08
1:D:351:GLU:OE1	1:H:213:TRP:CB[1_655]	2.15	0.05
1:H:215:ALA:N	3:D:666:HOH:O[1_455]	2.17	0.03
1:B:247:HIS:CE1	3:G:749:HOH:O[2_554]	2.18	0.02

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	471/488 (96%)	454 (96%)	15 (3%)	2 (0%)	30	28
1	B	471/488 (96%)	456 (97%)	14 (3%)	1 (0%)	43	44
1	C	471/488 (96%)	456 (97%)	14 (3%)	1 (0%)	43	44
1	D	471/488 (96%)	454 (96%)	15 (3%)	2 (0%)	30	28
1	E	471/488 (96%)	453 (96%)	16 (3%)	2 (0%)	30	28
1	F	471/488 (96%)	455 (97%)	14 (3%)	2 (0%)	30	28
1	G	471/488 (96%)	455 (97%)	15 (3%)	1 (0%)	43	44
1	H	471/488 (96%)	455 (97%)	15 (3%)	1 (0%)	43	44
All	All	3768/3904 (96%)	3638 (96%)	118 (3%)	12 (0%)	36	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	392	PRO
1	C	392	PRO
1	E	392	PRO
1	B	392	PRO
1	D	392	PRO
1	G	392	PRO
1	H	392	PRO
1	D	413	GLY
1	F	392	PRO
1	A	413	GLY
1	F	413	GLY
1	E	413	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	389/401 (97%)	374 (96%)	15 (4%)	28	31
1	B	389/401 (97%)	375 (96%)	14 (4%)	31	34
1	C	389/401 (97%)	375 (96%)	14 (4%)	31	34
1	D	389/401 (97%)	376 (97%)	13 (3%)	33	37
1	E	389/401 (97%)	372 (96%)	17 (4%)	25	26
1	F	389/401 (97%)	375 (96%)	14 (4%)	31	34
1	G	389/401 (97%)	374 (96%)	15 (4%)	28	31
1	H	389/401 (97%)	369 (95%)	20 (5%)	21	21
All	All	3112/3208 (97%)	2990 (96%)	122 (4%)	28	31

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	61	GLN
1	A	74	LEU
1	A	78	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	181	LYS
1	A	191	LEU
1	A	263	ILE
1	A	285	LYS
1	A	314	ARG
1	A	348	ARG
1	A	367	LEU
1	A	377	HIS
1	A	426	MET
1	A	427	GLN
1	A	447	ARG
1	B	12	HIS
1	B	41	THR
1	B	61	GLN
1	B	78	GLU
1	B	122	ARG
1	B	181	LYS
1	B	191	LEU
1	B	263	ILE
1	B	285	LYS
1	B	348	ARG
1	B	372	VAL
1	B	377	HIS
1	B	427	GLN
1	B	447	ARG
1	C	12	HIS
1	C	61	GLN
1	C	78	GLU
1	C	183	THR
1	C	191	LEU
1	C	263	ILE
1	C	285	LYS
1	C	314	ARG
1	C	344	GLU
1	C	348	ARG
1	C	367	LEU
1	C	377	HIS
1	C	427	GLN
1	C	447	ARG
1	D	12	HIS
1	D	24	THR
1	D	41	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	61	GLN
1	D	74	LEU
1	D	78	GLU
1	D	191	LEU
1	D	263	ILE
1	D	344	GLU
1	D	348	ARG
1	D	377	HIS
1	D	427	GLN
1	D	447	ARG
1	E	12	HIS
1	E	20	ARG
1	E	41	THR
1	E	51	ARG
1	E	61	GLN
1	E	74	LEU
1	E	78	GLU
1	E	122	ARG
1	E	183	THR
1	E	191	LEU
1	E	263	ILE
1	E	314	ARG
1	E	344	GLU
1	E	348	ARG
1	E	372	VAL
1	E	377	HIS
1	E	427	GLN
1	F	12	HIS
1	F	20	ARG
1	F	41	THR
1	F	61	GLN
1	F	74	LEU
1	F	78	GLU
1	F	122	ARG
1	F	191	LEU
1	F	263	ILE
1	F	285	LYS
1	F	348	ARG
1	F	377	HIS
1	F	427	GLN
1	F	447	ARG
1	G	12	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	20	ARG
1	G	24	THR
1	G	61	GLN
