



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:18 AM UTC

PDB ID : 7CE3 / pdb_00007ce3
Title : Crystal structure of human IDH3 holoenzyme in APO form.
Authors : Sun, P.K.; Ding, J.P.
Deposited on : 2020-06-21
Resolution : 3.47 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

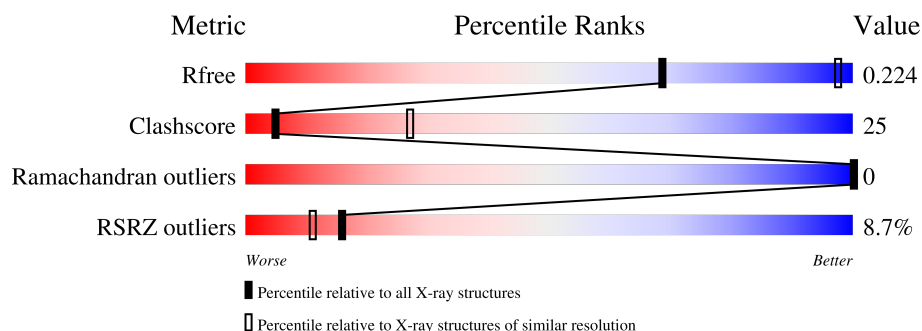
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	366	13% 49% 40% 11%
1	C	366	14% 55% 36% 8%
2	B	357	2% 58% 38%
3	D	359	3% 56% 36% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9853 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 Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	0	0
			2346	1475	403	450	18			
1	C	335	Total	C	N	O	S	0	0	0
			2371	1480	411	461	19			

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	345	Total	C	N	O	S	0	0	0
			2614	1630	476	490	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP P51553
B	-1	GLY	-	expression tag	UNP P51553
B	0	SER	-	expression tag	UNP P51553

- Molecule 3 is a protein called Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	332	Total	C	N	O	S	0	0	0
			2522	1594	439	470	19			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	MET	-	expression tag	UNP O43837
D	-1	GLY	-	expression tag	UNP O43837
D	0	SER	-	expression tag	UNP O43837
D	341	GLU	-	expression tag	UNP O43837
D	342	ILE	-	expression tag	UNP O43837

Continued on next page...

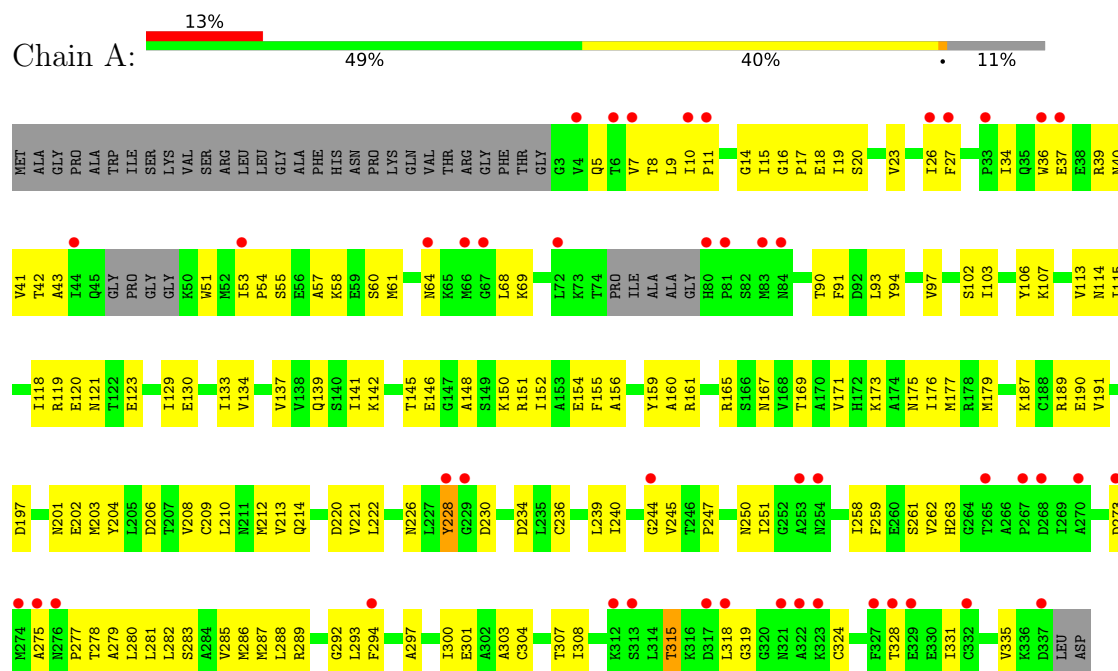
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	343	CYS	-	expression tag	UNP O43837
D	344	ARG	-	expression tag	UNP O43837
D	345	ARG	-	expression tag	UNP O43837
D	346	VAL	-	expression tag	UNP O43837
D	347	LYS	-	expression tag	UNP O43837
D	348	ASP	-	expression tag	UNP O43837
D	349	LEU	-	expression tag	UNP O43837
D	350	ASP	-	expression tag	UNP O43837
D	351	GLU	-	expression tag	UNP O43837
D	352	ASN	-	expression tag	UNP O43837
D	353	LEU	-	expression tag	UNP O43837
D	354	TYR	-	expression tag	UNP O43837
D	355	PHE	-	expression tag	UNP O43837
D	356	GLN	-	expression tag	UNP O43837

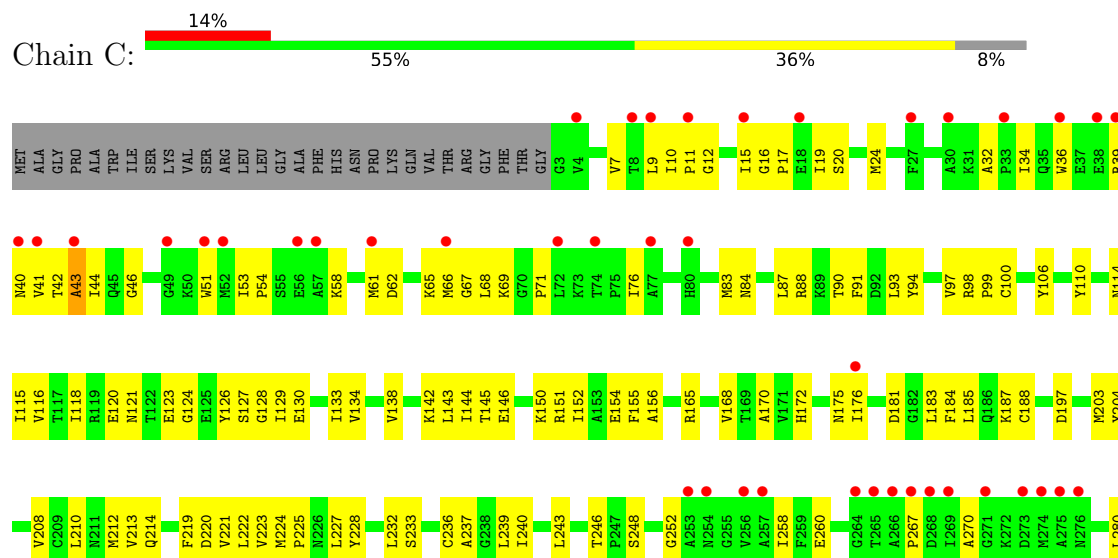
3 Residue-property plots

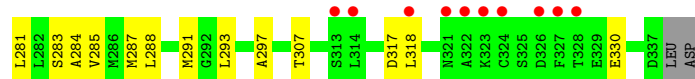
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

