



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:04 AM UTC

PDB ID : 4RS4 / pdb_00004rs4
Title : Crystal structure and mutational analysis of the endoribonuclease from human coronavirus 229E
Authors : Huo, T.; Liu, X.; Yang, C.; Rao, Z.
Deposited on : 2014-11-06
Resolution : 2.96 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:

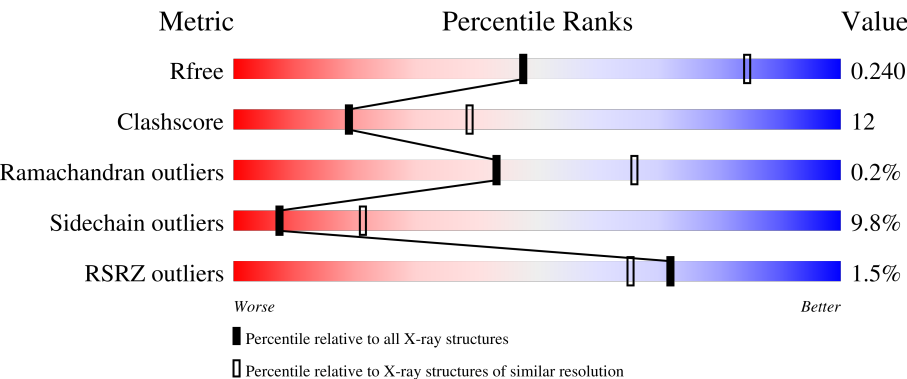
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	349	% 72%23%..
1	B	349	% 73%22%..
1	C	349	2% 58%33%.5%
1	D	349	4% 60%32%..
1	E	349	% 67%27%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	349	 70%25% . .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15989 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 Uridylate-specific endoribonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2674	1724	432	504	14			
1	B	345	Total	C	N	O	S	0	0	0
			2695	1735	437	509	14			
1	C	332	Total	C	N	O	S	0	0	0
			2601	1679	418	490	14			
1	D	337	Total	C	N	O	S	0	0	0
			2636	1703	424	495	14			
1	E	341	Total	C	N	O	S	0	0	0
			2669	1721	430	504	14			
1	F	346	Total	C	N	O	S	0	0	0
			2714	1746	439	515	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P0C6X1
A	17	SER	GLY	engineered mutation	UNP P0C6X1
A	142	ALA	THR	engineered mutation	UNP P0C6X1
A	219	MET	ILE	engineered mutation	UNP P0C6X1
A	252	SER	LEU	engineered mutation	UNP P0C6X1
B	0	SER	-	expression tag	UNP P0C6X1
B	17	SER	GLY	engineered mutation	UNP P0C6X1
B	142	ALA	THR	engineered mutation	UNP P0C6X1
B	219	MET	ILE	engineered mutation	UNP P0C6X1
B	252	SER	LEU	engineered mutation	UNP P0C6X1
C	0	SER	-	expression tag	UNP P0C6X1
C	17	SER	GLY	engineered mutation	UNP P0C6X1
C	142	ALA	THR	engineered mutation	UNP P0C6X1
C	219	MET	ILE	engineered mutation	UNP P0C6X1
C	252	SER	LEU	engineered mutation	UNP P0C6X1
D	0	SER	-	expression tag	UNP P0C6X1
D	17	SER	GLY	engineered mutation	UNP P0C6X1

Continued on next page...

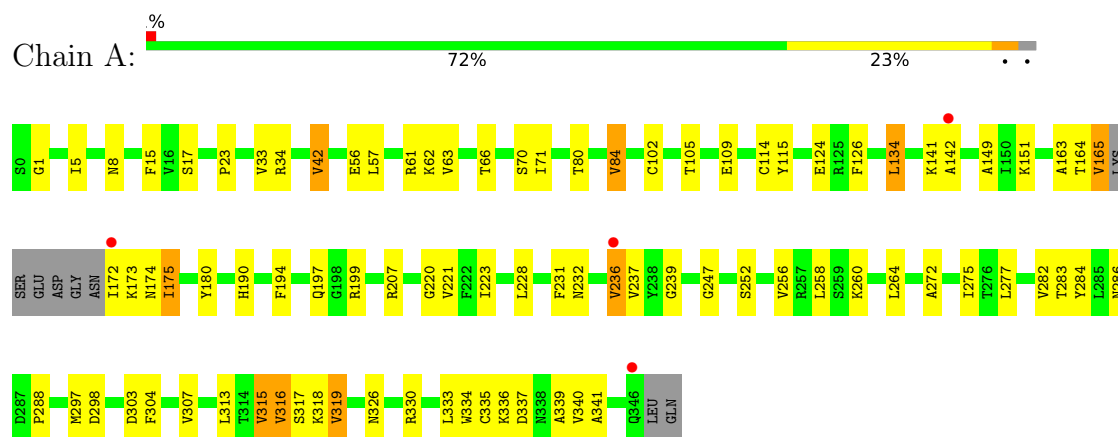
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	142	ALA	THR	engineered mutation	UNP P0C6X1
D	219	MET	ILE	engineered mutation	UNP P0C6X1
D	252	SER	LEU	engineered mutation	UNP P0C6X1
E	0	SER	-	expression tag	UNP P0C6X1
E	17	SER	GLY	engineered mutation	UNP P0C6X1
E	142	ALA	THR	engineered mutation	UNP P0C6X1
E	219	MET	ILE	engineered mutation	UNP P0C6X1
E	252	SER	LEU	engineered mutation	UNP P0C6X1
F	0	SER	-	expression tag	UNP P0C6X1
F	17	SER	GLY	engineered mutation	UNP P0C6X1
F	142	ALA	THR	engineered mutation	UNP P0C6X1
F	219	MET	ILE	engineered mutation	UNP P0C6X1
F	252	SER	LEU	engineered mutation	UNP P0C6X1

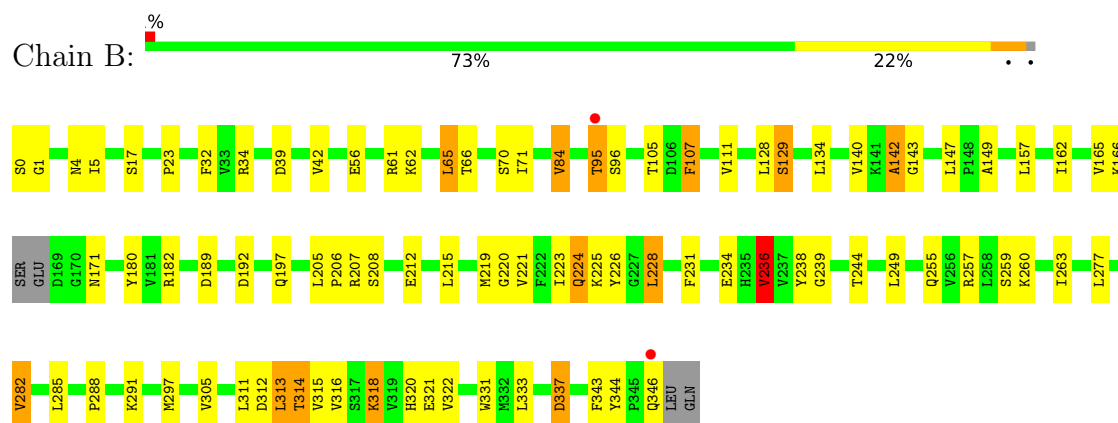
3 Residue-property plots [i](#)

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.