1	G	74	LEU
1	G	78	GLU
1	G	181	LYS
1	G	191	LEU
1	G	263	ILE
1	G	284	THR
1	G	314	ARG
1	G	348	ARG
1	G	367	LEU
1	G	377	HIS
1	G	427	GLN
1	H	12	HIS
1	H	41	THR
1	H	61	GLN
1	H	74	LEU
1	H	78	GLU
1	H	122	ARG
1	H	144	MET
1	H	181	LYS
1	H	191	LEU
1	H	263	ILE
1	H	285	LYS
1	H	335	HIS
1	H	344	GLU
1	H	348	ARG
1	H	372	VAL
1	H	377	HIS
1	H	424	ARG
1	H	426	MET
1	H	427	GLN
1	H	447	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	HIS
1	A	247	HIS
1	A	427	GLN
1	B	247	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	427	GLN
1	C	226	HIS
1	C	247	HIS
1	C	427	GLN
1	D	226	HIS
1	D	427	GLN
1	E	226	HIS
1	E	247	HIS
1	F	176	ASN
1	F	427	GLN
1	G	158	ASN
1	G	176	ASN
1	G	247	HIS
1	G	377	HIS
1	H	427	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 ⓘ

8 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
2	POA	D	500	1	6,6,6	2.26	4 (66%)	7,8,8	2.49	5 (71%)
2	POA	A	500	1	6,6,6	2.25	3 (50%)	7,8,8	2.31	4 (57%)
2	POA	G	500	1	6,6,6	2.28	3 (50%)	7,8,8	2.22	5 (71%)
2	POA	H	500	1	6,6,6	1.84	3 (50%)	7,8,8	2.54	4 (57%)
2	POA	E	500	1	6,6,6	2.21	3 (50%)	7,8,8	2.74	5 (71%)
2	POA	F	500	1	6,6,6	1.75	1 (16%)	7,8,8	2.81	4 (57%)
2	POA	B	500	1	6,6,6	1.88	2 (33%)	7,8,8	2.67	6 (85%)
2	POA	C	500	1	6,6,6	1.75	1 (16%)	7,8,8	2.23	5 (71%)

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
2	POA	D	500	1	-	0/3/4/4	-
2	POA	A	500	1	-	0/3/4/4	-
2	POA	G	500	1	-	0/3/4/4	-
2	POA	H	500	1	-	0/3/4/4	-
2	POA	E	500	1	-	0/3/4/4	-
2	POA	F	500	1	-	0/3/4/4	-
2	POA	B	500	1	-	0/3/4/4	-
2	POA	C	500	1	-	0/3/4/4	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	500	POA	O2-C2	3.65	1.40	1.20
2	A	500	POA	O2-C2	3.54	1.40	1.20
2	B	500	POA	O2-C2	3.41	1.39	1.20
2	F	500	POA	O2-C2	3.35	1.39	1.20
2	C	500	POA	O2-C2	3.30	1.38	1.20
2	D	500	POA	O2-C2	3.29	1.38	1.20
2	E	500	POA	O2-C2	3.22	1.38	1.20
2	H	500	POA	O2-C2	3.17	1.38	1.20
2	A	500	POA	P-C1	3.12	1.84	1.79
2	G	500	POA	P-C1	2.90	1.84	1.79
2	E	500	POA	P-O2P	-2.83	1.48	1.55
2	E	500	POA	P-O3P	-2.74	1.48	1.55
2	D	500	POA	P-O2P	-2.65	1.49	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	POA	P-O3P	-2.60	1.49	1.55
2	B	500	POA	P-C1	2.41	1.83	1.79
2	G	500	POA	P-O3P	-2.41	1.49	1.55
2	D	500	POA	P-C1	2.37	1.83	1.79
2	A	500	POA	P-O3P	-2.32	1.49	1.55
2	H	500	POA	P-O3P	-2.11	1.50	1.55
2	H	500	POA	P-C1	2.03	1.82	1.79

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	500	POA	O3P-P-C1	3.98	116.63	106.78
2	F	500	POA	O3P-P-O1P	-3.98	102.09	112.39
2	B	500	POA	O3P-P-O1P	-3.82	102.51	112.39
2	E	500	POA	O2P-P-C1	3.72	115.98	106.78
2	H	500	POA	O3P-P-O1P	-3.67	102.91	112.39
2	B	500	POA	O2P-P-C1	3.63	115.74	106.78