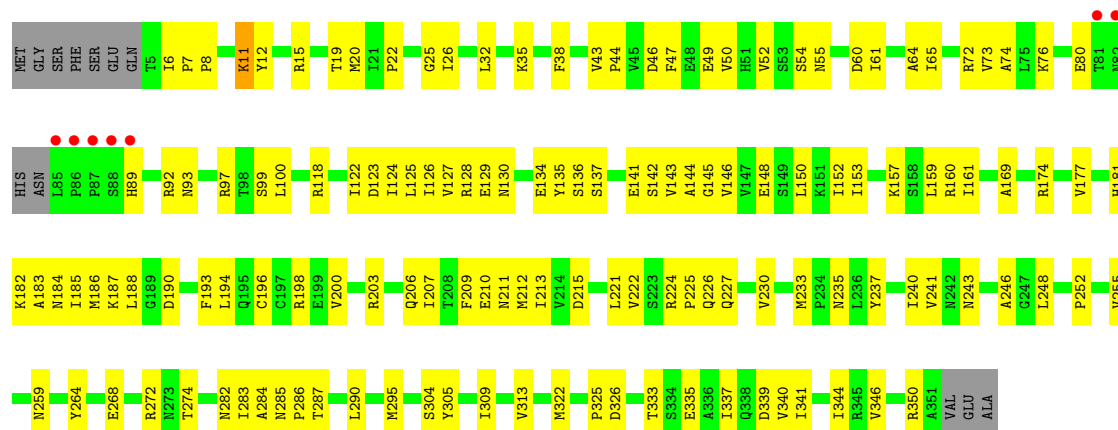


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit alpha, mitochondrial

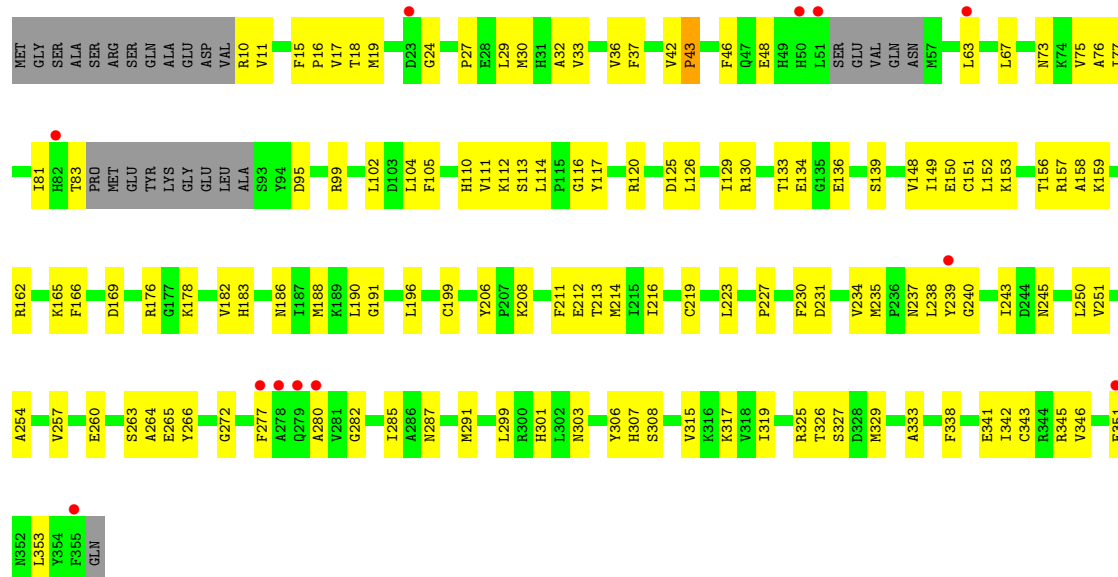




- Molecule 2: Isocitrate dehydrogenase [NAD] subunit gamma, mitochondrial



- Molecule 3: Isocitrate dehydrogenase [NAD] subunit beta, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	204.57Å 204.57Å 237.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.34 – 3.47 46.34 – 3.47	Depositor EDS
% Data completeness (in resolution range)	93.0 (46.34-3.47) 93.2 (46.34-3.47)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.213 , 0.246 (Not available) , 0.224	Depositor DCC
R_{free} test set	1572 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9853	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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 [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	0.59	1/2382 (0.0%)	0.91	4/3236 (0.1%)
1	C	0.54	0/2406	0.83	4/3273 (0.1%)
2	B	0.65	0/2653	0.88	3/3592 (0.1%)
3	D	0.68	2/2565 (0.1%)	0.89	1/3463 (0.0%)
All	All	0.62	3/10006 (0.0%)	0.88	12/13564 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	PRO	C-O	-7.28	1.14	1.24
3	D	308	SER	C-O	-5.31	1.18	1.24
3	D	43	PRO	C-O	-5.01	1.14	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	43	ALA	CB-CA-C	9.37	122.73	109.71
1	A	247	PRO	CB-CA-C	-7.01	100.00	111.56
1	C	43	ALA	N-CA-C	-6.80	100.49	110.42
1	C	44	ILE	N-CA-C	-6.54	98.20	108.86
2	B	11	LYS	CB-CA-C	-5.71	101.54	110.74
1	A	315	THR	CA-C-N	5.53	129.12	120.82
1	A	315	THR	C-N-CA	5.53	129.12	120.82
2	B	89	HIS	CB-CA-C	-5.53	109.21	115.79
1	A	228	TYR	N-CA-C	-5.37	106.78	113.38
1	C	100	CYS	N-CA-CB	5.12	118.88	110.90
3	D	43	PRO	N-CA-CB	-5.06	99.04	102.73
2	B	295	MET	CB-CG-SD	-5.05	97.56	112.70

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	2346	0	2220	147	0
1	C	2371	0	2214	138	0
2	B	2614	0	2625	120	1
3	D	2522	0	2475	132	1
All	All	9853	0	9534	489	1

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 25.