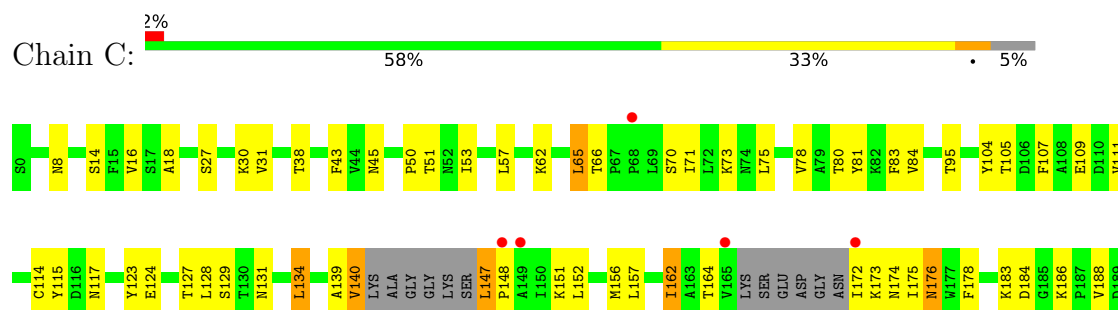
• Molecule 1: Uridylate-specific endoribonuclease

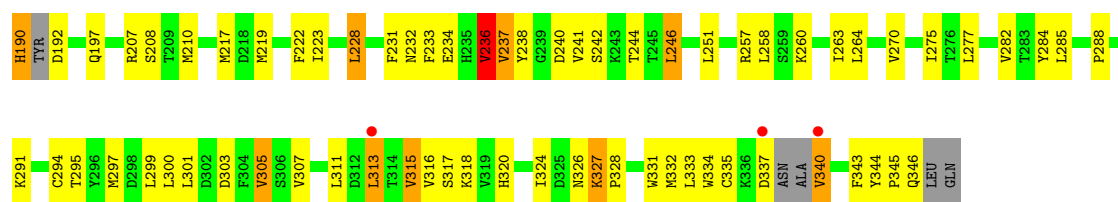


• Molecule 1: Uridylate-specific endoribonuclease

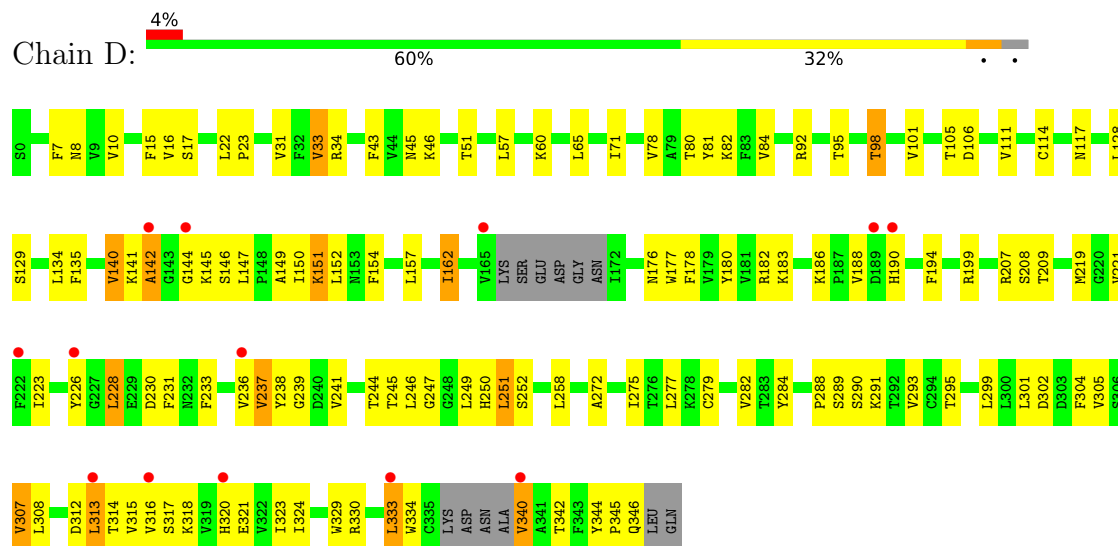


• Molecule 1: Uridylate-specific endoribonuclease

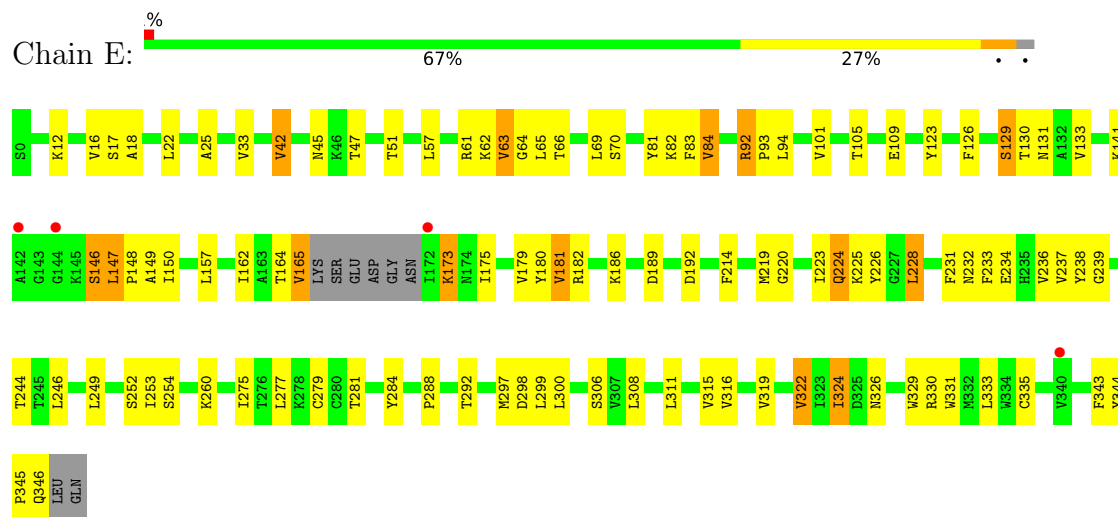




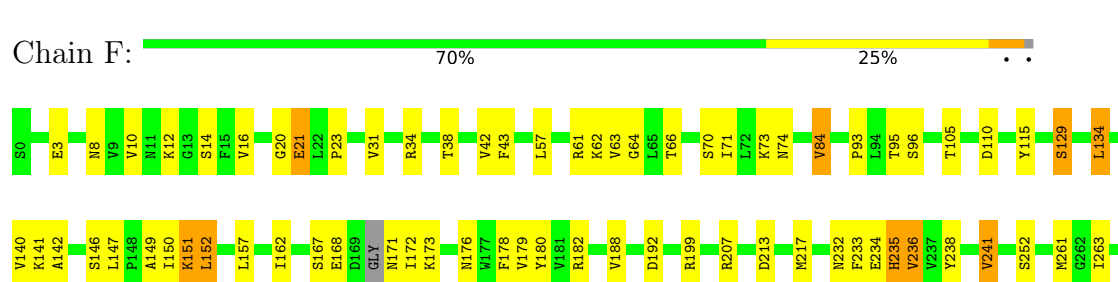
• Molecule 1: Uridylate-specific endoribonuclease