2	A	500	POA	O3P-P-C1	3.53	115.51	106.78
2	D	500	POA	P-C1-C2	-3.37	107.29	114.06
2	H	500	POA	O3P-P-C1	3.37	115.11	106.78
2	C	500	POA	O2P-P-C1	3.36	115.09	106.78
2	D	500	POA	O2P-P-C1	3.36	115.07	106.78
2	E	500	POA	O3P-P-O2P	-3.30	98.56	107.96
2	A	500	POA	O2P-P-O1P	-3.25	103.97	112.39
2	E	500	POA	O3P-P-C1	3.25	114.81	106.78
2	E	500	POA	O3P-P-O1P	-3.11	104.35	112.39
2	F	500	POA	O2P-P-O1P	-3.06	104.47	112.39
2	G	500	POA	O3P-P-C1	3.03	114.27	106.78
2	D	500	POA	O2P-P-O1P	-2.68	105.44	112.39
2	G	500	POA	O2P-P-C1	2.66	113.35	106.78
2	C	500	POA	O2P-P-O1P	-2.64	105.57	112.39
2	H	500	POA	O2P-P-O1P	-2.53	105.84	112.39
2	E	500	POA	P-C1-C2	-2.45	109.14	114.06
2	B	500	POA	O3P-P-O2P	-2.43	101.04	107.96
2	A	500	POA	O3P-P-O1P	-2.41	106.14	112.39
2	B	500	POA	O3P-P-C1	2.41	112.74	106.78
2	D	500	POA	O3P-P-C1	2.39	112.69	106.78
2	F	500	POA	P-C1-C2	-2.39	109.27	114.06
2	C	500	POA	O3P-P-C1	2.36	112.61	106.78
2	G	500	POA	O2P-P-O1P	-2.36	106.30	112.39
2	C	500	POA	P-C1-C2	-2.34	109.37	114.06
2	G	500	POA	O3P-P-O1P	-2.31	106.41	112.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	500	POA	P-C1-C2	-2.24	109.57	114.06
2	A	500	POA	O2P-P-C1	2.19	112.20	106.78
2	B	500	POA	O2P-P-O1P	-2.17	106.78	112.39
2	H	500	POA	O2P-P-C1	2.16	112.11	106.78
2	B	500	POA	O1P-P-C1	2.14	116.19	111.30
2	D	500	POA	O3P-P-O1P	-2.10	106.95	112.39
2	C	500	POA	O3P-P-O2P	-2.07	102.06	107.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	POA	2	0
2	A	500	POA	2	0
2	G	500	POA	3	0
2	H	500	POA	1	0
2	E	500	POA	2	0
2	F	500	POA	2	0
2	B	500	POA	2	0
2	C	500	POA	2	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	473/488 (96%)	-0.07	14 (2%)	52	55	13, 20, 38, 56	0
1	B	473/488 (96%)	0.09	19 (4%)	42	44	14, 22, 40, 57	0
1	C	473/488 (96%)	-0.05	11 (2%)	61	64	12, 21, 39, 58	0
1	D	473/488 (96%)	0.09	23 (4%)	35	37	13, 21, 39, 55	0
1	E	473/488 (96%)	0.19	19 (4%)	42	44	13, 21, 40, 58	0
1	F	473/488 (96%)	-0.05	12 (2%)	58	61	14, 22, 40, 58	0
1	G	473/488 (96%)	0.09	17 (3%)	46	48	15, 23, 41, 59	0
1	H	473/488 (96%)	0.21	31 (6%)	24	26	14, 22, 41, 57	0
All	All	3784/3904 (96%)	0.06	146 (3%)	43	45	12, 22, 40, 59	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	HIS	8.1
1	H	216	ASP	6.9
1	E	377	HIS	6.5
1	E	12	HIS	6.4
1	F	12	HIS	5.8
1	D	344	GLU	5.7
1	D	247	HIS	5.0
1	H	215	ALA	4.8
1	H	12	HIS	4.8
1	H	243	ALA	4.8
1	H	214	PRO	4.7
1	D	12	HIS	4.6
1	G	12	HIS	4.6
1	H	244	ALA	4.4
1	D	348	ARG	4.4
1	H	46	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	377	HIS	4.2
1	H	219	MET	4.2
1	G	247	HIS	4.2
1	G	241	LEU	4.2
1	H	241	LEU	4.1
1	G	377	HIS	4.0