All (489) 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:228:TYR:OH	2:B:134:GLU:OE2	1.72	1.05
1:C:61:MET:SD	1:C:67:GLY:HA3	1.97	1.04
1:A:102:SER:HA	1:A:240:ILE:HG22	1.41	1.03
2:B:181:HIS:HD2	2:B:194:LEU:HD23	1.32	0.95
3:D:63:LEU:O	3:D:67:LEU:HD12	1.67	0.94
3:D:42:VAL:HG12	3:D:307:HIS:CD2	2.02	0.93
1:A:68:LEU:HD12	1:A:287:MET:HE1	1.51	0.93
1:A:228:TYR:OH	2:B:134:GLU:CD	2.12	0.92
2:B:285:ASN:OD1	2:B:287:THR:HG22	1.71	0.88
1:C:61:MET:SD	1:C:67:GLY:CA	2.61	0.88
1:C:114:ASN:OD1	1:C:165:ARG:NH2	2.08	0.87
1:A:226:ASN:O	1:A:226:ASN:ND2	2.07	0.86
1:C:69:LYS:O	1:C:280:LEU:HD11	1.76	0.86
3:D:19:MET:HE3	3:D:46:PHE:CD2	2.12	0.84
3:D:214:MET:HG2	3:D:219:CYS:HB2	1.58	0.84
3:D:42:VAL:HG12	3:D:307:HIS:HD2	1.39	0.84
1:A:102:SER:CA	1:A:240:ILE:HG22	2.09	0.83
1:C:68:LEU:CD1	1:C:284:ALA:HB2	2.09	0.81
1:C:69:LYS:NZ	1:C:84:ASN:OD1	2.13	0.81
1:C:67:GLY:O	1:C:258:ILE:HA	1.80	0.81
1:A:102:SER:HA	1:A:240:ILE:CG2	2.11	0.80
1:A:39:ARG:HG3	1:A:57:ALA:HA	1.65	0.79
3:D:117:TYR:CE2	3:D:329:MET:HG2	2.17	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:GLU:HB3	2:B:274:THR:HG21	1.65	0.79
2:B:181:HIS:CD2	2:B:194:LEU:HD23	2.19	0.78
3:D:42:VAL:CG1	3:D:307:HIS:HD2	1.96	0.78
3:D:63:LEU:O	3:D:67:LEU:CD1	2.32	0.77
1:A:273:ASP:O	1:A:324:CYS:N	2.15	0.77
1:A:294:PHE:O	1:A:297:ALA:HB3	1.85	0.76
1:C:66:MET:SD	1:C:66:MET:N	2.59	0.76
2:B:26:ILE:HD12	2:B:284:ALA:HB1	1.69	0.75
2:B:123:ASP:OD1	2:B:174:ARG:NH2	2.20	0.75
2:B:159:LEU:HD22	2:B:196:CYS:HB3	1.69	0.75
1:A:150:LYS:HB2	1:A:187:LYS:HD2	1.69	0.74
1:A:289:ARG:NH2	1:A:301:GLU:OE2	2.20	0.74
3:D:19:MET:HE3	3:D:46:PHE:HD2	1.52	0.74
1:A:68:LEU:HD23	1:A:69:LYS:H	1.53	0.73
2:B:55:ASN:OD1	2:B:92:ARG:CZ	2.37	0.73
3:D:319:ILE:HD12	3:D:329:MET:HE1	1.69	0.73
2:B:322:MET:HE2	2:B:335:GLU:HB3	1.71	0.72
1:C:93:LEU:HD21	1:C:258:ILE:HG13	1.72	0.72
3:D:235:MET:HE1	3:D:243:ILE:HD12	1.71	0.72
1:C:9:LEU:HD13	1:C:24:MET:HE3	1.72	0.71
1:C:150:LYS:HB2	1:C:187:LYS:HD3	1.73	0.71
1:A:106:TYR:CE2	1:A:318:LEU:HD22	2.26	0.71
1:A:103:ILE:HD11	1:A:245:VAL:HG21	1.72	0.71
3:D:151:CYS:O	3:D:152:LEU:HD23	1.91	0.70
3:D:10:ARG:HG3	3:D:11:VAL:HG23	1.74	0.70
1:A:142:LYS:NZ	2:B:186:MET:HE2	2.06	0.70
1:A:123:GLU:OE1	1:A:145:THR:N	2.25	0.70
3:D:125:ASP:OD1	3:D:176:ARG:NH2	2.23	0.69
1:C:240:ILE:HD11	1:C:246:THR:HG22	1.73	0.69
1:C:146:GLU:HG3	1:C:187:LYS:HD2	1.73	0.69
1:A:303:ALA:O	1:A:307:THR:OG1	2.11	0.68
1:C:106:TYR:HE2	1:C:318:LEU:HD22	1.57	0.68
1:A:213:VAL:HG11	2:B:248:LEU:HD12	1.76	0.68
1:C:184:PHE:CE2	1:C:225:PRO:HD3	2.29	0.68
1:A:307:THR:HG21	1:A:331:ILE:CG1	2.24	0.68
1:C:83:MET:O	1:C:84:ASN:C	2.35	0.68
1:A:41:VAL:HG23	1:A:53:ILE:HB	1.75	0.67
2:B:233:MET:HE1	2:B:241:VAL:HG11	1.76	0.67
3:D:111:VAL:HG22	3:D:126:LEU:HB2	1.78	0.66
3:D:32:ALA:O	3:D:36:VAL:HG23	1.95	0.66
1:A:94:TYR:HE2	1:A:151:ARG:HG2	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:TYR:CE2	1:A:151:ARG:HG2	2.30	0.66
1:A:150:LYS:NZ	1:A:154:GLU:OE2	2.28	0.66
3:D:130:ARG:HD2	3:D:240:GLY:HA3	1.77	0.66
1:A:173:LYS:NZ	1:A:206:ASP:OD1	2.29	0.66
1:C:307:THR:HG23	1:C:330:GLU:HG2	1.76	0.66
1:A:16:GLY:O	1:A:20:SER:OG	2.11	0.65
3:D:176:ARG:HD2	3:D:231:ASP:OD1	1.96	0.65
1:A:9:LEU:HD13	1:A:68:LEU:HB3	1.78	0.65
3:D:111:VAL:CG2	3:D:126:LEU:HB2	2.27	0.65
2:B:206:GLN:HG2	2:B:207:ILE:HD12	1.79	0.65
3:D:117:TYR:CD2	3:D:329:MET:HE3	2.32	0.65
2:B:268:GLU:OE2	2:B:272:ARG:NH1	2.31	0.64
1:A:288:LEU:HD11	1:A:300:ILE:HD12	1.79	0.64
1:C:68:LEU:HD23	1:C:68:LEU:C	2.22	0.64
1:A:304:CYS:O	1:A:308:ILE:HG13	1.96	0.64
2:B:237:TYR:O	2:B:240:ILE:HG12	1.97	0.64
1:A:141:ILE:HG12	2:B:150:LEU:HD12	1.78	0.64
1:C:88:ARG:HA	1:C:93:LEU:HD13	1.78	0.64
2:B:226:GLN:H	2:B:226:GLN:CD	2.06	0.63
1:C:133:ILE:O	1:C:134:VAL:HG13	1.99	0.63
3:D:81:ILE:O	3:D:83:THR:HG23	1.98	0.63
1:A:203:MET:HE2	1:A:208:VAL:HG23	1.79	0.63
2:B:143:VAL:HG21	3:D:148:VAL:CG2	2.28	0.63
2:B:153:ILE:HD11	2:B:193:PHE:HB2	1.81	0.63
1:A:123:GLU:OE1	1:A:145:THR:OG1	2.14	0.62
1:A:307:THR:HG21	1:A:331:ILE:HG12	1.80	0.62
1:C:98:ARG:CB	1:C:98:ARG:HH11	2.12	0.62
2:B:337:ILE:O	2:B:341:ILE:HG13	1.99	0.62
1:A:278:THR:HG22	1:A:282:LEU:HD12	1.82	0.62
1:C:46:GLY:H	1:C:51:TRP:HA	1.65	0.61
2:B:97:ARG:HD3	2:B:130:ASN:OD1	2.01	0.61
3:D:24:GLY:O	3:D:27:PRO:HD2	2.00	0.61
