



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:52 AM UTC

PDB ID : 1UMF / pdb_00001umf
Title : crystal structure of chorismate synthase
Authors : Ahn, H.J.; Yoon, H.J.; Lee, B.; Suh, S.W.
Deposited on : 2003-09-30
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

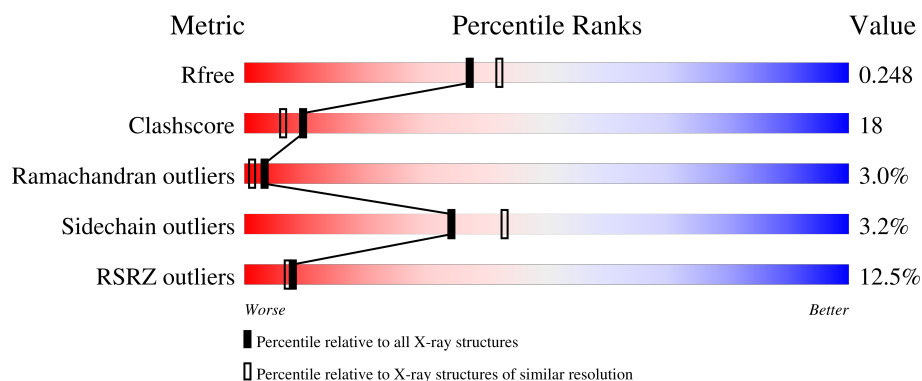
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	365	8% 74% 22% .
1	B	365	16% 68% 28% .
1	C	365	18% 66% 30% .
1	D	365	8% 67% 27% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11756 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 Chorismate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	B	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	C	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			
1	D	365	Total	C	N	O	S	36	0	0
			2816	1768	502	532	14			

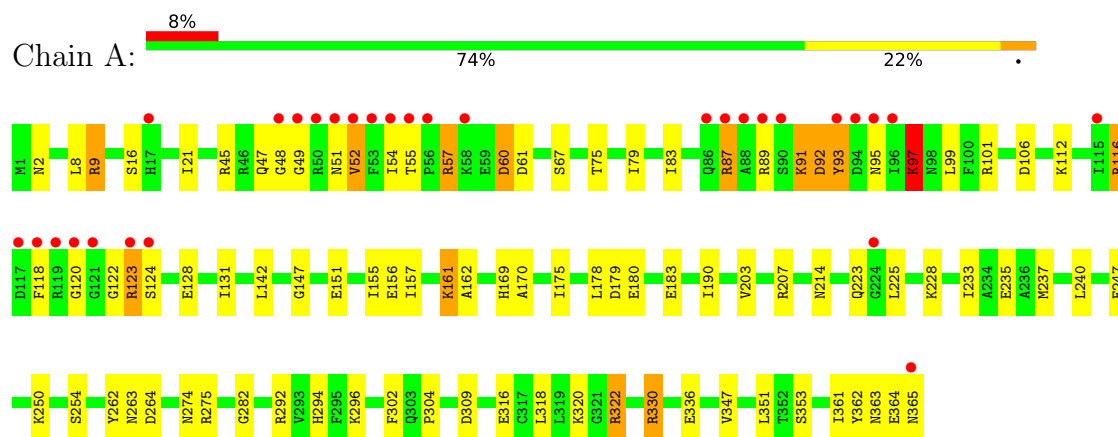
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	173	Total	O	0	0
			173	173		
2	B	82	Total	O	0	0
			82	82		
2	C	90	Total	O	0	0
			90	90		
2	D	147	Total	O	0	0
			147	147		

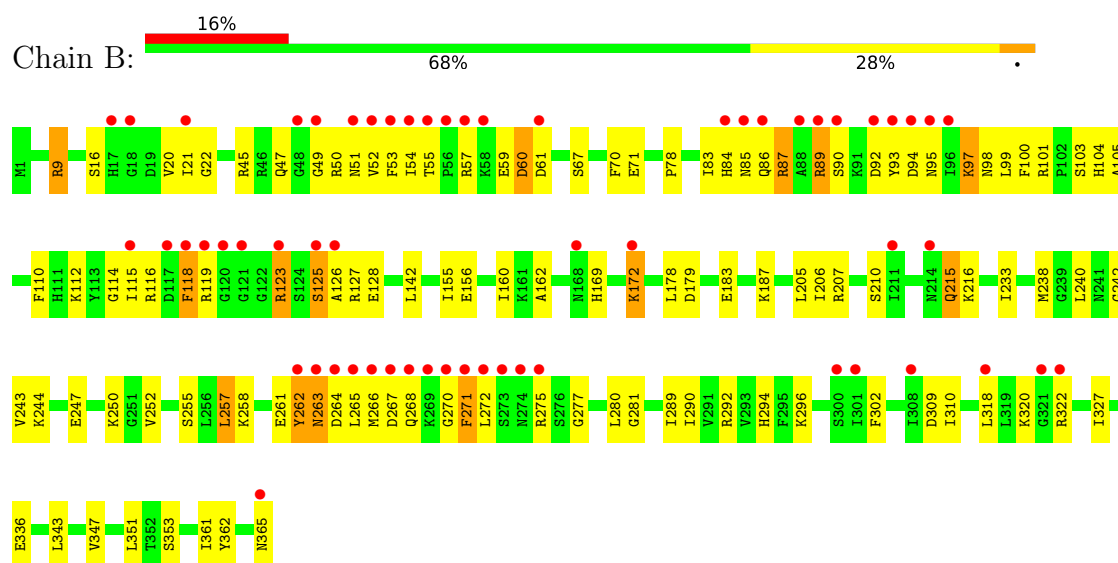
3 Residue-property plots [i](#)