• Molecule 1: Uridylate-specific endoribonuclease



• Molecule 1: Uridylate-specific endoribonuclease



V270	A271	A272	I275	T276	L277	K278	C279	Y284	L285	W286	D287	P288	K291	T292	V293	M297	S306	V307	L308	L311	D312	L313	T314	V315	V316	S317	K318	V322	I323	I324	D325	N326	K327	P328	W329	W334	T342	Q346	LEU	GLN
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.93Å 143.17Å 174.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.96 30.00 – 2.96	Depositor EDS
% Data completeness (in resolution range)	90.4 (30.00-2.96) 89.1 (30.00-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.208 , 0.255 0.194 , 0.240	Depositor DCC
R_{free} test set	3387 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15989	wwPDB-VP
Average B, all atoms (Å ²)	71.0	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 [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	0.37	0/2732	0.79	2/3708 (0.1%)
1	B	0.36	0/2753	0.78	4/3737 (0.1%)
1	C	0.34	0/2655	0.78	3/3604 (0.1%)
1	D	0.34	0/2692	0.78	2/3653 (0.1%)
1	E	0.36	0/2726	0.77	1/3700 (0.0%)
1	F	0.34	0/2772	0.76	1/3761 (0.0%)
All	All	0.35	0/16330	0.78	13/22163 (0.1%)

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	D	0	1
1	F	0	1
All	All	0	2

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	GLU	N-CA-C	-8.55	94.69	108.55
1	A	221	VAL	N-CA-C	-7.83	103.22	110.82
1	D	144	GLY	N-CA-C	7.47	124.91	115.42
1	B	221	VAL	N-CA-C	-6.27	104.17	111.00
1	B	142	ALA	N-CA-C	5.94	118.12	108.26
1	E	173	LYS	N-CA-C	5.89	118.33	108.96
1	F	168	GLU	CB-CA-C	-5.47	109.79	117.23
1	C	236	VAL	N-CA-C	5.40	116.13	110.62
1	C	344	TYR	CA-C-N	5.37	126.55	119.84
1	C	344	TYR	C-N-CA	5.37	126.55	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	LEU	N-CA-C	-5.31	106.58	113.16
1	B	344	TYR	CA-C-N	5.06	124.96	119.85
1	B	344	TYR	C-N-CA	5.06	124.96	119.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	142	ALA	Peptide
1	F	142	ALA	Peptide