1:C:69:LYS:HE3	1:C:87:LEU:HD12	1.83	0.61
1:A:93:LEU:HD11	1:A:258:ILE:HD12	1.83	0.60
1:C:9:LEU:HD12	1:C:36:TRP:CE3	2.35	0.60
1:A:288:LEU:HD22	1:A:293:LEU:HD12	1.83	0.60
1:C:130:GLU:OE2	3:D:188:MET:HG3	2.00	0.60
1:A:61:MET:HE1	1:A:91:PHE:CE2	2.36	0.60
3:D:263:SER:HB3	3:D:266:TYR:HB2	1.83	0.60
1:A:119:ARG:NH1	1:A:226:ASN:OD1	2.35	0.59
1:A:133:ILE:HG22	1:A:134:VAL:HG13	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ASN:ND2	1:C:204:TYR:CE1	2.70	0.59
1:C:236:CYS:O	1:C:239:LEU:N	2.35	0.59
1:A:102:SER:CB	1:A:240:ILE:HG22	2.32	0.59
2:B:346:VAL:HG12	2:B:350:ARG:O	2.03	0.59
1:A:187:LYS:NZ	1:A:190:GLU:OE2	2.33	0.59
2:B:283:ILE:HB	2:B:325:PRO:HG2	1.85	0.59
2:B:52:VAL:HG12	2:B:52:VAL:O	2.03	0.59
1:C:42:THR:O	1:C:43:ALA:C	2.46	0.59
2:B:11:LYS:O	2:B:11:LYS:HG2	2.02	0.59
1:C:129:ILE:N	1:C:129:ILE:HD12	2.18	0.59
3:D:165:LYS:HE2	3:D:206:TYR:OH	2.02	0.58
1:C:128:GLY:C	1:C:129:ILE:HD12	2.29	0.58
2:B:143:VAL:HG21	3:D:148:VAL:HG21	1.85	0.58
2:B:38:PHE:CD2	2:B:43:VAL:HG21	2.38	0.58
2:B:224:ARG:O	2:B:227:GLN:HG2	2.03	0.58
1:A:169:THR:HA	1:A:201:ASN:O	2.03	0.58
3:D:102:LEU:HG	3:D:266:TYR:HD2	1.68	0.58
2:B:54:SER:N	2:B:60:ASP:OD2	2.36	0.58
3:D:183:HIS:HD2	3:D:214:MET:O	1.86	0.58
2:B:20:MET:HE3	2:B:47:PHE:CD1	2.38	0.58
2:B:38:PHE:O	2:B:43:VAL:HG22	2.04	0.58
1:C:12:GLY:HA3	1:C:71:PRO:HD2	1.85	0.58
1:C:176:ILE:HG21	3:D:136:GLU:HG2	1.86	0.57
3:D:30:MET:HE1	3:D:77:ILE:HG22	1.85	0.57
1:A:165:ARG:NH1	1:A:220:ASP:OD1	2.37	0.57
2:B:181:HIS:HD2	2:B:194:LEU:CD2	2.10	0.57
1:C:93:LEU:HD12	1:C:93:LEU:H	1.70	0.57
3:D:129:ILE:O	3:D:234:VAL:HA	2.03	0.57
1:A:37:GLU:O	1:A:39:ARG:NH1	2.38	0.57
2:B:127:VAL:HG12	2:B:161:ILE:HD11	1.87	0.57
2:B:322:MET:SD	2:B:339:ASP:OD1	2.61	0.57
1:C:68:LEU:HD23	1:C:68:LEU:O	2.05	0.57
1:C:155:PHE:CD1	1:C:155:PHE:C	2.81	0.57
3:D:99:ARG:HG2	3:D:104:LEU:HD12	1.87	0.57
3:D:63:LEU:HD23	3:D:67:LEU:CD1	2.34	0.57
1:C:98:ARG:HH11	1:C:98:ARG:HB3	1.69	0.57
3:D:37:PHE:CZ	3:D:299:LEU:HD11	2.40	0.57
1:C:123:GLU:HG2	1:C:124:GLY:N	2.20	0.57
1:A:161:ARG:NH1	1:A:197:ASP:OD2	2.35	0.56
1:A:15:ILE:HD12	1:A:275:ALA:HB1	1.87	0.56
1:A:102:SER:HB3	1:A:240:ILE:HG22	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:PHE:N	1:A:259:PHE:HD1	2.02	0.56
2:B:20:MET:O	2:B:22:PRO:HD3	2.05	0.56
1:C:99:PRO:HB3	1:C:116:VAL:HG22	1.87	0.56
1:C:236:CYS:HA	1:C:239:LEU:HD12	1.87	0.56
1:A:189:ARG:HH21	1:A:202:GLU:CD	2.14	0.56
2:B:181:HIS:CD2	2:B:194:LEU:CD2	2.88	0.56
2:B:246:ALA:HA	2:B:255:VAL:HG21	1.88	0.56
2:B:190:ASP:OD2	2:B:237:TYR:OH	2.24	0.56
1:A:68:LEU:HD23	1:A:69:LYS:N	2.18	0.55
1:A:281:LEU:O	1:A:285:VAL:HG23	2.06	0.55
2:B:32:LEU:O	2:B:35:LYS:HB2	2.06	0.55
1:C:98:ARG:HB3	1:C:98:ARG:NH1	2.22	0.55
1:C:9:LEU:HD21	1:C:20:SER:HB3	1.87	0.55
1:A:259:PHE:N	1:A:259:PHE:CD1	2.75	0.55
2:B:221:LEU:O	2:B:225:PRO:HB3	2.07	0.55
1:C:168:VAL:HA	1:C:221:VAL:HG23	1.88	0.55
1:A:288:LEU:HD12	1:A:297:ALA:HA	1.89	0.55
2:B:152:ILE:HG13	1:C:133:ILE:HG23	1.87	0.55
1:C:185:LEU:O	1:C:188:CYS:N	2.35	0.55
1:A:201:ASN:N	1:A:201:ASN:OD1	2.38	0.55
1:C:214:GLN:O	3:D:120:ARG:NH2	2.40	0.55
1:A:169:THR:HG22	1:A:201:ASN:CG	2.31	0.55
1:C:68:LEU:HD11	1:C:284:ALA:HB2	1.87	0.54
3:D:287:ASN:ND2	3:D:329:MET:SD	2.81	0.54
2:B:286:PRO:HB2	2:B:290:LEU:HD12	1.90	0.54
1:C:93:LEU:HA	1:C:252:GLY:HA2	1.89	0.54
1:A:171:VAL:HG22	1:A:208:VAL:HG21	1.90	0.54
3:D:341:GLU:HG3	3:D:341:GLU:O	2.07	0.54
1:C:210:LEU:HD12	3:D:245:ASN:ND2	2.22	0.53
1:A:179:MET:HE2	2:B:141:GLU:HB2	1.90	0.53
1:C:120:GLU:HB2	1:C:152:ILE:HG21	1.90	0.53
1:C:220:ASP:OD1	1:C:221:VAL:N	2.41	0.53
1:A:114:ASN:OD1	1:A:165:ARG:NH2	2.36	0.53
2:B:203:ARG:HG3	2:B:203:ARG:HH11	1.73	0.53
3:D:18:THR:O	3:D:76:ALA:HA	2.08	0.53
2:B:184:ASN:OD1	2:B:213:ILE:HD12	2.09	0.53
3:D:196:LEU:HD23	3:D:213:THR:HG21	1.91	0.53
1:A:23:VAL:HA	1:A:26:ILE:HG12	1.91	0.53
1:A:176:ILE:HD13	2:B:134:GLU:HB3	1.91	0.53
2:B:184:ASN:ND2	2:B:185:ILE:HG12	2.24	0.53
1:A:228:TYR:OH	2:B:134:GLU:OE1	2.27	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:GLN:CD	2:B:206:GLN:H	2.17	0.52
1:C:97:VAL:HG22	1:C:118:ILE:HG12	1.90	0.52
1:C:168:VAL:HG22	1:C:221:VAL:HG21	1.91	0.52
2:B:177:VAL:HG22	2:B:230:VAL:HB	1.89	0.52
2:B:184:ASN:O	2:B:187:LYS:NZ	2.41	0.52
2:B:55:ASN:OD1	2:B:92:ARG:NH2	2.41	0.52
1:C:110:TYR:CD2	1:C:239:LEU:HD23	2.44	0.52