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

• Molecule 1: Chorismate synthase

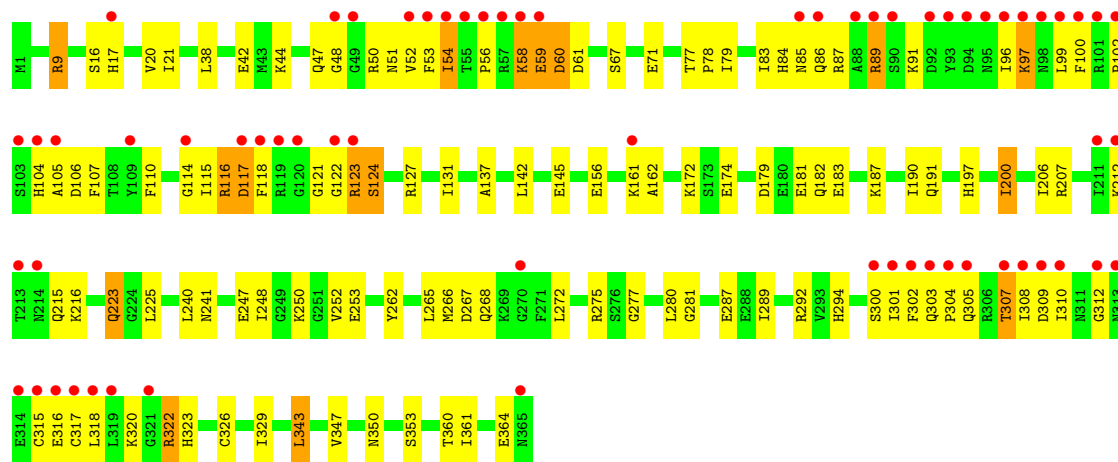


• Molecule 1: Chorismate synthase

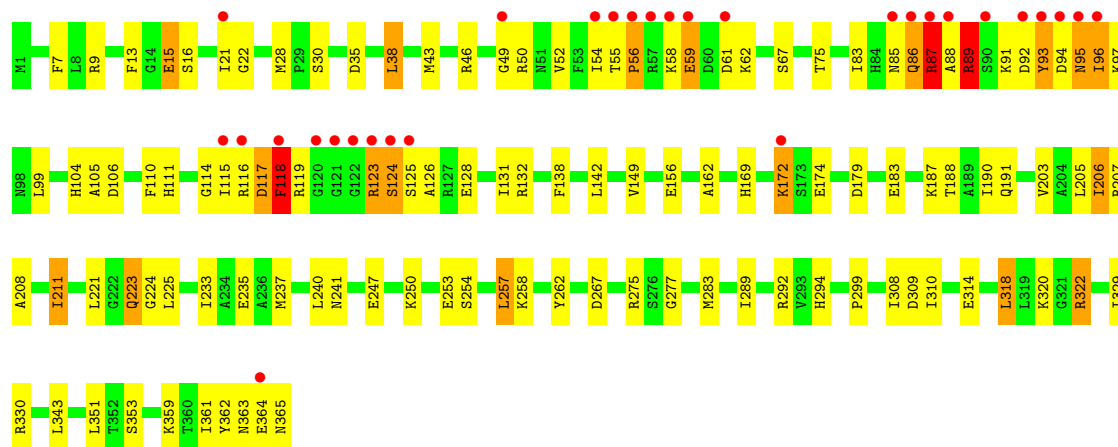


• Molecule 1: Chorismate synthase





• Molecule 1: Chorismate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	146.48Å 146.48Å 132.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.13 – 2.25 21.13 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.5 (21.13-2.25) 98.5 (21.13-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.248 0.202 , 0.248	Depositor DCC
R_{free} test set	6567 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.026 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11756	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2857	0.90	11/3833 (0.3%)
1	B	0.37	0/2857	0.86	6/3833 (0.2%)
1	C	0.38	0/2857	0.87	6/3833 (0.2%)
1	D	0.39	0/2857	0.88	7/3833 (0.2%)
All	All	0.39	0/11428	0.88	30/15332 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	SER	N-CA-C	9.24	120.96	111.07
1	C	353	SER	N-CA-C	8.98	120.68	111.07
1	A	353	SER	N-CA-C	8.29	120.32	111.28
1	D	353	SER	N-CA-C	7.13	119.67	111.11
1	D	211	ILE	N-CA-C	-6.67	106.23	112.83
1	A	223	GLN	N-CA-C	6.60	119.17	108.41
1	A	8	LEU	N-CA-C	-6.52	96.52	107.99
1	C	223	GLN	N-CA-C	6.39	119.20	108.02
1	D	223	GLN	N-CA-C	6.27	118.74	108.52
1	A	161	LYS	N-CA-C	5.93	119.72	110.17
1	B	233	ILE	N-CA-C	-5.86	105.02	110.53
1	A	60	ASP	N-CA-C	5.79	116.72	108.74
1	D	364	GLU	N-CA-C	-5.78	106.56	113.21
1	B	60	ASP	N-CA-C	5.55	117.06	109.18
1	B	9	ARG	N-CA-C	5.47	117.44	108.52
1	C	89	ARG	NE-CZ-NH2	5.32	123.98	119.20
1	C	87	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	89	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	89	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	A	87	ARG	NE-CZ-NH2	5.27	123.95	119.20
1	B	89	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	B	87	ARG	NE-CZ-NH2	5.25	123.93	119.20
1	D	87	ARG	NE-CZ-NH2	5.22	123.90	119.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ASN	N-CA-C	5.21	116.69	110.44
1	A	9	ARG	N-CA-C	5.20	117.00	108.52
1	C	9	ARG	N-CA-C	5.19	116.98	108.52
1	A	214	ASN	N-CA-C	5.07	118.75	112.47
1	D	257	LEU	N-CA-C	5.06	118.27	110.42
1	A	147	GLY	N-CA-C	5.03	122.65	114.90
1	C	60	ASP	N-CA-C	5.02	114.78	108.45

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	2816	0	2852	85	0
1	B	2816	0	2852	111	1
1	C	2816	0	2852	130	6
1	D	2816	0	2852	111	5
2	A	173	0	0	6	0
2	B	82	0	0	4	0
2	C	90	0	0	1	0
2	D	147	0	0	5	0
All	All	11756	0	11408	396	7