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	2674	0	2657	59	0
1	B	2695	0	2668	59	0
1	C	2601	0	2568	75	0
1	D	2636	0	2621	77	0
1	E	2669	0	2652	67	0
1	F	2714	0	2691	52	0
All	All	15989	0	15857	375	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (375) 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:B:315:VAL:HG11	1:B:318:LYS:HE2	1.42	1.01
1:F:157:LEU:HB2	1:F:162:ILE:HD13	1.58	0.86
1:A:288:PRO:HG3	1:D:162:ILE:HD11	1.57	0.85
1:D:334:TRP:HZ3	1:D:344:TYR:HE2	1.24	0.84
1:A:164:THR:HG23	1:A:174:ASN:HA	1.61	0.82
1:B:236:VAL:HG21	1:B:343:PHE:H	1.45	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:CYS:HB2	1:A:339:ALA:O	1.82	0.80
1:D:145:LYS:HG3	1:D:146:SER:H	1.50	0.76
1:E:315:VAL:HG12	1:E:316:VAL:H	1.51	0.76
1:B:263:ILE:HG21	1:B:285:LEU:HD22	1.68	0.75
1:D:334:TRP:CZ3	1:D:344:TYR:HE2	2.05	0.74
1:B:0:SER:HB2	1:B:4:ASN:HB2	1.69	0.74
1:D:233:PHE:HB3	1:D:238:TYR:HD2	1.53	0.73
1:C:62:LYS:HG2	1:C:66:THR:HG22	1.70	0.73
1:D:236:VAL:HG22	1:D:237:VAL:HG23	1.70	0.73
1:A:335:CYS:HA	1:A:341:ALA:H	1.53	0.72
1:C:210:MET:HE1	1:C:305:VAL:HG21	1.72	0.72
1:A:232:ASN:O	1:A:236:VAL:HB	1.90	0.72
1:A:236:VAL:HG12	1:A:237:VAL:HG23	1.72	0.71
1:B:111:VAL:HG12	1:C:109:GLU:HG2	1.73	0.71
1:E:149:ALA:HB2	1:E:180:TYR:CE1	2.25	0.70
1:C:151:LYS:HE2	1:C:178:PHE:CZ	2.25	0.70
1:E:277:LEU:HD13	1:E:297:MET:HE2	1.72	0.70
1:B:315:VAL:HG11	1:B:318:LYS:CE	2.21	0.70
1:D:117:ASN:HB2	1:D:134:LEU:HD11	1.74	0.69
1:B:220:GLY:H	1:B:223:ILE:HG13	1.58	0.69
1:D:45:ASN:HB2	1:D:51:THR:HG23	1.75	0.69
1:C:327:LYS:HG3	1:C:328:PRO:HD2	1.74	0.68
1:D:334:TRP:HZ3	1:D:344:TYR:CE2	2.11	0.68
1:C:277:LEU:HD13	1:C:297:MET:HE3	1.76	0.68
1:E:284:TYR:O	1:E:288:PRO:HA	1.94	0.68
1:A:220:GLY:H	1:A:223:ILE:HG13	1.57	0.67
1:B:226:TYR:HB2	1:B:228:LEU:CD2	2.24	0.67
1:C:313:LEU:HD11	1:C:337:ASP:O	1.93	0.67
1:D:299:LEU:HD21	1:D:324:ILE:HD13	1.76	0.67
1:A:71:ILE:HD12	1:A:71:ILE:H	1.58	0.67
1:A:61:ARG:HA	1:A:84:VAL:HG22	1.78	0.66
1:D:71:ILE:HD12	1:D:71:ILE:H	1.61	0.65
1:A:57:LEU:HD11	1:A:105:THR:HG21	1.78	0.65
1:E:12:LYS:HG2	1:E:16:VAL:HG21	1.78	0.65
1:B:149:ALA:HB2	1:B:180:TYR:CE1	2.32	0.65
1:A:239:GLY:HA2	1:A:247:GLY:O	1.97	0.64
1:D:249:LEU:HD11	1:D:258:LEU:HD23	1.78	0.64
1:E:62:LYS:HG2	1:E:66:THR:HG22	1.79	0.64
1:E:315:VAL:HG12	1:E:316:VAL:N	2.13	0.63
1:B:197:GLN:HB3	1:B:207:ARG:NH2	2.12	0.63
1:D:152:LEU:HD12	1:D:154:PHE:CE2	2.33	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ARG:HA	1:B:84:VAL:HG22	1.80	0.62
1:D:145:LYS:HG3	1:D:146:SER:N	2.14	0.62
1:F:62:LYS:HG2	1:F:66:THR:HG22	1.81	0.62
1:B:206:PRO:HG3	1:B:215:LEU:HD12	1.81	0.62
1:C:295:THR:OG1	1:C:345:PRO:HG2	1.99	0.62
1:D:318:LYS:HD3	1:D:320:HIS:CE1	2.33	0.62
1:E:22:LEU:HD13	1:E:33:VAL:HG11	1.81	0.62
1:E:299:LEU:HD21	1:E:324:ILE:HD13	1.82	0.61
1:F:23:PRO:HG2	1:F:34:ARG:HB3	1.82	0.61
1:B:23:PRO:HG2	1:B:34:ARG:HB3	1.83	0.61
1:D:231:PHE:HA	1:D:340:VAL:HG11	1.81	0.60
1:E:224:GLN:HG3	1:E:225:LYS:N	2.14	0.60
1:F:276:THR:HB	1:F:325:ASP:OD2	2.01	0.60
1:B:42:VAL:HG12	1:F:270:VAL:HG22	1.83	0.60
1:A:33:VAL:HG13	1:A:42:VAL:HG21	1.84	0.60
1:D:302:ASP:O	1:D:305:VAL:HG22	2.02	0.59
1:D:272:ALA:HB3	1:D:275:ILE:HG13	1.84	0.59
1:F:241:VAL:HG11	1:F:284:TYR:CD1	2.37	0.59
1:D:142:ALA:H	1:D:147:LEU:CD1	2.15	0.59
1:B:311:LEU:HD22	1:B:333:LEU:HD22	1.83	0.59
1:B:315:VAL:CG1	1:B:318:LYS:HE2	2.26	0.59
1:A:23:PRO:HG2	1:A:34:ARG:HB3	1.84	0.59
1:E:150:ILE:HB	1:E:179:VAL:HB	1.83	0.59
1:A:173:LYS:HE3	1:C:242:SER:O	2.02	0.58
1:E:232:ASN:HB3	1:E:236:VAL:HG23	1.85	0.58
1:D:151:LYS:C	1:D:152:LEU:HD22	2.27	0.58
1:A:258:LEU:HD23	1:A:264:LEU:HD22	1.85	0.58
1:F:149:ALA:HB2	1:F:180:TYR:CE1	2.38	0.58
1:D:65:LEU:HG	1:D:157:LEU:HD13	1.85	0.58
1:D:317:SER:O	1:D:318:LYS:HB3	2.03	0.58
1:C:236:VAL:HG12	1:C:237:VAL:HG12	1.86	0.58
1:B:224:GLN:HG3	1:B:225:LYS:N	2.19	0.57
1:E:45:ASN:ND2	1:E:51:THR:HA	2.20	0.57
1:D:312:ASP:CG	1:D:314:THR:HG22	2.30	0.57
1:C:164:THR:HG23	1:C:174:ASN:HA	1.85	0.57
1:E:331:TRP:HB3	1:E:343:PHE:CE2	2.40	0.57
1:F:129:SER:O	1:F:182:ARG:NH1	2.37	0.57
1:E:63:VAL:HG12	1:E:64:GLY:H	1.68	0.57
1:E:164:THR:O	1:E:165:VAL:HG23	2.05	0.57
1:C:291:LYS:HG2	1:C:294:CYS:HB2	1.86	0.56