2:B:141:GLU:OE1	2:B:144:ALA:HA	2.09	0.52
1:C:98:ARG:HG2	1:C:248:SER:HB2	1.92	0.52
1:A:213:VAL:HG11	2:B:248:LEU:CD1	2.39	0.52
1:A:236:CYS:O	1:A:239:LEU:HB2	2.10	0.52
1:C:15:ILE:HG13	1:C:270:ALA:HB2	1.92	0.52
1:A:209:CYS:SG	2:B:240:ILE:HG23	2.50	0.52
2:B:6:ILE:HG12	2:B:7:PRO:HD2	1.91	0.52
2:B:35:LYS:NZ	2:B:49:GLU:OE1	2.43	0.52
1:C:53:ILE:HD11	1:C:90:THR:HG21	1.90	0.51
1:C:130:GLU:HB3	3:D:190:LEU:HD13	1.93	0.51
1:A:288:LEU:O	1:A:292:GLY:N	2.42	0.51
2:B:157:LYS:HD3	2:B:160:ARG:HH21	1.75	0.51
1:A:210:LEU:HD21	2:B:252:PRO:HD3	1.93	0.51
1:C:94:TYR:CD2	1:C:151:ARG:NH2	2.79	0.51
1:C:121:ASN:O	1:C:121:ASN:ND2	2.37	0.51
3:D:166:PHE:CD1	3:D:166:PHE:C	2.87	0.51
1:A:118:ILE:HG22	1:A:152:ILE:HD11	1.92	0.51
1:A:234:ASP:OD2	2:B:215:ASP:HB3	2.11	0.51
2:B:76:LYS:HG3	2:B:268:GLU:HB3	1.92	0.51
1:C:210:LEU:HD12	3:D:245:ASN:HD22	1.74	0.51
3:D:77:ILE:CG2	3:D:291:MET:HE1	2.41	0.51
1:A:145:THR:HG22	2:B:146:VAL:HG22	1.93	0.51
1:C:34:ILE:HD11	1:C:291:MET:HE1	1.93	0.51
1:A:129:ILE:HG12	1:A:141:ILE:HB	1.93	0.51
1:A:331:ILE:O	1:A:335:VAL:HG23	2.11	0.51
2:B:125:LEU:HD12	2:B:174:ARG:NE	2.26	0.51
1:C:127:SER:O	1:C:129:ILE:HD12	2.11	0.51
3:D:105:PHE:HA	3:D:133:THR:HG23	1.93	0.51
1:A:160:ALA:HA	1:A:165:ARG:HB2	1.93	0.51
2:B:50:VAL:HG11	2:B:64:ALA:HA	1.93	0.51
1:A:27:PHE:CE1	1:A:300:ILE:HD13	2.45	0.51
2:B:25:GLY:HA3	2:B:274:THR:O	2.11	0.50
1:C:168:VAL:HG22	1:C:221:VAL:CG2	2.41	0.50
1:A:129:ILE:HG13	1:A:129:ILE:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:20:MET:HE3	2:B:47:PHE:CG	2.45	0.50
1:C:68:LEU:HD12	1:C:284:ALA:HB2	1.93	0.50
3:D:126:LEU:CD2	3:D:230:PHE:HB2	2.41	0.50
1:A:118:ILE:HD13	1:A:156:ALA:HA	1.93	0.50
1:C:288:LEU:HD22	1:C:293:LEU:HD12	1.92	0.50
1:C:130:GLU:OE2	3:D:188:MET:HA	2.11	0.50
3:D:183:HIS:CG	3:D:196:LEU:HD11	2.46	0.50
1:C:76:ILE:HG13	1:C:76:ILE:O	2.11	0.50
2:B:97:ARG:NH1	2:B:135:TYR:OH	2.45	0.50
1:C:15:ILE:HD12	1:C:15:ILE:H	1.76	0.50
1:C:280:LEU:HA	1:C:283:SER:HB2	1.94	0.50
1:A:53:ILE:HB	1:A:54:PRO:HD2	1.94	0.49
1:A:259:PHE:HD2	1:A:283:SER:O	1.95	0.49
2:B:15:ARG:HA	2:B:44:PRO:HB2	1.94	0.49
3:D:199:CYS:HB3	3:D:211:PHE:CZ	2.47	0.49
1:A:39:ARG:NH2	1:A:60:SER:HB3	2.27	0.49
3:D:301:HIS:C	3:D:303:ASN:H	2.21	0.49
2:B:285:ASN:HB2	2:B:326:ASP:OD1	2.11	0.49
1:C:156:ALA:HB1	1:C:223:VAL:HG11	1.94	0.49
3:D:183:HIS:CB	3:D:196:LEU:HD11	2.42	0.49
3:D:315:VAL:O	3:D:319:ILE:HG12	2.11	0.49
1:A:9:LEU:HD23	1:A:36:TRP:HB3	1.93	0.49
1:A:167:ASN:N	1:A:220:ASP:OD2	2.42	0.49
2:B:19:THR:HB	2:B:74:ALA:HB2	1.94	0.49
3:D:110:HIS:NE2	3:D:260:GLU:OE2	2.45	0.49
1:A:18:GLU:HG2	1:A:324:CYS:SG	2.53	0.49
2:B:194:LEU:HD12	2:B:198:ARG:CZ	2.42	0.49
3:D:42:VAL:CG1	3:D:307:HIS:CD2	2.78	0.49
3:D:126:LEU:HD21	3:D:230:PHE:HB2	1.94	0.49
3:D:277:PHE:CE1	3:D:280:ALA:HB2	2.48	0.49
1:A:97:VAL:HG11	1:A:159:TYR:CE2	2.48	0.49
1:C:219:PHE:HB3	1:C:222:LEU:HD21	1.95	0.49
3:D:102:LEU:HG	3:D:266:TYR:CD2	2.46	0.49
1:A:210:LEU:O	1:A:214:GLN:HG3	2.12	0.49
3:D:338:PHE:O	3:D:342:ILE:HG12	2.13	0.49
1:C:208:VAL:HG11	1:C:232:LEU:HD11	1.96	0.48
1:A:259:PHE:CE2	1:A:287:MET:HA	2.48	0.48
3:D:238:LEU:HD22	3:D:238:LEU:H	1.78	0.48
1:A:142:LYS:HZ2	2:B:186:MET:HE2	1.77	0.48
1:A:318:LEU:N	1:A:318:LEU:HD23	2.29	0.48
2:B:122:ILE:HD13	2:B:248:LEU:HD23	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ASN:O	1:C:54:PRO:HG2	2.14	0.48
3:D:19:MET:HE2	3:D:30:MET:SD	2.54	0.48
2:B:15:ARG:NH2	2:B:46:ASP:OD1	2.46	0.48
1:A:19:ILE:O	1:A:23:VAL:HG23	2.13	0.48
1:C:115:ILE:HD11	1:C:236:CYS:SG	2.53	0.48
1:A:139:GLN:HB2	2:B:152:ILE:CD1	2.43	0.48
1:C:69:LYS:HB3	1:C:260:GLU:HB2	1.96	0.48
1:C:127:SER:O	1:C:129:ILE:CD1	2.61	0.48
3:D:216:ILE:HG12	3:D:239:TYR:HD2	1.79	0.48
3:D:151:CYS:C	3:D:152:LEU:HD23	2.38	0.48
3:D:263:SER:OG	3:D:264:ALA:N	2.47	0.48
3:D:116:GLY:C	3:D:325:ARG:HH22	2.22	0.48
1:A:97:VAL:HG11	1:A:159:TYR:HE2	1.79	0.47
3:D:117:TYR:HD2	3:D:329:MET:HE3	1.75	0.47
1:C:91:PHE:N	1:C:91:PHE:CD1	2.82	0.47
1:C:232:LEU:O	1:C:232:LEU:HD23	2.14	0.47
2:B:309:ILE:O	2:B:313:VAL:HG23	2.13	0.47
1:C:10:ILE:HG22	1:C:11:PRO:HD2	1.96	0.47
1:A:236:CYS:O	1:A:239:LEU:N	2.44	0.47
3:D:105:PHE:CG	3:D:162:ARG:HD3	2.49	0.47
1:A:239:LEU:CD2	2:B:222:VAL:HG21	2.45	0.47
2:B:169:ALA:HB2	2:B:230:VAL:HG21	1.96	0.47
1:C:41:VAL:HA	1:C:54:PRO:HD2	1.97	0.47