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 (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:HIS:HB3	1:C:302:PHE:HB3	1.40	0.99
1:C:307:THR:HG23	1:C:308:ILE:H	1.34	0.92
1:B:47:GLN:HE22	1:B:60:ASP:HB3	1.35	0.89
1:C:102:PRO:HG2	1:C:305:GLN:HB3	1.56	0.88
1:A:322:ARG:HH11	1:A:322:ARG:H	1.21	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:LEU:HD12	1:A:320:LYS:HE3	1.55	0.85
1:D:322:ARG:HB2	1:D:322:ARG:HH11	1.40	0.84
1:D:104:HIS:HB3	1:D:123:ARG:NH2	1.93	0.82
1:D:105:ALA:N	1:D:123:ARG:HH22	1.77	0.82
1:A:128:GLU:HG3	1:D:225:LEU:HD13	1.62	0.81
1:D:322:ARG:HB2	1:D:322:ARG:NH1	1.95	0.81
1:D:105:ALA:H	1:D:123:ARG:HH12	1.29	0.80
1:B:281:GLY:HA3	1:C:105:ALA:HB2	1.64	0.80
1:B:105:ALA:HB3	1:B:123:ARG:HH22	1.49	0.78
1:D:105:ALA:H	1:D:123:ARG:NH1	1.82	0.77
1:D:115:ILE:HD12	1:D:115:ILE:O	1.84	0.77
1:B:250:LYS:HE2	1:B:257:LEU:HD21	1.66	0.76
1:B:67:SER:HB3	1:D:16:SER:HB3	1.66	0.76
1:B:238:MET:HE1	1:B:244:LYS:HA	1.66	0.76
1:C:305:GLN:HB2	1:C:317:CYS:SG	2.25	0.76
1:C:117:ASP:CG	1:C:118:PHE:H	1.93	0.75
1:B:54:ILE:HB	1:B:59:GLU:HG3	1.69	0.75
1:D:21:ILE:HG13	1:D:131:ILE:HD11	1.68	0.75
1:D:123:ARG:HG2	1:D:124:SER:N	2.00	0.74
1:D:169:HIS:CD2	1:D:172:LYS:HE3	2.22	0.74
1:C:322:ARG:H	1:C:322:ARG:HD3	1.53	0.73
1:A:361:ILE:HD11	1:B:361:ILE:HD11	1.69	0.73
1:A:45:ARG:HD2	2:A:491:HOH:O	1.88	0.73
1:C:47:GLN:HE22	1:C:60:ASP:HB2	1.53	0.73
1:B:302:PHE:HE2	1:B:318:LEU:HD11	1.55	0.72
1:B:318:LEU:HD12	1:B:320:LYS:HE3	1.70	0.72
1:C:48:GLY:HA2	1:C:52:VAL:HG21	1.69	0.72
1:D:50:ARG:HD3	1:D:52:VAL:O	1.91	0.71
1:B:169:HIS:HA	1:B:172:LYS:HE3	1.72	0.71
1:A:322:ARG:HB2	1:A:322:ARG:NH1	2.08	0.69
1:D:104:HIS:HB3	1:D:123:ARG:HH22	1.55	0.69
1:D:116:ARG:H	1:D:116:ARG:HD2	1.56	0.69
1:D:247:GLU:OE1	1:D:294:HIS:HE1	1.76	0.69
1:B:320:LYS:H	1:B:320:LYS:HD2	1.58	0.68
1:A:75:THR:HA	1:C:115:ILE:HD12	1.73	0.68
1:A:21:ILE:HG13	1:A:131:ILE:HD11	1.76	0.68
1:B:262:TYR:HD1	1:B:263:ASN:N	1.92	0.68
1:A:302:PHE:HE2	1:A:318:LEU:HD11	1.56	0.68
1:D:97:LYS:HA	2:D:463:HOH:O	1.93	0.68
1:C:97:LYS:HZ2	1:C:97:LYS:HB2	1.59	0.68
1:C:197:HIS:CB	1:C:302:PHE:HB3	2.22	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LYS:H	1:C:320:LYS:HD2	1.58	0.67
1:A:262:TYR:O	1:A:275:ARG:HD3	1.94	0.67
1:A:361:ILE:HD12	1:B:351:LEU:HD22	1.76	0.67
1:C:97:LYS:HB2	1:C:97:LYS:NZ	2.09	0.67
1:C:247:GLU:HB2	1:C:292:ARG:HB2	1.76	0.67
1:C:247:GLU:OE2	1:C:252:VAL:HG22	1.95	0.67
1:C:322:ARG:HB2	1:C:322:ARG:NH1	2.11	0.66
1:D:105:ALA:N	1:D:123:ARG:NH2	2.44	0.66
1:D:116:ARG:HE	1:D:310:ILE:HD12	1.60	0.66
1:B:247:GLU:OE2	1:B:252:VAL:HG22	1.96	0.66
1:A:97:LYS:HB2	1:A:97:LYS:NZ	2.10	0.65
1:B:100:PHE:HB2	1:C:266:MET:HE1	1.77	0.65
1:D:99:LEU:HA	1:D:309:ASP:HA	1.77	0.65
1:B:169:HIS:HE1	1:B:183:GLU:OE2	1.79	0.65
1:C:197:HIS:HB2	1:C:303:GLN:HG3	1.78	0.65
1:D:85:ASN:ND2	1:D:86:GLN:HG3	2.12	0.65
1:B:101:ARG:HG3	1:B:101:ARG:HH11	1.62	0.64
1:C:322:ARG:HD3	1:C:322:ARG:N	2.11	0.64
1:C:361:ILE:HD12	1:D:351:LEU:HD22	1.80	0.64
1:C:21:ILE:HG13	1:C:131:ILE:HD11	1.80	0.64
1:D:162:ALA:HB1	1:D:179:ASP:HB2	1.79	0.64
1:B:128:GLU:HG3	1:C:225:LEU:HD13	1.81	0.63
1:B:206:ILE:HD12	1:B:206:ILE:N	2.13	0.63
1:A:47:GLN:HE22	1:A:60:ASP:CG	2.06	0.63
2:A:501:HOH:O	1:D:258:LYS:HE3	1.99	0.62
1:B:264:ASP:C	1:B:265:LEU:HD12	2.25	0.62
1:C:322:ARG:H	1:C:322:ARG:HH11	1.48	0.62
1:D:206:ILE:HD12	1:D:206:ILE:N	2.14	0.62
1:C:212:LYS:HD3	1:C:215:GLN:HG2	1.82	0.62
1:C:100:PHE:CE2	1:C:310:ILE:HA	2.34	0.61
1:C:308:ILE:HD11	1:C:312:GLY:HA2	1.83	0.61
1:A:330:ARG:HH21	1:A:330:ARG:HB3	1.65	0.61
1:B:262:TYR:CD1	1:B:263:ASN:N	2.68	0.61
1:C:320:LYS:HD2	1:C:320:LYS:N	2.16	0.61
1:C:142:LEU:C	1:C:142:LEU:HD23	2.26	0.61
1:A:322:ARG:HH11	1:A:322:ARG:N	1.96	0.60
1:D:169:HIS:O	1:D:172:LYS:HD3	2.01	0.60
1:D:58:LYS:HG3	1:D:59:GLU:HG2	1.84	0.60
1:C:307:THR:HG23	1:C:308:ILE:N	2.11	0.60
1:C:308:ILE:HG12	1:C:309:ASP:N	2.16	0.60
1:D:190:ILE:HD11	1:D:329:ILE:HD11	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ARG:HH11	1:A:322:ARG:HB2	1.68	0.59
1:D:54:ILE:CG2	1:D:58:LYS:HD2	2.33	0.59
1:D:207:ARG:HG2	1:D:208:ALA:N	2.17	0.59
1:D:318:LEU:HD13	1:D:320:LYS:HE3	1.83	0.59
1:A:123:ARG:HG3	1:A:124:SER:H	1.65	0.59
1:A:45:ARG:HH22	1:A:336:GLU:CD	2.10	0.59
1:A:320:LYS:HD2	1:A:320:LYS:H	1.68	0.59
1:A:225:LEU:HD13	1:D:128:GLU:HG3	1.84	0.58
1:D:169:HIS:HE1	1:D:183:GLU:OE2	1.86	0.58
1:B:16:SER:HB3	1:D:67:SER:HB3	1.84	0.58
1:A:16:SER:HB3	1:C:67:SER:HB3	1.84	0.58
1:D:322:ARG:HH11	1:D:322:ARG:CB	2.16	0.58
1:B:322:ARG:HD3	1:B:322:ARG:N	2.19	0.58
1:C:48:GLY:HA2	1:C:52:VAL:CG2	2.33	0.58
1:D:106:ASP:H	1:D:123:ARG:NH2	2.00	0.58
1:D:361:ILE:O	1:D:365:ASN:HB2	2.04	0.57
1:A:142:LEU:HD23	1:A:142:LEU:C	2.29	0.57
1:B:267:ASP:O	1:B:268:GLN:HG3	2.03	0.57
1:B:118:PHE:O	1:B:119:ARG:HD2	2.05	0.57
1:D:54:ILE:HG22	1:D:58:LYS:HD2	1.87	0.57
1:A:161:LYS:HE2	2:A:409:HOH:O	2.04	0.57
1:B:247:GLU:OE1	1:B:294:HIS:HE1	1.88	0.57
1:C:322:ARG:HB2	1:C:322:ARG:HH11	1.68	0.57
1:D:28:MET:HE2	1:D:138:PHE:HB3	1.87	0.56
1:D:49:GLY:O	1:D:174:GLU:HA	2.05	0.56
1:A:156:GLU:HB2	1:A:203:VAL:HB	1.88	0.56
1:A:169:HIS:HE1	1:A:183:GLU:OE2	1.89	0.56
2:B:433:HOH:O	1:D:115:ILE:HD11	2.06	0.56
1:D:105:ALA:H	1:D:123:ARG:CZ	2.18	0.56
1:C:59:GLU:O	1:C:59:GLU:HG2	2.06	0.56
1:D:116:ARG:HD2	1:D:116:ARG:N	2.20	0.56
1:B:104:HIS:CD2	1:B:123:ARG:HH11	2.24	0.56
1:D:253:GLU:O	1:D:257:LEU:HD13	2.06	0.56
1:C:100:PHE:CZ	1:C:310:ILE:HA	2.41	0.56
1:B:258:LYS:HZ3	1:B:261:GLU:HG3	1.71	0.55
1:D:116:ARG:HG2	1:D:310:ILE:HD13	1.88	0.55
1:A:264:ASP:OD1	1:A:275:ARG:HD2	2.07	0.55
1:A:363:ASN:C	1:A:364:GLU:HG3	2.31	0.55
1:C:304:PRO:HG3	1:C:318:LEU:CD2	2.36	0.55
1:D:247:GLU:HB2	1:D:292:ARG:HB2	1.87	0.55
1:C:162:ALA:HB1	1:C:179:ASP:HB2	1.86	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:NH1	1:A:106:ASP:OD2	2.39	0.55