1:E:220:GLY:HA2	1:E:223:ILE:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LEU:HD13	1:C:337:ASP:HA	1.88	0.56
1:D:315:VAL:HG11	1:D:318:LYS:HD2	1.88	0.56
1:B:129:SER:O	1:B:182:ARG:NH1	2.39	0.56
1:B:220:GLY:O	1:B:224:GLN:HB3	2.05	0.56
1:C:197:GLN:HB3	1:C:207:ARG:NH2	2.21	0.55
1:C:315:VAL:HG21	1:C:318:LYS:HB2	1.86	0.55
1:A:197:GLN:HB2	1:A:298:ASP:OD2	2.06	0.55
1:C:57:LEU:HD11	1:C:105:THR:HG21	1.89	0.55
1:E:231:PHE:CE1	1:E:308:LEU:HB3	2.41	0.55
1:A:272:ALA:HB3	1:A:275:ILE:HG13	1.87	0.55
1:C:315:VAL:HG11	1:C:318:LYS:HD2	1.88	0.55
1:E:226:TYR:CB	1:E:228:LEU:HD21	2.36	0.55
1:F:141:LYS:HG3	1:F:146:SER:HA	1.88	0.55
1:D:151:LYS:HD2	1:D:151:LYS:O	2.05	0.55
1:C:71:ILE:HD12	1:C:71:ILE:H	1.71	0.55
1:D:246:LEU:HD13	1:D:289:SER:OG	2.07	0.55
1:E:47:THR:HG22	1:E:92:ARG:HB3	1.89	0.55
1:D:152:LEU:O	1:D:176:ASN:HA	2.07	0.54
1:C:147:LEU:HD22	1:C:148:PRO:HD2	1.89	0.54
1:D:277:LEU:HD11	1:D:295:THR:HG22	1.89	0.54
1:F:316:VAL:HG23	1:F:317:SER:H	1.72	0.54
1:B:257:ARG:O	1:B:260:LYS:HG2	2.08	0.54
1:B:337:ASP:OD1	1:B:337:ASP:N	2.39	0.54
1:C:147:LEU:HD22	1:C:148:PRO:CD	2.37	0.54
1:A:141:LYS:O	1:A:142:ALA:HB2	2.08	0.53
1:D:78:VAL:HG11	1:D:111:VAL:HG21	1.88	0.53
1:E:226:TYR:HB2	1:E:228:LEU:HD21	1.89	0.53
1:C:297:MET:HB3	1:C:299:LEU:HD13	1.91	0.53
1:E:133:VAL:HG22	1:E:181:VAL:HG13	1.91	0.53
1:E:239:GLY:HA3	1:E:249:LEU:HD13	1.91	0.53
1:C:233:PHE:HB3	1:C:238:TYR:HD1	1.74	0.53
1:D:152:LEU:HB2	1:D:177:TRP:HB2	1.91	0.52
1:F:233:PHE:HB3	1:F:238:TYR:CD1	2.44	0.52
1:B:311:LEU:HD23	1:B:320:HIS:CE1	2.44	0.52
1:A:252:SER:O	1:A:256:VAL:HG23	2.10	0.52
1:E:329:TRP:O	1:E:331:TRP:HD1	1.91	0.52
1:D:16:VAL:O	1:D:17:SER:HB2	2.10	0.52
1:D:284:TYR:O	1:D:288:PRO:HA	2.10	0.52
1:E:126:PHE:CZ	1:E:182:ARG:HG3	2.45	0.52
1:A:71:ILE:HD12	1:A:71:ILE:N	2.23	0.51
1:E:219:MET:HB2	1:E:238:TYR:CZ	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:NH1	1:A:207:ARG:HG2	2.26	0.51
1:C:313:LEU:CD1	1:C:337:ASP:HA	2.40	0.51
1:E:252:SER:OG	1:E:298:ASP:HB2	2.10	0.51
1:E:288:PRO:O	1:F:173:LYS:HE2	2.11	0.51
1:C:78:VAL:O	1:C:95:THR:HB	2.11	0.51
1:C:172:ILE:N	1:C:172:ILE:HD12	2.26	0.51
1:C:210:MET:HE2	1:C:301:LEU:HG	1.92	0.51
1:D:304:PHE:O	1:D:307:VAL:HG12	2.10	0.51
1:F:31:VAL:HB	1:F:43:PHE:HB3	1.93	0.51
1:B:277:LEU:HD13	1:B:297:MET:HE3	1.92	0.51
1:C:208:SER:OG	1:C:300:LEU:HD11	2.10	0.51
1:F:167:SER:OG	1:F:171:ASN:HB2	2.11	0.51
1:F:233:PHE:HB3	1:F:238:TYR:HD1	1.76	0.51
1:F:308:LEU:O	1:F:311:LEU:HB2	2.11	0.51
1:B:220:GLY:HA2	1:B:223:ILE:HB	1.92	0.50
1:D:231:PHE:HA	1:D:340:VAL:CG1	2.42	0.50
1:B:157:LEU:HB2	1:B:162:ILE:HD13	1.92	0.50
1:F:279:CYS:SG	1:F:293:VAL:HG13	2.51	0.50
1:B:107:PHE:HZ	1:C:107:PHE:CZ	2.29	0.50
1:C:117:ASN:HB2	1:C:134:LEU:HD21	1.93	0.50
1:D:22:LEU:HD13	1:D:33:VAL:HG21	1.93	0.50
1:C:223:ILE:HG23	1:C:228:LEU:HB2	1.92	0.50
1:D:182:ARG:C	1:D:183:LYS:HD2	2.35	0.50
1:A:115:TYR:HB2	1:A:134:LEU:HD12	1.93	0.50
1:B:288:PRO:O	1:E:173:LYS:HE2	2.11	0.50
1:E:311:LEU:HD13	1:E:333:LEU:HD22	1.94	0.50
1:A:149:ALA:HB2	1:A:180:TYR:CE1	2.47	0.50
1:E:344:TYR:HB2	1:E:345:PRO:HD2	1.94	0.50
1:F:284:TYR:O	1:F:288:PRO:HA	2.11	0.50
1:F:317:SER:HB2	1:F:334:TRP:CZ3	2.47	0.50
1:F:61:ARG:HA	1:F:84:VAL:HG22	1.93	0.50
1:F:315:VAL:HG11	1:F:318:LYS:HB2	1.93	0.49
1:C:263:ILE:HB	1:C:285:LEU:HB2	1.94	0.49
1:B:140:VAL:HG12	1:B:147:LEU:HD13	1.93	0.49
1:B:282:VAL:HG23	1:B:291:LYS:HB3	1.94	0.49
1:F:140:VAL:HG12	1:F:147:LEU:HD22	1.94	0.49
1:A:335:CYS:HB2	1:A:340:VAL:HA	1.93	0.49
1:D:241:VAL:HG11	1:D:284:TYR:CD1	2.47	0.49
1:E:281:THR:HG23	1:E:292:THR:HA	1.94	0.49
1:E:33:VAL:HG23	1:E:42:VAL:HG21	1.94	0.49
1:A:264:LEU:HD11	1:A:282:VAL:HG12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ASN:OD1	1:F:276:THR:HG21	2.12	0.49
1:F:235:HIS:ND1	1:F:235:HIS:C	2.70	0.49
1:C:75:LEU:CD2	1:C:326:ASN:HD22	2.26	0.49
1:F:272:ALA:HB3	1:F:275:ILE:HG13	1.95	0.49
1:D:334:TRP:CZ3	1:D:344:TYR:CE2	2.94	0.49
1:D:149:ALA:HB2	1:D:180:TYR:CE1	2.48	0.49
1:C:335:CYS:HB3	1:C:340:VAL:HG23	1.95	0.48
1:E:330:ARG:NH1	1:E:346:GLN:O	2.46	0.48
1:B:312:ASP:H	1:B:318:LYS:HZ1	1.61	0.48
1:C:303:ASP:O	1:C:307:VAL:HG23	2.14	0.48
1:A:172:ILE:O	1:A:172:ILE:HG13	2.14	0.48
1:A:284:TYR:O	1:A:288:PRO:HA	2.12	0.48