3:D:186:ASN:OD1	3:D:186:ASN:N	2.47	0.47
1:A:175:ASN:ND2	1:A:204:TYR:CE1	2.83	0.47
1:C:127:SER:O	1:C:127:SER:OG	2.27	0.47
1:C:156:ALA:HB1	1:C:223:VAL:CG1	2.45	0.47
2:B:183:ALA:HA	2:B:190:ASP:HB2	1.98	0.46
1:A:159:TYR:CD1	1:A:159:TYR:C	2.93	0.46
1:A:315:THR:O	1:A:319:GLY:N	2.48	0.46
3:D:63:LEU:HD23	3:D:67:LEU:HD11	1.97	0.46
1:A:113:VAL:HG13	1:A:115:ILE:HD12	1.98	0.46
1:A:206:ASP:HB3	2:B:243:ASN:HD21	1.81	0.46
1:C:181:ASP:OD2	1:C:228:TYR:OH	2.34	0.46
3:D:17:VAL:HG22	3:D:75:VAL:CG2	2.45	0.46
1:A:261:SER:OG	1:A:263:HIS:NE2	2.48	0.46
2:B:226:GLN:OE1	2:B:226:GLN:N	2.29	0.46
1:C:210:LEU:HB2	3:D:245:ASN:HB3	1.98	0.46
1:C:212:MET:HE1	1:C:232:LEU:HD21	1.97	0.46
1:C:88:ARG:CZ	1:C:126:TYR:HD2	2.28	0.46
3:D:43:PRO:O	3:D:43:PRO:HG2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:17:VAL:HG22	3:D:75:VAL:HG21	1.97	0.46
3:D:95:ASP:OD1	3:D:99:ARG:NH1	2.48	0.46
1:A:43:ALA:HB1	1:A:51:TRP:CE3	2.51	0.46
2:B:129:GLU:O	2:B:235:ASN:HB2	2.16	0.46
3:D:77:ILE:HG23	3:D:291:MET:HE1	1.98	0.46
1:C:19:ILE:HG13	1:C:20:SER:N	2.31	0.45
3:D:112:LYS:HE3	3:D:125:ASP:OD2	2.16	0.45
3:D:237:ASN:C	3:D:237:ASN:HD22	2.22	0.45
2:B:100:LEU:HD22	2:B:264:TYR:CD2	2.51	0.45
1:A:212:MET:HE2	1:A:212:MET:HB2	1.72	0.45
1:A:133:ILE:HB	1:A:137:VAL:HG12	1.99	0.45
1:C:142:LYS:HZ3	3:D:153:LYS:HZ3	1.64	0.45
3:D:277:PHE:CD1	3:D:280:ALA:HB2	2.51	0.45
2:B:282:ASN:ND2	2:B:333:THR:HB	2.31	0.45
1:C:32:ALA:O	1:C:34:ILE:N	2.48	0.45
3:D:30:MET:SD	3:D:291:MET:HE2	2.56	0.45
1:A:280:LEU:HD12	1:A:280:LEU:HA	1.47	0.45
1:C:91:PHE:HB2	1:C:93:LEU:HD11	1.98	0.45
1:C:129:ILE:HG22	1:C:129:ILE:O	2.15	0.45
3:D:351:GLU:OE1	3:D:353:LEU:HB2	2.17	0.45
2:B:340:VAL:O	2:B:344:ILE:HG13	2.16	0.45
3:D:29:LEU:O	3:D:33:VAL:HG23	2.17	0.45
3:D:257:VAL:HG12	3:D:272:GLY:HA3	1.98	0.45
3:D:291:MET:HE3	3:D:291:MET:HB3	1.62	0.45
1:A:324:CYS:O	1:A:328:THR:OG1	2.25	0.45
1:C:16:GLY:N	1:C:17:PRO:HD2	2.32	0.45
3:D:18:THR:HG23	3:D:76:ALA:HB2	1.99	0.45
1:A:262:VAL:HG12	1:A:262:VAL:O	2.17	0.45
2:B:65:ILE:HD13	2:B:99:SER:OG	2.17	0.45
2:B:196:CYS:O	2:B:200:VAL:HG23	2.17	0.45
1:C:69:LYS:HE3	1:C:87:LEU:CD1	2.46	0.45
1:A:177:MET:HE3	1:A:177:MET:HB3	1.84	0.44
1:C:236:CYS:O	1:C:237:ALA:C	2.59	0.44
3:D:16:PRO:O	3:D:73:ASN:HB3	2.17	0.44
1:A:107:LYS:HD2	1:A:107:LYS:HA	1.81	0.44
3:D:317:LYS:O	3:D:317:LYS:HG2	2.18	0.44
1:A:307:THR:CG2	1:A:331:ILE:HG12	2.48	0.44
3:D:113:SER:HA	3:D:251:VAL:HG13	1.98	0.44
1:C:67:GLY:O	1:C:258:ILE:HG23	2.18	0.44
2:B:61:ILE:HD12	2:B:92:ARG:HB3	1.99	0.44
1:C:130:GLU:OE1	3:D:190:LEU:HB2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:GLU:OE1	3:D:191:GLY:N	2.44	0.44
1:C:281:LEU:O	1:C:285:VAL:HG23	2.18	0.44
1:A:60:SER:O	1:A:64:ASN:N	2.41	0.44
1:A:69:LYS:O	1:A:280:LEU:HD11	2.18	0.44
1:A:155:PHE:HE1	1:A:251:ILE:HG21	1.83	0.44
1:C:142:LYS:NZ	3:D:153:LYS:HZ3	2.15	0.44
3:D:134:GLU:HB3	3:D:159:LYS:HD3	2.00	0.44
1:C:61:MET:SD	1:C:67:GLY:N	2.91	0.44
1:A:8:THR:HG22	1:A:9:LEU:H	1.82	0.44
2:B:93:ASN:C	2:B:93:ASN:HD22	2.24	0.44
1:C:145:THR:HG22	3:D:148:VAL:HG22	1.99	0.44
1:C:224:MET:HE3	1:C:224:MET:HB2	1.79	0.44
1:A:187:LYS:O	1:A:191:VAL:HG23	2.18	0.44
3:D:117:TYR:HE2	3:D:329:MET:HG2	1.75	0.44
1:C:144:ILE:HG13	1:C:227:LEU:HD11	2.00	0.43
1:C:267:PRO:HA	1:C:270:ALA:HB3	2.00	0.43
1:A:5:GLN:O	1:A:34:ILE:HA	2.18	0.43
1:A:40:ASN:O	1:A:54:PRO:HG3	2.19	0.43
1:A:113:VAL:HG21	1:A:239:LEU:HB3	2.00	0.43
2:B:304:SER:OG	2:B:305:TYR:N	2.50	0.43
3:D:263:SER:HB3	3:D:266:TYR:H	1.83	0.43
1:A:42:THR:H	1:A:54:PRO:HD3	1.83	0.43
1:C:130:GLU:OE1	3:D:190:LEU:N	2.51	0.43
1:A:10:ILE:HG21	1:A:41:VAL:HG12	2.00	0.43
1:A:90:THR:HG23	1:A:91:PHE:CD1	2.53	0.43
1:A:239:LEU:HD21	2:B:222:VAL:HG21	2.00	0.43
1:A:41:VAL:HA	1:A:54:PRO:HG3	2.00	0.43
3:D:196:LEU:CD2	3:D:213:THR:HG21	2.49	0.43
3:D:315:VAL:HG22	3:D:342:ILE:HD12	2.00	0.43
3:D:317:LYS:HD3	3:D:345:ARG:HD2	2.01	0.43
3:D:325:ARG:O	3:D:333:ALA:HB3	2.19	0.43
1:A:189:ARG:NE	1:A:202:GLU:OE2	2.47	0.43
2:B:8:PRO:HA	2:B:72:ARG:HH21	1.83	0.43
2:B:209:PHE:CG	2:B:210:GLU:N	2.86	0.43
1:C:210:LEU:HD11	3:D:254:ALA:HB2	2.00	0.43
3:D:15:PHE:N	3:D:15:PHE:CD1	2.87	0.43
1:A:130:GLU:OE2	2:B:188:LEU:N	2.52	0.43
2:B:212:MET:HG2	2:B:213:ILE:O	2.19	0.43
1:C:98:ARG:CB	1:C:98:ARG:NH1	2.82	0.43
1:C:154:GLU:O	1:C:155:PHE:C	2.62	0.43