1:C:206:ILE:N	1:C:206:ILE:HD12	2.21	0.55
1:C:247:GLU:OE1	1:C:294:HIS:HE1	1.88	0.55
1:A:247:GLU:OE1	1:A:294:HIS:HE1	1.90	0.55
1:D:116:ARG:H	1:D:116:ARG:CD	2.18	0.55
1:B:162:ALA:HB1	1:B:179:ASP:HB2	1.89	0.55
1:C:301:ILE:H	1:C:305:GLN:NE2	2.06	0.54
1:A:67:SER:HB3	1:C:16:SER:HB3	1.89	0.54
1:B:205:LEU:C	1:B:206:ILE:HD12	2.33	0.54
1:B:266:MET:HE3	1:C:307:THR:OG1	2.06	0.54
1:C:44:LYS:HE2	1:C:56:PRO:HG2	1.89	0.54
1:C:85:ASN:O	1:C:86:GLN:HB2	2.07	0.54
1:B:97:LYS:HB3	1:B:118:PHE:CE2	2.43	0.54
1:A:162:ALA:HB1	1:A:179:ASP:HB2	1.88	0.54
1:B:115:ILE:HD12	1:D:75:THR:HA	1.90	0.54
1:B:277:GLY:O	1:B:289:ILE:HA	2.08	0.54
1:A:157:ILE:HD13	1:A:190:ILE:HD11	1.89	0.54
1:A:363:ASN:O	1:A:364:GLU:HG3	2.07	0.54
1:B:266:MET:H	1:C:307:THR:HA	1.73	0.53
1:A:51:ASN:OD1	1:A:52:VAL:HG23	2.08	0.53
1:A:99:LEU:HA	1:A:309:ASP:HA	1.90	0.53
1:D:169:HIS:NE2	1:D:172:LYS:HE3	2.22	0.53
1:C:100:PHE:HD1	1:C:106:ASP:HB3	1.73	0.53
1:B:142:LEU:C	1:B:142:LEU:HD23	2.34	0.53
1:A:21:ILE:HG23	1:A:83:ILE:HB	1.90	0.52
1:A:362:TYR:CE2	1:B:347:VAL:HG13	2.45	0.52
1:A:122:GLY:O	1:A:124:SER:N	2.43	0.52
1:C:38:LEU:HD23	1:C:42:GLU:HG2	1.90	0.52
1:C:277:GLY:O	1:C:289:ILE:HA	2.09	0.52
1:C:262:TYR:O	1:C:275:ARG:HD2	2.10	0.52
1:A:351:LEU:HD22	1:B:361:ILE:HD12	1.91	0.52
1:C:360:THR:HG23	1:C:364:GLU:OE1	2.09	0.52
1:A:112:LYS:HZ1	1:D:223:GLN:HE22	1.58	0.52
1:A:250:LYS:HB3	1:A:254:SER:OG	2.10	0.52
1:D:330:ARG:HG3	2:D:392:HOH:O	2.09	0.52
1:C:38:LEU:HD23	1:C:38:LEU:C	2.36	0.51
1:D:320:LYS:HD2	1:D:320:LYS:N	2.26	0.51
1:B:20:VAL:HG22	1:B:84:HIS:ND1	2.26	0.51
1:D:205:LEU:C	1:D:206:ILE:HD12	2.36	0.51
1:C:117:ASP:CG	1:C:118:PHE:N	2.64	0.51
1:D:142:LEU:HD23	1:D:142:LEU:C	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:PHE:N	1:C:323:HIS:HD2	2.09	0.51
1:C:318:LEU:O	1:C:320:LYS:HD2	2.10	0.51
1:A:322:ARG:H	1:A:322:ARG:NH1	2.00	0.51
1:D:128:GLU:HG2	2:D:469:HOH:O	2.11	0.51
1:B:99:LEU:HA	1:B:309:ASP:HA	1.92	0.51
1:B:238:MET:HE3	1:B:243:VAL:O	2.10	0.51
1:D:15:GLU:H	1:D:15:GLU:CD	2.18	0.51
1:A:97:LYS:HB2	1:A:97:LYS:HZ2	1.75	0.51
1:C:77:THR:HB	1:C:78:PRO:CD	2.41	0.51
1:C:122:GLY:O	1:C:123:ARG:HG2	2.10	0.51
1:B:266:MET:HB2	1:C:308:ILE:HG22	1.93	0.50
1:B:261:GLU:O	1:B:275:ARG:NH1	2.39	0.50
1:A:302:PHE:HE2	1:A:318:LEU:CD1	2.25	0.50
1:B:105:ALA:HB3	1:B:123:ARG:NH2	2.22	0.50
1:B:169:HIS:O	1:B:172:LYS:HD3	2.11	0.50
1:A:330:ARG:HH21	1:A:330:ARG:CB	2.24	0.50
1:B:238:MET:HE1	1:B:244:LYS:CA	2.39	0.50
1:C:197:HIS:O	1:C:303:GLN:HG3	2.11	0.50
1:B:155:ILE:CG2	1:B:178:LEU:HD12	2.42	0.50
1:B:271:PHE:CZ	1:B:280:LEU:HD22	2.47	0.50
1:D:97:LYS:HB2	1:D:97:LYS:NZ	2.26	0.50
1:D:363:ASN:C	1:D:365:ASN:H	2.19	0.50
1:B:264:ASP:HB3	1:B:271:PHE:HD2	1.77	0.50
1:C:9:ARG:HD2	2:C:446:HOH:O	2.11	0.50
1:D:106:ASP:N	1:D:123:ARG:NH2	2.60	0.50
1:A:233:ILE:O	1:A:237:MET:HG2	2.12	0.50
1:C:100:PHE:CD1	1:C:106:ASP:HB3	2.47	0.50
1:D:95:ASN:O	1:D:96:ILE:HB	2.11	0.50
1:D:99:LEU:C	1:D:99:LEU:HD12	2.37	0.50
1:D:106:ASP:H	1:D:123:ARG:HH22	1.58	0.50
1:A:180:GLU:HG2	2:A:535:HOH:O	2.11	0.49
1:C:265:LEU:HD22	1:C:265:LEU:N	2.27	0.49
1:C:360:THR:O	1:C:364:GLU:HB2	2.13	0.49
1:C:123:ARG:HG3	1:C:124:SER:N	2.27	0.49
1:D:105:ALA:H	1:D:123:ARG:NH2	2.09	0.49
1:B:110:PHE:O	1:B:114:GLY:HA2	2.11	0.49
1:D:124:SER:O	1:D:126:ALA:N	2.46	0.49
1:C:267:ASP:CG	1:C:268:GLN:H	2.21	0.49
1:D:320:LYS:HD2	1:D:320:LYS:H	1.77	0.49
1:A:304:PRO:HB3	1:A:316:GLU:OE1	2.13	0.49
1:A:330:ARG:HB3	1:A:330:ARG:NH2	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:99:LEU:HD12	1:C:99:LEU:O	2.12	0.49
1:B:97:LYS:HB2	1:B:97:LYS:NZ	2.27	0.49
1:B:104:HIS:HD2	1:B:123:ARG:HH11	1.60	0.48
1:B:105:ALA:H	1:B:123:ARG:HH12	1.61	0.48
1:C:58:LYS:H	1:C:58:LYS:HD3	1.78	0.48
1:A:54:ILE:HG22	1:A:55:THR:N	2.29	0.48
1:B:238:MET:HE2	1:C:248:ILE:HG13	1.96	0.48
1:B:247:GLU:HB2	1:B:292:ARG:HB2	1.94	0.48
1:B:9:ARG:HD2	2:B:386:HOH:O	2.13	0.48
1:C:20:VAL:HG22	1:C:84:HIS:ND1	2.29	0.48
1:C:265:LEU:HB2	1:C:272:LEU:HD12	1.95	0.48
1:A:361:ILE:O	1:A:365:ASN:OXT	2.30	0.48
1:B:92:ASP:C	1:B:94:ASP:H	2.22	0.48
1:B:54:ILE:HG22	1:B:55:THR:N	2.29	0.47
1:B:302:PHE:CE2	1:B:318:LEU:HD11	2.42	0.47
1:A:318:LEU:O	1:A:320:LYS:HD2	2.14	0.47
1:B:116:ARG:HG3	1:B:116:ARG:HH11	1.78	0.47
1:C:123:ARG:HG3	1:C:123:ARG:HH11	1.79	0.47
1:C:21:ILE:HG23	1:C:83:ILE:HB	1.96	0.47
1:C:99:LEU:HD12	1:C:99:LEU:C	2.38	0.47
1:C:316:GLU:HG2	1:C:318:LEU:H	1.80	0.47
1:B:215:GLN:OE1	1:B:216:LYS:N	2.47	0.47
1:B:101:ARG:O	1:B:104:HIS:HB2	2.14	0.47
1:C:110:PHE:O	1:C:114:GLY:HA2	2.15	0.47
1:C:145:GLU:OE1	1:D:359:LYS:HE2	2.15	0.47
1:C:190:ILE:HD11	1:C:329:ILE:HD11	1.96	0.47
1:C:267:ASP:HB2	1:C:272:LEU:CD2	2.45	0.47
1:A:93:TYR:HA	1:A:320:LYS:O	2.15	0.47
1:C:240:LEU:HD23	1:C:241:ASN:N	2.30	0.47
1:A:302:PHE:CE2	1:A:318:LEU:HD11	2.44	0.47
1:C:100:PHE:CD2	1:C:107:PHE:HA	2.50	0.47
1:D:132:ARG:NH1	2:D:416:HOH:O	2.47	0.47
1:B:45:ARG:HH22	1:B:336:GLU:CD	2.23	0.47
1:C:99:LEU:HD23	1:C:315:CYS:HB2	1.96	0.47
1:A:322:ARG:HH11	1:A:322:ARG:CB	2.28	0.46
1:B:54:ILE:HD12	1:B:59:GLU:OE2	2.15	0.46
1:D:85:ASN:HD22	1:D:86:GLN:HG3	1.77	0.46
1:A:247:GLU:HB2	1:A:292:ARG:HB2	1.96	0.46
1:C:309:ASP:HB3	1:C:315:CYS:SG	2.56	0.46
1:D:314:GLU:HG3	2:D:502:HOH:O	2.15	0.46
1:A:170:ALA:HB2	1:A:178:LEU:HD23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:ASN:O	1:B:310:ILE:HG13	2.15	0.46
1:B:103:SER:C	1:C:280:LEU:HD11	2.40	0.46
1:C:308:ILE:CG1	1:C:312:GLY:HA2	2.45	0.46
1:A:75:THR:HA	1:C:115:ILE:CD1	2.45	0.46
1:B:112:LYS:HZ3	1:C:223:GLN:NE2	2.13	0.46
1:C:161:LYS:O	1:C:182:GLN:HG3	2.16	0.46
1:A:347:VAL:HG13	1:B:362:TYR:CE2	2.50	0.46
1:C:38:LEU:HD22	1:C:137:ALA:HB1	1.97	0.46
1:B:116:ARG:HG2	1:B:310:ILE:HD13	1.99	0.45
1:C:322:ARG:HH11	1:C:322:ARG:CB	2.29	0.45