1:A:284:TYR:CE1	1:A:286:ASN:HB2	2.49	0.48
1:A:319:VAL:CG1	1:A:330:ARG:HH11	2.26	0.48
1:D:333:LEU:HG	1:D:334:TRP:N	2.28	0.48
1:D:81:TYR:CE2	1:D:82:LYS:HG3	2.48	0.48
1:A:313:LEU:HA	1:A:335:CYS:SG	2.54	0.48
1:C:152:LEU:O	1:C:176:ASN:HA	2.14	0.48
1:A:164:THR:O	1:A:173:LYS:O	2.32	0.47
1:A:165:VAL:O	1:A:165:VAL:HG13	2.14	0.47
1:B:312:ASP:H	1:B:318:LYS:NZ	2.12	0.47
1:C:31:VAL:HB	1:C:43:PHE:HB3	1.96	0.47
1:D:31:VAL:HB	1:D:43:PHE:HB3	1.95	0.47
1:D:150:ILE:HG22	1:D:152:LEU:HD21	1.95	0.47
1:E:81:TYR:O	1:E:83:PHE:HD2	1.97	0.47
1:B:95:THR:HG23	1:B:96:SER:H	1.79	0.47
1:F:57:LEU:HD11	1:F:105:THR:HG21	1.95	0.47
1:A:173:LYS:HE2	1:C:288:PRO:O	2.15	0.47
1:A:223:ILE:HG23	1:A:228:LEU:HB2	1.95	0.47
1:D:23:PRO:HG2	1:D:34:ARG:HB3	1.96	0.47
1:E:322:VAL:HG13	1:E:331:TRP:CD1	2.48	0.47
1:A:62:LYS:HG2	1:A:66:THR:HG22	1.96	0.47
1:B:32:PHE:HB3	1:B:39:ASP:HB3	1.96	0.47
1:B:239:GLY:HA3	1:B:249:LEU:HD13	1.97	0.47
1:D:134:LEU:HD12	1:D:135:PHE:N	2.29	0.47
1:D:150:ILE:HG22	1:D:152:LEU:CD2	2.44	0.47
1:E:277:LEU:CD1	1:E:297:MET:HE2	2.43	0.47
1:F:151:LYS:HD3	1:F:178:PHE:CE1	2.49	0.47
1:F:308:LEU:HA	1:F:311:LEU:HD22	1.97	0.47
1:C:65:LEU:HD22	1:C:157:LEU:HD13	1.96	0.47
1:C:345:PRO:O	1:C:346:GLN:C	2.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:SER:O	1:B:105:THR:HG23	2.15	0.47
1:C:313:LEU:HD22	1:C:340:VAL:HG22	1.96	0.47
1:D:317:SER:HA	1:D:333:LEU:O	2.14	0.46
1:C:157:LEU:HD21	1:D:290:SER:HB3	1.97	0.46
1:C:217:MET:HE1	1:C:222:PHE:HA	1.98	0.46
1:C:50:PRO:HB2	1:C:53:ILE:HG12	1.97	0.46
1:B:206:PRO:HG3	1:B:215:LEU:CD1	2.46	0.46
1:E:162:ILE:HD12	1:E:175:ILE:HG12	1.98	0.46
1:B:263:ILE:CG2	1:B:285:LEU:HD22	2.41	0.46
1:A:126:PHE:CD1	1:A:134:LEU:HB2	2.50	0.46
1:B:228:LEU:HD12	1:B:231:PHE:CD2	2.50	0.46
1:C:139:ALA:HB2	1:C:178:PHE:CE1	2.51	0.46
1:C:188:VAL:HG21	1:C:190:HIS:CD2	2.50	0.46
1:D:231:PHE:HB2	1:D:233:PHE:HE1	1.80	0.46
1:E:141:LYS:HG3	1:E:146:SER:HA	1.97	0.46
1:C:257:ARG:O	1:C:260:LYS:HB2	2.16	0.45
1:E:94:LEU:O	1:F:38:THR:HG21	2.16	0.45
1:B:1:GLY:O	1:B:5:ILE:HG13	2.15	0.45
1:C:162:ILE:HG12	1:D:288:PRO:HB3	1.98	0.45
1:C:284:TYR:O	1:C:288:PRO:HA	2.16	0.45
1:D:321:GLU:O	1:D:321:GLU:HG3	2.15	0.45
1:D:330:ARG:NH1	1:D:346:GLN:OE1	2.49	0.45
1:A:264:LEU:HD11	1:A:282:VAL:CG1	2.47	0.45
1:A:239:GLY:HA2	1:A:247:GLY:C	2.42	0.45
1:C:38:THR:HB	1:D:92:ARG:HE	1.81	0.45
1:C:45:ASN:HB2	1:C:51:THR:HG23	1.98	0.45
1:D:219:MET:HE3	1:D:238:TYR:CD2	2.51	0.45
1:F:12:LYS:HG3	1:F:16:VAL:HG21	1.97	0.45
1:F:152:LEU:O	1:F:176:ASN:HA	2.16	0.45
1:A:102:CYS:HB3	1:A:105:THR:OG1	2.17	0.45
1:F:277:LEU:HD13	1:F:297:MET:HE3	1.98	0.45
1:A:194:PHE:CD2	1:A:303:ASP:HB3	2.52	0.45
1:C:164:THR:HG23	1:C:173:LYS:O	2.16	0.45
1:E:81:TYR:CE2	1:E:82:LYS:HG3	2.52	0.45
1:E:239:GLY:HA3	1:E:249:LEU:CD1	2.47	0.45
1:C:316:VAL:HG23	1:C:317:SER:N	2.32	0.45
1:F:334:TRP:HD1	1:F:342:THR:OG1	2.00	0.45
1:A:304:PHE:O	1:A:307:VAL:HB	2.16	0.45
1:C:140:VAL:O	1:C:147:LEU:HB2	2.16	0.45
1:E:147:LEU:HG	1:E:148:PRO:HD2	1.98	0.45
1:F:93:PRO:HB2	1:F:95:THR:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:TYR:HB2	1:D:228:LEU:HD22	1.99	0.44
1:D:150:ILE:O	1:D:178:PHE:HA	2.16	0.44
1:D:78:VAL:O	1:D:95:THR:HB	2.17	0.44
1:D:134:LEU:HD12	1:D:135:PHE:H	1.82	0.44
1:E:92:ARG:HD2	1:E:93:PRO:O	2.17	0.44
1:C:124:GLU:O	1:C:128:LEU:HD23	2.18	0.44
1:E:232:ASN:HB3	1:E:236:VAL:CG2	2.48	0.44
1:F:10:VAL:HG22	1:F:42:VAL:HG11	1.98	0.44
1:C:210:MET:HE1	1:C:305:VAL:CG2	2.45	0.44
1:C:241:VAL:HG11	1:C:284:TYR:CD1	2.52	0.44
1:D:324:ILE:HB	1:D:329:TRP:CD1	2.53	0.44
1:E:123:TYR:O	1:E:126:PHE:HB3	2.18	0.44
1:A:80:THR:HG22	1:A:114:CYS:HB3	1.99	0.44
1:E:219:MET:HB2	1:E:238:TYR:CE2	2.53	0.44
1:F:3:GLU:OE1	1:F:3:GLU:N	2.48	0.44
1:F:115:TYR:HB2	1:F:134:LEU:HD12	1.98	0.44
1:B:62:LYS:HG2	1:B:66:THR:HG22	2.00	0.43
1:C:217:MET:HE3	1:C:217:MET:HB3	1.87	0.43
1:E:69:LEU:HD22	1:E:94:LEU:HD22	1.99	0.43
1:A:260:LYS:HB3	1:A:260:LYS:HE3	1.84	0.43
1:B:142:ALA:HA	1:B:143:GLY:HA2	1.48	0.43
1:E:233:PHE:CE1	1:E:237:VAL:HG21	2.53	0.43
1:B:312:ASP:HB3	1:B:318:LYS:NZ	2.34	0.43
1:C:190:HIS:C	1:C:192:ASP:HB2	2.44	0.43
1:E:45:ASN:HD22	1:E:51:THR:HA	1.83	0.43
1:A:1:GLY:O	1:A:5:ILE:HG13	2.18	0.43
1:A:163:ALA:HB2	1:A:207:ARG:NH2	2.33	0.43