2:B:143:VAL:HG21	3:D:148:VAL:HG22	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:ILE:HA	1:C:220:ASP:HA	1.99	0.42
1:C:183:LEU:HD23	3:D:149:ILE:HG13	2.00	0.42
1:A:11:PRO:HB3	1:A:17:PRO:HA	2.00	0.42
1:C:58:LYS:O	1:C:62:ASP:HB2	2.19	0.42
1:C:172:HIS:CD2	1:C:203:MET:O	2.73	0.42
1:C:210:LEU:O	1:C:214:GLN:HG3	2.19	0.42
3:D:139:SER:O	3:D:139:SER:OG	2.35	0.42
3:D:157:ARG:O	3:D:158:ALA:C	2.59	0.42
1:A:230:ASP:HB2	2:B:215:ASP:OD2	2.19	0.42
2:B:142:SER:HB2	1:C:143:LEU:CD1	2.50	0.42
3:D:114:LEU:HD13	3:D:319:ILE:HG13	2.00	0.42
3:D:206:TYR:CD1	3:D:206:TYR:N	2.87	0.42
2:B:305:TYR:O	2:B:309:ILE:HG13	2.19	0.42
1:C:65:LYS:C	1:C:66:MET:SD	3.02	0.42
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.83	0.42
3:D:211:PHE:O	3:D:212:GLU:HG3	2.19	0.42
1:A:169:THR:OG1	1:A:222:LEU:HD23	2.19	0.42
2:B:182:LYS:HD3	2:B:215:ASP:OD1	2.19	0.42
3:D:287:ASN:OD1	3:D:287:ASN:C	2.63	0.42
1:A:8:THR:HG22	1:A:9:LEU:N	2.35	0.42
1:A:93:LEU:HB3	1:A:250:ASN:HB3	2.01	0.42
1:A:307:THR:HG21	1:A:331:ILE:HG13	1.99	0.42
2:B:210:GLU:HG2	2:B:211:ASN:H	1.83	0.42
1:C:11:PRO:HD3	1:C:39:ARG:O	2.20	0.42
1:C:213:VAL:HG11	3:D:250:LEU:HD23	2.01	0.42
3:D:19:MET:HE3	3:D:46:PHE:CE2	2.52	0.42
1:A:55:SER:HA	1:A:58:LYS:HB3	2.00	0.42
2:B:128:ARG:NH2	2:B:130:ASN:ND2	2.68	0.42
1:C:7:VAL:HG11	1:C:287:MET:SD	2.60	0.42
3:D:15:PHE:HD1	3:D:15:PHE:H	1.68	0.42
3:D:266:TYR:N	3:D:266:TYR:CD1	2.85	0.42
2:B:183:ALA:O	2:B:187:LYS:HA	2.20	0.42
1:C:197:ASP:OD1	1:C:197:ASP:N	2.46	0.42
1:C:317:ASP:O	1:C:318:LEU:HD23	2.20	0.42
3:D:282:GLY:O	3:D:285:ILE:HG12	2.20	0.42
2:B:72:ARG:O	2:B:73:VAL:HG23	2.20	0.42
1:C:155:PHE:C	1:C:155:PHE:HD1	2.27	0.42
1:C:287:MET:HE2	1:C:287:MET:HB3	1.87	0.42
1:A:214:GLN:O	2:B:118:ARG:NH2	2.52	0.41
1:C:116:VAL:N	1:C:220:ASP:O	2.46	0.41
3:D:29:LEU:HD23	3:D:291:MET:HG2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:343:CYS:O	3:D:346:VAL:HG22	2.19	0.41
1:A:41:VAL:HA	1:A:54:PRO:CG	2.49	0.41
1:A:154:GLU:HA	1:A:191:VAL:HG11	2.02	0.41
2:B:136:SER:O	2:B:137:SER:C	2.63	0.41
2:B:183:ALA:HA	2:B:190:ASP:CB	2.50	0.41
1:C:110:TYR:CE2	1:C:239:LEU:HD23	2.56	0.41
3:D:19:MET:O	3:D:48:GLU:HA	2.20	0.41
2:B:135:TYR:N	2:B:135:TYR:CD1	2.89	0.41
1:C:12:GLY:C	1:C:16:GLY:HA3	2.46	0.41
3:D:208:LYS:H	3:D:208:LYS:HG2	1.43	0.41
1:A:123:GLU:CD	1:A:148:ALA:HB3	2.46	0.41
1:A:220:ASP:HB3	1:A:221:VAL:H	1.56	0.41
2:B:148:GLU:OE1	3:D:150:GLU:OE2	2.38	0.41
1:C:76:ILE:O	1:C:76:ILE:CG1	2.69	0.41
3:D:169:ASP:OD1	3:D:206:TYR:OH	2.16	0.41
1:A:14:GLY:C	1:A:16:GLY:H	2.26	0.41
1:A:139:GLN:HB2	2:B:152:ILE:HD13	2.01	0.41
2:B:124:ILE:HG22	2:B:125:LEU:N	2.35	0.41
1:C:138:VAL:HG11	3:D:191:GLY:CA	2.51	0.41
1:A:7:VAL:HG12	1:A:8:THR:O	2.21	0.41
1:A:93:LEU:O	1:A:121:ASN:HB3	2.21	0.41
1:A:94:TYR:CD2	1:A:151:ARG:NH1	2.89	0.41
1:C:24:MET:HG2	1:C:36:TRP:CD1	2.56	0.41
1:C:24:MET:HE2	1:C:36:TRP:CB	2.50	0.41
1:C:170:ALA:HA	1:C:223:VAL:HG22	2.02	0.41
1:C:288:LEU:HB2	1:C:297:ALA:HB2	2.03	0.41
3:D:216:ILE:HG21	3:D:239:TYR:CD2	2.56	0.41
1:A:146:GLU:HB2	2:B:145:GLY:HA2	2.03	0.41
2:B:26:ILE:O	2:B:26:ILE:HG13	2.21	0.41
1:C:184:PHE:CZ	1:C:225:PRO:HD3	2.56	0.41
3:D:235:MET:HE2	3:D:235:MET:HB3	1.77	0.41
3:D:306:TYR:N	3:D:306:TYR:CD1	2.89	0.41
2:B:11:LYS:HA	2:B:15:ARG:O	2.20	0.40
2:B:259:ASN:ND2	2:B:268:GLU:OE1	2.54	0.40
1:C:61:MET:HE1	1:C:67:GLY:N	2.36	0.40
3:D:326:THR:O	3:D:327:SER:C	2.64	0.40
1:A:120:GLU:OE2	1:A:148:ALA:HB1	2.21	0.40
2:B:126:ILE:HD13	2:B:126:ILE:HG21	1.78	0.40
3:D:156:THR:OG1	3:D:159:LYS:HG3	2.21	0.40
3:D:223:LEU:O	3:D:227:PRO:HB3	2.21	0.40
1:A:93:LEU:HD22	1:A:250:ASN:O	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:ASN:C	1:A:115:ILE:HG13	2.46	0.40
1:A:244:GLY:O	1:A:279:ALA:HB2	2.22	0.40
1:A:277:PRO:O	1:A:278:THR:C	2.65	0.40
1:A:286:MET:HE2	1:A:286:MET:HB3	1.95	0.40
2:B:142:SER:HB2	1:C:143:LEU:HD13	2.03	0.40
1:C:98:ARG:HA	1:C:99:PRO:HD3	1.93	0.40
3:D:182:VAL:HB	3:D:235:MET:HE2	2.02	0.40
3:D:265:GLU:HG3	3:D:266:TYR:CD1	2.55	0.40
1:A:23:VAL:O	1:A:27:PHE:HB2	2.21	0.40
1:A:27:PHE:CZ	1:A:288:LEU:HD21	2.56	0.40
2:B:182:LYS:N	2:B:190:ASP:OD2	2.46	0.40
1:C:98:ARG:NH1	1:C:233:SER:OG	2.54	0.40
1:C:150:LYS:HB3	1:C:150:LYS:HE3	1.75	0.40
3:D:18:THR:HG22	3:D:75:VAL:O	2.21	0.40
3:D:178:LYS:O	3:D:231:ASP:HB3	2.21	0.40