1:D:117:ASP:O	1:D:119:ARG:HD3	2.16	0.45
1:A:228:LYS:HD3	1:A:282:GLY:HA3	1.98	0.45
1:C:58:LYS:HD3	1:C:58:LYS:N	2.31	0.45
1:D:61:ASP:O	1:D:62:LYS:HB2	2.15	0.45
1:A:47:GLN:HE22	1:A:60:ASP:CB	2.28	0.45
1:C:322:ARG:N	1:C:322:ARG:HH11	2.12	0.45
1:D:267:ASP:OD2	1:D:267:ASP:C	2.58	0.45
1:B:101:ARG:HG3	1:B:101:ARG:NH1	2.30	0.45
1:B:207:ARG:HG3	1:B:290:ILE:HD13	1.98	0.45
1:B:322:ARG:HD3	1:B:322:ARG:H	1.81	0.45
1:C:77:THR:HB	1:C:78:PRO:HD2	1.99	0.45
1:C:308:ILE:CD1	1:C:312:GLY:HA2	2.46	0.45
1:A:322:ARG:N	1:A:322:ARG:HD3	2.32	0.45
1:A:47:GLN:HE22	1:A:60:ASP:HB3	1.81	0.45
1:B:128:GLU:CG	1:C:225:LEU:HD13	2.45	0.45
1:D:21:ILE:HG23	1:D:83:ILE:HB	1.99	0.45
1:A:296:LYS:HD2	1:D:262:TYR:CE1	2.52	0.44
1:B:361:ILE:O	1:B:365:ASN:HB3	2.17	0.44
1:C:58:LYS:C	1:C:60:ASP:H	2.26	0.44
1:C:127:ARG:NH1	1:C:127:ARG:HG2	2.31	0.44
1:C:207:ARG:HA	1:C:289:ILE:O	2.17	0.44
1:A:9:ARG:HD2	2:A:416:HOH:O	2.17	0.44
1:C:200:ILE:CD1	1:C:326:CYS:HB2	2.47	0.44
1:B:21:ILE:HG23	1:B:83:ILE:HB	1.98	0.44
1:A:128:GLU:CG	1:D:225:LEU:HD13	2.42	0.44
1:B:327:ILE:HA	2:B:399:HOH:O	2.16	0.44
1:C:122:GLY:O	1:C:124:SER:N	2.45	0.44
1:D:188:THR:HA	1:D:191:GLN:NE2	2.33	0.44
1:D:247:GLU:OE1	1:D:294:HIS:CE1	2.65	0.44
1:A:67:SER:O	1:A:79:ILE:HA	2.17	0.44
1:B:93:TYR:HA	1:B:320:LYS:HB2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ALA:HB2	1:C:281:GLY:HA3	2.00	0.44
1:C:174:GLU:H	1:C:174:GLU:CD	2.25	0.44
1:A:116:ARG:HG3	1:A:116:ARG:HH11	1.81	0.44
1:B:156:GLU:HG2	2:B:371:HOH:O	2.17	0.44
1:C:67:SER:O	1:C:79:ILE:HA	2.18	0.44
1:C:99:LEU:HA	1:C:309:ASP:HA	1.99	0.44
1:C:116:ARG:NH1	1:C:310:ILE:HG21	2.33	0.44
1:D:88:ALA:O	1:D:89:ARG:HB2	2.16	0.43
1:C:47:GLN:NE2	1:C:60:ASP:HB2	2.27	0.43
1:C:127:ARG:HG2	1:C:127:ARG:HH11	1.82	0.43
1:D:262:TYR:O	1:D:275:ARG:HD2	2.19	0.43
1:A:361:ILE:HD11	1:B:361:ILE:CD1	2.45	0.43
1:B:61:ASP:OD2	1:B:85:ASN:HB3	2.18	0.43
1:B:97:LYS:HB3	1:B:118:PHE:CD2	2.53	0.43
1:C:115:ILE:C	1:C:117:ASP:H	2.25	0.43
1:C:216:LYS:NZ	1:C:287:GLU:OE1	2.50	0.43
1:B:265:LEU:HD12	1:B:265:LEU:N	2.32	0.43
1:C:304:PRO:HG3	1:C:318:LEU:HD23	1.99	0.43
1:B:116:ARG:HG3	1:B:116:ARG:NH1	2.33	0.43
1:A:2:ASN:OD1	1:C:9:ARG:NH1	2.52	0.43
1:B:270:GLY:O	1:B:271:PHE:C	2.61	0.43
1:D:206:ILE:N	1:D:206:ILE:CD1	2.82	0.43
1:C:183:GLU:HG2	1:C:187:LYS:HE3	2.01	0.43
1:A:99:LEU:C	1:A:99:LEU:HD12	2.42	0.43
1:A:155:ILE:CG2	1:A:178:LEU:HD12	2.49	0.43
1:A:320:LYS:HD2	1:A:320:LYS:N	2.32	0.43
1:B:99:LEU:C	1:B:99:LEU:HD12	2.44	0.43
1:D:221:LEU:O	1:D:283:MET:HA	2.19	0.43
1:D:308:ILE:HG22	1:D:314:GLU:HG2	2.01	0.43
1:B:85:ASN:O	1:B:86:GLN:HB2	2.18	0.43
1:B:156:GLU:HA	1:B:160:ILE:O	2.18	0.43
1:B:242:GLY:HA2	1:B:296:LYS:HE2	2.01	0.43
1:C:50:ARG:O	1:C:51:ASN:HB2	2.19	0.43
1:D:233:ILE:O	1:D:237:MET:HG2	2.19	0.43
1:D:169:HIS:CE1	1:D:183:GLU:OE2	2.69	0.42
1:D:54:ILE:HG21	1:D:58:LYS:HD2	2.01	0.42
1:B:318:LEU:C	1:B:318:LEU:HD13	2.44	0.42
1:A:106:ASP:HA	1:A:118:PHE:CZ	2.54	0.42
1:C:187:LYS:O	1:C:191:GLN:HG3	2.18	0.42
1:C:250:LYS:HE3	1:C:253:GLU:HB3	2.00	0.42
2:A:519:HOH:O	1:D:111:HIS:HD2	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:106:ASP:HA	1:C:118:PHE:CZ	2.54	0.42
1:A:351:LEU:HD22	1:B:361:ILE:CD1	2.49	0.42
1:B:183:GLU:HG2	1:B:187:LYS:HE3	2.01	0.42
1:C:200:ILE:H	1:C:200:ILE:HD12	1.85	0.42
1:D:35:ASP:CG	1:D:38:LEU:HB2	2.45	0.42
1:D:104:HIS:CE1	1:D:299:PRO:HB2	2.55	0.42
1:C:300:SER:HA	1:C:305:GLN:HE22	1.85	0.42
1:D:43:MET:O	1:D:46:ARG:HG2	2.20	0.42
1:A:262:TYR:O	1:A:263:ASN:C	2.62	0.42
1:B:155:ILE:HG22	1:B:178:LEU:HD12	2.00	0.42
1:C:104:HIS:C	1:C:106:ASP:H	2.28	0.42
1:D:55:THR:O	1:D:58:LYS:HG2	2.19	0.42
1:D:110:PHE:O	1:D:114:GLY:N	2.50	0.42
1:D:149:VAL:HG11	1:D:211:ILE:HD12	2.01	0.42
1:B:78:PRO:HB2	1:D:13:PHE:O	2.20	0.42
1:B:255:SER:OG	1:C:294:HIS:HD2	2.03	0.42
1:C:156:GLU:OE1	1:C:161:LYS:HG2	2.20	0.42
1:D:104:HIS:C	1:D:123:ARG:HH22	2.27	0.42
1:D:156:GLU:HB2	1:D:203:VAL:HB	2.02	0.42
1:B:21:ILE:HD12	1:B:22:GLY:H	1.84	0.41
1:B:53:PHE:CD1	1:B:53:PHE:C	2.98	0.41
1:D:172:LYS:O	1:D:172:LYS:HG2	2.19	0.41
1:B:125:SER:O	1:B:127:ARG:N	2.53	0.41
1:C:121:GLY:C	1:C:123:ARG:N	2.77	0.41
1:A:55:THR:C	1:A:57:ARG:H	2.28	0.41
1:B:262:TYR:HD1	1:B:263:ASN:H	1.59	0.41
1:C:320:LYS:H	1:C:320:LYS:CD	2.29	0.41
1:A:48:GLY:O	1:A:49:GLY:C	2.63	0.41
1:C:343:LEU:O	1:C:347:VAL:HG23	2.20	0.41
1:C:350:ASN:HB3	1:D:362:TYR:OH	2.21	0.41
1:B:55:THR:C	1:B:57:ARG:H	2.28	0.41
1:B:101:ARG:NH1	1:B:118:PHE:CE1	2.88	0.41
1:D:56:PRO:C	1:D:58:LYS:H	2.27	0.41
1:A:235:GLU:HB2	1:D:235:GLU:HB2	2.03	0.41
1:D:105:ALA:N	1:D:123:ARG:HH12	2.06	0.41
1:B:210:SER:HB3	1:B:215:GLN:O	2.20	0.41
1:C:53:PHE:O	1:C:54:ILE:HB	2.20	0.41
1:A:91:LYS:HB2	1:A:92:ASP:H	1.64	0.41
1:B:47:GLN:O	1:B:49:GLY:N	2.46	0.41
1:B:70:PHE:CE2	1:B:71:GLU:HG3	2.56	0.41
1:B:115:ILE:CD1	1:D:30:SER:HB2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:SER:O	1:B:126:ALA:HB3	2.21	0.41
1:B:320:LYS:H	1:B:320:LYS:CD	2.31	0.41
1:C:267:ASP:HB2	1:C:272:LEU:HD21	2.03	0.41
1:D:115:ILE:O	1:D:115:ILE:CD1	2.63	0.41
1:A:123:ARG:CG	1:A:124:SER:H	2.30	0.41
1:A:175:ILE:HG21	1:A:190:ILE:HD12	2.03	0.41
1:D:250:LYS:HB3	1:D:254:SER:OG	2.20	0.41
1:D:174:GLU:CD	1:D:187:LYS:NZ	2.79	0.40
1:A:151:GLU:OE2	1:A:207:ARG:NH1	2.45	0.40
1:A:235:GLU:OE2	1:D:235:GLU:OE2	2.38	0.40
1:C:38:LEU:HD23	1:C:38:LEU:O	2.20	0.40
1:C:215:GLN:OE1	1:C:215:GLN:HA	2.21	0.40
1:C:302:PHE:O	1:C:302:PHE:HD2	2.04	0.40
1:D:118:PHE:CD1	1:D:118:PHE:N	2.88	0.40
1:D:277:GLY:O	1:D:289:ILE:HA	2.22	0.40
1:B:100:PHE:CB	1:C:266:MET:HE1	2.47	0.40
1:B:250:LYS:HE2	1:B:257:LEU:CD2	2.46	0.40
1:D:7:PHE:O	1:D:9:ARG:HG3	2.21	0.40
1:D:21:ILE:HD12	1:D:22:GLY:H	1.86	0.40
1:A:225:LEU:HD13	1:D:128:GLU:CG	2.50	0.40
1:B:47:GLN:C	1:B:49:GLY:H	2.30	0.40
1:D:322:ARG:HH11	1:D:322:ARG:H	1.69	0.40