1:B:239:GLY:HA3	1:B:249:LEU:CD1	2.48	0.43
1:B:331:TRP:HB3	1:B:343:PHE:CE2	2.53	0.43
1:D:80:THR:HG22	1:D:114:CYS:HB3	1.99	0.43
1:D:279:CYS:SG	1:D:293:VAL:HG13	2.58	0.43
1:D:194:PHE:HB2	1:D:323:ILE:O	2.18	0.43
1:E:226:TYR:HB2	1:E:228:LEU:CD2	2.49	0.43
1:F:192:ASP:N	1:F:192:ASP:OD1	2.49	0.43
1:C:16:VAL:HG23	1:C:18:ALA:H	1.84	0.43
1:F:150:ILE:HB	1:F:179:VAL:HB	2.00	0.43
1:A:335:CYS:CB	1:A:340:VAL:HA	2.49	0.43
1:A:277:LEU:HD13	1:A:297:MET:HE3	2.01	0.43
1:C:311:LEU:HD22	1:C:320:HIS:CD2	2.54	0.43
1:D:141:LYS:HA	1:D:141:LYS:HD3	1.72	0.43
1:E:84:VAL:HG12	1:E:101:VAL:HG11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:PRO:HD2	1:E:173:LYS:HG3	2.01	0.42
1:E:157:LEU:HB2	1:E:162:ILE:HD13	2.01	0.42
1:E:315:VAL:O	1:E:335:CYS:HB2	2.19	0.42
1:F:199:ARG:NH1	1:F:207:ARG:HG3	2.34	0.42
1:F:324:ILE:HB	1:F:329:TRP:CD1	2.54	0.42
1:E:57:LEU:HD11	1:E:105:THR:HG21	2.02	0.42
1:B:312:ASP:OD1	1:B:314:THR:HG23	2.19	0.42
1:E:246:LEU:HD13	1:E:249:LEU:HD22	2.01	0.42
1:D:239:GLY:HA2	1:D:247:GLY:O	2.19	0.42
1:C:30:LYS:HE3	1:C:30:LYS:HB2	1.92	0.42
1:E:16:VAL:HG23	1:E:18:ALA:H	1.85	0.42
1:A:315:VAL:HG11	1:A:318:LYS:HB2	2.01	0.42
1:A:317:SER:HB2	1:A:334:TRP:CZ3	2.55	0.42
1:A:336:LYS:HG2	1:A:337:ASP:OD1	2.19	0.42
1:B:313:LEU:HD12	1:B:313:LEU:HA	1.83	0.42
1:C:80:THR:HG22	1:C:114:CYS:HB3	2.02	0.42
1:D:301:LEU:O	1:D:305:VAL:HG13	2.20	0.42
1:E:233:PHE:CZ	1:E:237:VAL:HG21	2.54	0.42
1:F:232:ASN:O	1:F:236:VAL:HG23	2.20	0.42
1:A:8:ASN:HB3	1:A:15:PHE:HA	2.02	0.42
1:C:258:LEU:HB3	1:C:264:LEU:HD22	2.00	0.42
1:F:172:ILE:C	1:F:172:ILE:HD12	2.44	0.42
1:B:226:TYR:HB2	1:B:228:LEU:HD21	1.98	0.42
1:A:175:ILE:HD13	1:A:175:ILE:HA	1.84	0.42
1:A:316:VAL:HG23	1:A:317:SER:H	1.85	0.42
1:D:140:VAL:HG12	1:D:147:LEU:HD13	2.02	0.42
1:D:250:HIS:O	1:D:251:LEU:HD23	2.20	0.42
1:B:65:LEU:HD23	1:B:162:ILE:HD11	2.01	0.41
1:B:236:VAL:CG2	1:B:343:PHE:H	2.23	0.41
1:C:291:LYS:CG	1:C:294:CYS:HB2	2.50	0.41
1:D:60:LYS:HD2	1:D:101:VAL:HG12	2.02	0.41
1:F:8:ASN:HB3	1:F:14:SER:O	2.20	0.41
1:C:333:LEU:HD12	1:C:334:TRP:N	2.35	0.41
1:B:65:LEU:HG	1:B:157:LEU:HD13	2.01	0.41
1:C:183:LYS:HG2	1:C:184:ASP:OD2	2.19	0.41
1:E:61:ARG:HA	1:E:84:VAL:HG22	2.02	0.41
1:F:263:ILE:HG21	1:F:285:LEU:HD22	2.03	0.41
1:B:255:GLN:O	1:B:259:SER:HB2	2.20	0.41
1:F:63:VAL:HG12	1:F:64:GLY:N	2.35	0.41
1:A:57:LEU:HD22	1:A:84:VAL:HG11	2.02	0.41
1:C:8:ASN:HB3	1:C:14:SER:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:ARG:NH1	1:D:207:ARG:HG3	2.35	0.41
1:E:129:SER:O	1:E:182:ARG:NH2	2.52	0.41
1:F:20:GLY:C	1:F:21:GLU:HG2	2.46	0.41
1:F:213:ASP:HB3	1:F:217:MET:SD	2.60	0.41
1:A:319:VAL:HG11	1:A:330:ARG:HH11	1.84	0.41
1:A:336:LYS:HG2	1:A:337:ASP:N	2.35	0.41
1:D:7:PHE:HA	1:D:22:LEU:HD12	2.02	0.41
1:E:131:ASN:HA	1:E:182:ARG:O	2.20	0.41
1:F:115:TYR:CB	1:F:134:LEU:HD12	2.51	0.41
1:C:197:GLN:HB3	1:C:207:ARG:HH21	1.85	0.41
1:B:5:ILE:HD13	1:B:56:GLU:HG3	2.03	0.41
1:E:214:PHE:CD2	1:E:253:ILE:HG12	2.55	0.41
1:A:5:ILE:HD13	1:A:56:GLU:HG3	2.03	0.41
1:B:166:LYS:HA	1:B:171:ASN:O	2.20	0.41
1:C:75:LEU:HD23	1:C:326:ASN:HD22	1.86	0.41
1:C:104:TYR:CE1	1:E:25:ALA:HB2	2.56	0.41
1:C:162:ILE:HD12	1:C:162:ILE:HA	1.75	0.41
1:E:186:LYS:HB2	1:E:186:LYS:HE2	1.89	0.41
1:F:287:ASP:O	1:F:288:PRO:C	2.63	0.41
1:F:313:LEU:HD12	1:F:313:LEU:HA	1.88	0.41
1:A:163:ALA:HB3	1:A:207:ARG:HD2	2.02	0.40
1:C:331:TRP:HB3	1:C:343:PHE:CE2	2.56	0.40
1:E:324:ILE:HB	1:E:329:TRP:CD1	2.57	0.40
1:F:74:ASN:HB3	1:F:327:LYS:HG3	2.03	0.40
1:B:208:SER:O	1:B:212:GLU:HG3	2.21	0.40
1:B:219:MET:H	1:B:219:MET:HG2	1.71	0.40
1:C:81:TYR:O	1:C:83:PHE:HD2	2.04	0.40
1:C:123:TYR:O	1:C:127:THR:HG23	2.22	0.40
1:D:57:LEU:HD11	1:D:105:THR:HG21	2.02	0.40
1:D:142:ALA:H	1:D:147:LEU:HD11	1.85	0.40
1:D:344:TYR:HB2	1:D:345:PRO:HD2	2.04	0.40
1:B:157:LEU:HB2	1:B:162:ILE:CD1	2.51	0.40
1:B:219:MET:HB3	1:B:238:TYR:CZ	2.56	0.40
1:C:115:TYR:HB2	1:C:134:LEU:HD12	2.03	0.40
1:D:219:MET:HE3	1:D:238:TYR:CG	2.56	0.40
1:E:82:LYS:O	1:E:83:PHE:HB3	2.21	0.40
1:A:333:LEU:HD11	1:A:335:CYS:HB3	2.03	0.40
1:B:205:LEU:HA	1:B:206:PRO:HD3	1.96	0.40
1:D:8:ASN:HB3	1:D:15:PHE:HA	2.04	0.40
1:D:98:THR:HG22	1:D:105:THR:C	2.46	0.40
1:D:98:THR:HG22	1:D:106:ASP:HA	2.03	0.40