All (1) 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)
2:B:12:TYR:OH	3:D:169:ASP:OD2[5_454]	2.00	0.20

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/366 (87%)	260 (81%)	60 (19%)	0	100	100
1	C	333/366 (91%)	281 (84%)	52 (16%)	0	100	100
2	B	341/357 (96%)	306 (90%)	35 (10%)	0	100	100
3	D	326/359 (91%)	284 (87%)	42 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1320/1448 (91%)	1131 (86%)	189 (14%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	326/366 (89%)	0.92	46 (14%) 6 5	22, 72, 133, 151	0
1	C	335/366 (91%)	0.93	52 (15%) 5 5	17, 80, 129, 158	0
2	B	345/357 (96%)	-0.11	7 (2%) 65 40	8, 32, 67, 100	0
3	D	332/359 (92%)	0.10	12 (3%) 46 26	14, 37, 82, 114	0
All	All	1338/1448 (92%)	0.45	117 (8%) 16 11	8, 47, 122, 158	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	ASP	7.8
1	A	327	PHE	6.3
1	C	273	ASP	5.2
1	C	275	ALA	5.1
1	C	266	ALA	4.7
1	C	276	ASN	4.5
1	A	322	ALA	4.4
1	C	18	GLU	4.1
3	D	278	ALA	4.1
1	C	43	ALA	4.0
1	A	275	ALA	3.8
1	C	313	SER	3.7
1	A	337	ASP	3.6
1	A	265	THR	3.6
1	C	265	THR	3.6
1	A	274	MET	3.5
1	A	27	PHE	3.4
1	A	228	TYR	3.4
3	D	82	HIS	3.4
1	C	269	ILE	3.4
1	A	329	GLU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	280	ALA	3.3
1	C	33	PRO	3.3
1	C	326	ASP	3.2
2	B	89	HIS	3.2
1	C	254	ASN	3.2
1	C	41	VAL	3.2
1	C	314	LEU	3.1
1	C	15	ILE	3.1
1	C	176	ILE	3.1
1	A	328	THR	3.1
1	A	244	GLY	3.1
1	A	254	ASN	3.1
1	C	322	ALA	3.1
1	A	83	MET	3.0
1	C	4	VAL	3.0
1	A	80	HIS	2.9
1	A	312	LYS	2.9
1	A	313	SER	2.9
3	D	351	GLU	2.9
2	B	88	SER	2.9
1	C	268	ASP	2.9
2	B	81	THR	2.9
1	A	37	GLU	2.9
2	B	82	ASN	2.9
1	A	4	VAL	2.9
1	A	270	ALA	2.8
2	B	86	PRO	2.8
3	D	51	LEU	2.8
1	C	321	ASN	2.7
1	C	324	CYS	2.7
1	A	276	ASN	2.7
1	A	67	GLY	2.7
1	C	267	PRO	2.7
3	D	279	GLN	2.7
1	C	51	TRP	2.7
2	B	85	LEU	2.7
1	A	321	ASN	2.7
1	A	229	GLY	2.6
1	C	74	THR	2.6
1	C	257	ALA	2.6
1	A	26	ILE	2.6
1	A	332	CYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	264	GLY	2.6
1	C	56	GLU	2.6
1	C	36	TRP	2.6
1	C	274	MET	2.6
1	C	39	ARG	2.6
1	A	66	MET	2.6
1	A	81	PRO	2.6
1	C	77	ALA	2.5
1	A	64	ASN	2.5
1	C	80	HIS	2.5
3	D	239	TYR	2.5
1	C	271	GLY	2.5
1	A	53	ILE	2.5
1	A	36	TRP	2.5
1	A	267	PRO	2.5
1	A	72	LEU	2.5
1	A	11	PRO	2.5
1	A	268	ASP	2.4
1	A	7	VAL	2.4
3	D	277	PHE	2.4
1	C	9	LEU	2.4
3	D	63	LEU	2.4
1	C	328	THR	2.4
1	A	273	ASP	2.4
1	A	6	THR	2.3
1	A	84	ASN	2.3
1	C	49	GLY	2.3
3	D	50	HIS	2.3
1	C	27	PHE	2.3
1	A	10	ILE	2.3
1	C	318	LEU	2.3
1	A	294	PHE	2.3
1	C	38	GLU	2.3
1	C	66	MET	2.3
1	C	8	THR	2.2
1	C	256	VAL	2.2
1	A	253	ALA	2.2
1	C	253	ALA	2.2
1	A	323	LYS	2.2
2	B	87	PRO	2.2
3	D	23	ASP	2.2
1	C	61	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	72	LEU	2.1
1	C	57	ALA	2.1
1	C	327	PHE	2.1
1	A	44	ILE	2.1
3	D	355	PHE	2.1
1	C	40	ASN	2.1
1	C	30	ALA	2.1
1	C	52	MET	2.1
1	A	318	LEU	2.0
1	A	33	PRO	2.0
1	C	11	PRO	2.0
1	C	323	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.