All (7) 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:C:182:GLN:NE2	1:D:89:ARG:NH2[7_545]	1.37	0.83
1:C:316:GLU:OE1	1:C:316:GLU:OE1[2_655]	1.70	0.50
1:C:71:GLU:OE2	1:D:87:ARG:CG[6_555]	1.71	0.49
1:C:71:GLU:OE2	1:D:87:ARG:NE[6_555]	1.92	0.28
1:C:181:GLU:O	1:D:89:ARG:NH1[7_545]	2.05	0.15
1:B:272:LEU:CD2	1:B:272:LEU:CD2[2_655]	2.07	0.13
1:C:71:GLU:OE2	1:D:87:ARG:CD[6_555]	2.14	0.06

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	363/365 (100%)	323 (89%)	30 (8%)	10 (3%)	4	2
1	B	363/365 (100%)	318 (88%)	34 (9%)	11 (3%)	3	1
1	C	363/365 (100%)	323 (89%)	31 (8%)	9 (2%)	4	2
1	D	363/365 (100%)	333 (92%)	17 (5%)	13 (4%)	2	1
All	All	1452/1460 (100%)	1297 (89%)	112 (8%)	43 (3%)	3	1

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ARG
1	A	95	ASN
1	A	116	ARG
1	A	123	ARG
1	B	95	ASN
1	B	118	PHE
1	B	125	SER
1	B	262	TYR
1	B	263	ASN
1	B	271	PHE
1	C	61	ASP
1	C	117	ASP
1	C	307	THR
1	D	124	SER
1	A	52	VAL
1	B	50	ARG
1	B	51	ASN
1	B	123	ARG
1	C	124	SER
1	D	56	PRO
1	D	92	ASP
1	A	61	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	54	ILE
1	C	116	ARG
1	C	123	ARG
1	D	59	GLU
1	D	86	GLN
1	D	94	ASP
1	D	96	ILE
1	D	117	ASP
1	D	125	SER
1	A	87	ARG
1	A	97	LYS
1	A	120	GLY
1	D	89	ARG
1	A	92	ASP
1	C	59	GLU
1	D	93	TYR
1	D	118	PHE
1	B	90	SER
1	D	224	GLY
1	B	52	VAL
1	C	96	ILE