1	G	246	ALA	4.0
1	D	241	LEU	3.9
1	D	377	HIS	3.9
1	D	351	GLU	3.9
1	D	248	TYR	3.8
1	H	245	ASN	3.8
1	H	213	TRP	3.7
1	E	122	ARG	3.6
1	E	383	LEU	3.6
1	G	248	TYR	3.6
1	A	247	HIS	3.5
1	F	377	HIS	3.5
1	H	240	LYS	3.5
1	B	247	HIS	3.4
1	D	380	ASP	3.4
1	B	241	LEU	3.4
1	B	377	HIS	3.3
1	H	377	HIS	3.3
1	C	244	ALA	3.3
1	C	12	HIS	3.2
1	H	246	ALA	3.2
1	E	24	THR	3.2
1	A	351	GLU	3.1
1	H	237	PRO	3.1
1	D	285	LYS	3.1
1	G	326	ARG	3.0
1	H	25	ASP	3.0
1	C	122	ARG	3.0
1	B	254	GLU	2.9
1	B	351	GLU	2.9
1	G	245	ASN	2.9
1	D	122	ARG	2.9
1	D	383	LEU	2.9
1	A	241	LEU	2.8
1	G	325	ASP	2.8
1	H	236	VAL	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	242	ILE	2.8
1	H	248	TYR	2.8
1	A	122	ARG	2.8
1	F	248	TYR	2.8
1	G	254	GLU	2.8
1	H	247	HIS	2.8
1	H	360	PRO	2.8
1	F	122	ARG	2.7
1	G	122	ARG	2.7
1	E	344	GLU	2.7
1	B	122	ARG	2.7
1	A	285	LYS	2.7
1	C	243	ALA	2.7
1	D	319	ARG	2.7
1	H	24	THR	2.7
1	A	254	GLU	2.7
1	B	12	HIS	2.7
1	H	238	VAL	2.7
1	D	384	GLU	2.6
1	F	246	ALA	2.6
1	B	383	LEU	2.6
1	A	344	GLU	2.6
1	D	326	ARG	2.6
1	E	384	GLU	2.6
1	C	377	HIS	2.6
1	B	245	ASN	2.6
1	E	241	LEU	2.6
1	E	385	GLU	2.5
1	D	244	ALA	2.5
1	E	348	ARG	2.5
1	D	336	GLU	2.5
1	C	241	LEU	2.5
1	D	378	GLN	2.5
1	C	246	ALA	2.5
1	D	350	ALA	2.5
1	C	222	ILE	2.5
1	A	378	GLN	2.4
1	B	347	MET	2.4
1	D	246	ALA	2.4
1	B	348	ARG	2.4
1	E	254	GLU	2.4
1	F	24	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	24	THR	2.4
1	F	254	GLU	2.4
1	D	24	THR	2.3
1	A	245	ASN	2.3
1	E	245	ASN	2.3
1	E	345	ARG	2.3
1	H	122	ARG	2.3
1	B	240	LYS	2.3
1	H	285	LYS	2.3
1	H	222	ILE	2.3
1	E	134	PRO	2.2
1	G	348	ARG	2.2
1	G	424	ARG	2.2
1	H	26	ASP	2.2
1	E	20	ARG	2.2
1	H	348	ARG	2.2
1	D	245	ASN	2.2
1	D	355	ASP	2.2
1	E	244	ALA	2.2
1	H	254	GLU	2.2
1	E	378	GLN	2.2
1	C	245	ASN	2.2
1	F	25	ASP	2.2
1	G	285	LYS	2.2
1	F	355	ASP	2.2
1	B	256	GLY	2.1
1	B	460	GLY	2.1
1	H	349	ALA	2.1
1	G	20	ARG	2.1
1	F	247	HIS	2.1
1	G	319	ARG	2.1
1	B	363	SER	2.1
1	A	348	ARG	2.1
1	B	285	LYS	2.1
1	E	341	LEU	2.1
1	C	51	ARG	2.1
1	F	27	ARG	2.1
1	H	335	HIS	2.1
1	B	385	GLU	2.0
1	B	255	LEU	2.0
1	F	285	LYS	2.0
1	G	222	ILE	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	421	ASN	2.0
1	C	74	LEU	2.0
1	B	135	HIS	2.0
1	A	143	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	POA	G	500	7/7	0.96	0.07	17,25,31,31	0
2	POA	B	500	7/7	0.98	0.05	14,17,24,26	0
2	POA	C	500	7/7	0.98	0.05	14,16,22,23	0
2	POA	D	500	7/7	0.98	0.06	13,21,26,34	0
2	POA	E	500	7/7	0.98	0.05	18,21,23,27	0
2	POA	F	500	7/7	0.98	0.05	19,21,28,29	0
2	POA	A	500	7/7	0.98	0.05	6,15,17,19	0
2	POA	H	500	7/7	0.98	0.05	18,24,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.