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	300/300 (100%)	294 (98%)	6 (2%)	48	59
1	B	300/300 (100%)	292 (97%)	8 (3%)	39	49
1	C	300/300 (100%)	291 (97%)	9 (3%)	36	45
1	D	300/300 (100%)	285 (95%)	15 (5%)	22	24
All	All	1200/1200 (100%)	1162 (97%)	38 (3%)	34	43

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	LYS
1	A	93	TYR
1	A	97	LYS
1	A	240	LEU
1	A	322	ARG
1	A	330	ARG
1	B	87	ARG
1	B	89	ARG
1	B	97	LYS
1	B	172	LYS
1	B	215	GLN
1	B	240	LEU
1	B	257	LEU
1	B	343	LEU
1	C	17	HIS
1	C	58	LYS
1	C	89	ARG
1	C	91	LYS
1	C	97	LYS
1	C	172	LYS
1	C	200	ILE
1	C	322	ARG
1	C	343	LEU
1	D	15	GLU
1	D	38	LEU
1	D	87	ARG
1	D	91	LYS
1	D	93	TYR
1	D	95	ASN
1	D	118	PHE
1	D	123	ARG
1	D	172	LYS
1	D	206	ILE
1	D	240	LEU
1	D	241	ASN
1	D	318	LEU
1	D	322	ARG
1	D	343	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	104	HIS
1	A	168	ASN
1	A	169	HIS
1	A	182	GLN
1	A	186	GLN
1	A	223	GLN
1	A	294	HIS
1	A	313	ASN
1	B	47	GLN
1	B	51	ASN
1	B	86	GLN
1	B	98	ASN
1	B	168	ASN
1	B	186	GLN
1	B	191	GLN
1	B	196	ASN
1	B	223	GLN
1	B	241	ASN
1	B	263	ASN
1	B	294	HIS
1	B	313	ASN
1	B	323	HIS
1	C	47	GLN
1	C	51	ASN
1	C	98	ASN
1	C	168	ASN
1	C	182	GLN
1	C	186	GLN
1	C	191	GLN
1	C	214	ASN
1	C	223	GLN
1	C	294	HIS
1	C	303	GLN
1	C	305	GLN
1	C	313	ASN
1	C	323	HIS
1	D	47	GLN
1	D	85	ASN
1	D	104	HIS
1	D	111	HIS
1	D	169	HIS
1	D	186	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	191	GLN
1	D	196	ASN
1	D	215	GLN
1	D	223	GLN
1	D	294	HIS

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/365 (100%)	0.04	30 (8%) 17 16	19, 30, 119, 176	9 (2%)
1	B	365/365 (100%)	0.55	59 (16%) 4 4	23, 41, 134, 167	9 (2%)
1	C	365/365 (100%)	0.59	64 (17%) 4 3	22, 39, 166, 183	9 (2%)
1	D	365/365 (100%)	0.07	30 (8%) 17 16	20, 34, 95, 137	9 (2%)
All	All	1460/1460 (100%)	0.31	183 (12%) 8 7	19, 36, 133, 183	36 (2%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	ILE	6.9
1	C	300	SER	6.3
1	A	54	ILE	5.8
1	B	270	GLY	5.6
1	A	96	ILE	5.5
1	C	302	PHE	5.4
1	A	118	PHE	5.2
1	B	56	PRO	5.2
1	A	93	TYR	5.1
1	C	58	LYS	5.1
1	A	52	VAL	5.1
1	A	49	GLY	5.1
1	A	56	PRO	4.9
1	C	54	ILE	4.8
1	B	271	PHE	4.7
1	C	55	THR	4.7
1	A	94	ASP	4.5
1	C	52	VAL	4.4
1	D	115	ILE	4.4
1	C	93	TYR	4.4
1	C	49	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	115	ILE	4.3
1	C	56	PRO	4.3
1	D	49	GLY	4.3
1	C	310	ILE	4.3
1	C	105	ALA	4.1
1	D	122	GLY	4.1
1	B	263	ASN	4.1
1	C	304	PRO	4.1
1	C	118	PHE	4.0
1	A	53	PHE	4.0
1	A	95	ASN	3.9
1	C	103	SER	3.8
1	A	55	THR	3.8
1	B	118	PHE	3.8
1	D	55	THR	3.8
1	C	90	SER	3.7
1	C	100	PHE	3.7
1	C	96	ILE	3.7
1	C	308	ILE	3.7
1	B	265	LEU	3.7
1	B	54	ILE	3.6
1	B	93	TYR	3.6
1	C	314	GLU	3.6
1	B	269	LYS	3.6
1	C	104	HIS	3.6
1	C	213	THR	3.6
1	D	56	PRO	3.6
1	C	53	PHE	3.5
1	B	264	ASP	3.5
1	C	212	LYS	3.5
1	A	17	HIS	3.5
1	C	92	ASP	3.5
1	B	52	VAL	3.5
1	A	117	ASP	3.5
1	D	118	PHE	3.4
1	A	88	ALA	3.4
1	D	88	ALA	3.4
1	C	99	LEU	3.4
1	C	365	ASN	3.4
1	B	53	PHE	3.4
1	C	315	CYS	3.4
1	C	214	ASN	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	95	ASN	3.3
1	B	272	LEU	3.3
1	C	102	PRO	3.3
1	C	312	GLY	3.2
1	B	267	ASP	3.2
1	C	98	ASN	3.2
1	B	55	THR	3.2
1	C	307	THR	3.2
1	B	51	ASN	3.2
1	C	318	LEU	3.2
1	C	211	ILE	3.1
1	B	48	GLY	3.1
1	B	321	GLY	3.1
1	B	274	ASN	3.1
1	A	87	ARG	3.1
1	B	318	LEU	3.1
1	B	21	ILE	3.0
1	D	94	ASP	3.0
1	B	90	SER	3.0
1	C	85	ASN	3.0
1	D	93	TYR	3.0
1	C	101	ARG	3.0
1	B	120	GLY	3.0
1	A	58	LYS	2.9
1	D	59	GLU	2.9
1	C	305	GLN	2.9
1	B	266	MET	2.9
1	D	364	GLU	2.9
1	D	90	SER	2.9
1	D	172	LYS	2.9
1	D	123	ARG	2.9
1	A	86	GLN	2.9
1	C	303	GLN	2.8
1	C	88	ALA	2.8
1	B	172	LYS	2.8
1	B	214	ASN	2.8
1	C	313	ASN	2.8
1	B	17	HIS	2.8
1	A	123	ARG	2.8
1	A	365	ASN	2.7
1	B	268	GLN	2.7
1	C	86	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	301	ILE	2.7
1	B	96	ILE	2.7
1	B	273	SER	2.7
1	D	85	ASN	2.7
1	D	120	GLY	2.7
1	A	50	ARG	2.7
1	B	126	ALA	2.6
1	B	58	LYS	2.6
1	C	309	ASP	2.6
1	D	92	ASP	2.6
1	C	316	GLU	2.6
1	D	87	ARG	2.6
1	B	275	ARG	2.6
1	C	48	GLY	2.6
1	D	125	SER	2.6
1	D	86	GLN	2.5
1	A	120	GLY	2.5
1	C	321	GLY	2.5
1	A	90	SER	2.5
1	B	86	GLN	2.5
1	C	59	GLU	2.5
1	C	161	LYS	2.5
1	D	58	LYS	2.5
1	D	121	GLY	2.5
1	B	95	ASN	2.5
1	C	17	HIS	2.5
1	B	115	ILE	2.5
1	B	61	ASP	2.5
1	A	224	GLY	2.5
1	C	122	GLY	2.5
1	C	270	GLY	2.5
1	D	124	SER	2.4
1	A	48	GLY	2.4
1	A	89	ARG	2.4
1	B	49	GLY	2.4
1	B	300	SER	2.4
1	B	262	TYR	2.4
1	A	51	ASN	2.4
1	B	92	ASP	2.4
1	B	88	ALA	2.4
1	C	119	ARG	2.4
1	C	123	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	168	ASN	2.4
1	C	120	GLY	2.4
1	C	94	ASP	2.3
1	B	125	SER	2.3
1	B	89	ARG	2.3
1	C	319	LEU	2.3
1	B	57	ARG	2.3
1	C	317	CYS	2.3
1	D	21	ILE	2.3
1	D	96	ILE	2.3
1	D	61	ASP	2.3
1	B	85	ASN	2.2
1	B	121	GLY	2.2
1	D	54	ILE	2.2
1	B	119	ARG	2.2
1	C	109	TYR	2.2
1	B	94	ASP	2.2
1	B	365	ASN	2.2
1	D	57	ARG	2.2
1	A	124	SER	2.2
1	B	117	ASP	2.2
1	C	97	LYS	2.2
1	B	123	ARG	2.1
1	C	95	ASN	2.1
1	A	119	ARG	2.1
1	C	57	ARG	2.1
1	C	117	ASP	2.1
1	A	121	GLY	2.1
1	C	89	ARG	2.1
1	B	84	HIS	2.1
1	B	18	GLY	2.1
1	C	114	GLY	2.1
1	B	322	ARG	2.1
1	B	211	ILE	2.0
1	B	308	ILE	2.0
1	D	116	ARG	2.0

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

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.