There are no symmetry-related clashes.

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	337/349 (97%)	325 (96%)	12 (4%)	0	100	100
1	B	341/349 (98%)	328 (96%)	12 (4%)	1 (0%)	36	59
1	C	322/349 (92%)	307 (95%)	14 (4%)	1 (0%)	36	59
1	D	331/349 (95%)	311 (94%)	18 (5%)	2 (1%)	21	45
1	E	337/349 (97%)	321 (95%)	16 (5%)	0	100	100
1	F	342/349 (98%)	332 (97%)	10 (3%)	0	100	100
All	All	2010/2094 (96%)	1924 (96%)	82 (4%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	VAL
1	D	237	VAL
1	D	190	HIS
1	C	246	LEU

5.3.2 Protein sidechains [i](#)

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	298/306 (97%)	280 (94%)	18 (6%)	17	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	299/306 (98%)	271 (91%)	28 (9%)	8	22
1	C	290/306 (95%)	252 (87%)	38 (13%)	4	12
1	D	293/306 (96%)	262 (89%)	31 (11%)	6	19
1	E	297/306 (97%)	267 (90%)	30 (10%)	7	20
1	F	303/306 (99%)	274 (90%)	29 (10%)	8	22
All	All	1780/1836 (97%)	1606 (90%)	174 (10%)	7	21

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	SER
1	A	42	VAL
1	A	63	VAL
1	A	70	SER
1	A	84	VAL
1	A	124	GLU
1	A	134	LEU
1	A	151	LYS
1	A	165	VAL
1	A	175	ILE
1	A	190	HIS
1	A	231	PHE
1	A	236	VAL
1	A	283	THR
1	A	315	VAL
1	A	316	VAL
1	A	319	VAL
1	A	326	ASN
1	B	17	SER
1	B	65	LEU
1	B	70	SER
1	B	71	ILE
1	B	84	VAL
1	B	95	THR
1	B	107	PHE
1	B	128	LEU
1	B	129	SER
1	B	134	LEU
1	B	165	VAL
1	B	189	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	192	ASP
1	B	224	GLN
1	B	228	LEU
1	B	234	GLU
1	B	236	VAL
1	B	244	THR
1	B	282	VAL
1	B	305	VAL
1	B	313	LEU
1	B	314	THR
1	B	316	VAL
1	B	318	LYS
1	B	321	GLU
1	B	322	VAL
1	B	337	ASP
1	B	346	GLN
1	C	27	SER
1	C	65	LEU
1	C	70	SER
1	C	73	LYS
1	C	84	VAL
1	C	111	VAL
1	C	129	SER
1	C	131	ASN
1	C	134	LEU
1	C	140	VAL
1	C	147	LEU
1	C	156	MET
1	C	162	ILE
1	C	175	ILE
1	C	176	ASN
1	C	186	LYS
1	C	190	HIS
1	C	219	MET
1	C	228	LEU
1	C	231	PHE
1	C	232	ASN
1	C	234	GLU
1	C	236	VAL
1	C	237	VAL
1	C	240	ASP
1	C	244	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	246	LEU
1	C	251	LEU
1	C	270	VAL
1	C	275	ILE
1	C	282	VAL
1	C	305	VAL
1	C	313	LEU
1	C	315	VAL
1	C	324	ILE
1	C	327	LYS
1	C	332	MET
1	C	340	VAL
1	D	10	VAL
1	D	33	VAL
1	D	46	LYS
1	D	84	VAL
1	D	98	THR
1	D	128	LEU
1	D	129	SER
1	D	140	VAL
1	D	151	LYS
1	D	162	ILE
1	D	186	LYS
1	D	188	VAL
1	D	208	SER
1	D	209	THR
1	D	221	VAL
1	D	223	ILE
1	D	228	LEU
1	D	230	ASP
1	D	244	THR
1	D	245	THR
1	D	251	LEU
1	D	252	SER
1	D	282	VAL
1	D	291	LYS
1	D	307	VAL
1	D	308	LEU
1	D	313	LEU
1	D	316	VAL
1	D	333	LEU
1	D	340	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	342	THR
1	E	17	SER
1	E	42	VAL
1	E	63	VAL
1	E	65	LEU
1	E	70	SER
1	E	84	VAL
1	E	92	ARG
1	E	109	GLU
1	E	129	SER
1	E	130	THR
1	E	146	SER
1	E	147	LEU
1	E	165	VAL
1	E	181	VAL
1	E	189	ASP
1	E	192	ASP
1	E	224	GLN
1	E	228	LEU
1	E	234	GLU
1	E	244	THR
1	E	254	SER
1	E	260	LYS
1	E	275	ILE
1	E	279	CYS
1	E	300	LEU
1	E	306	SER
1	E	319	VAL
1	E	322	VAL
1	E	324	ILE
1	E	326	ASN
1	F	21	GLU
1	F	70	SER
1	F	71	ILE
1	F	73	LYS
1	F	84	VAL
1	F	96	SER
1	F	110	ASP
1	F	129	SER
1	F	134	LEU
1	F	151	LYS
1	F	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	188	VAL
1	F	234	GLU
1	F	235	HIS
1	F	236	VAL
1	F	241	VAL
1	F	252	SER
1	F	261	MET
1	F	276	THR
1	F	278	LYS
1	F	291	LYS
1	F	292	THR
1	F	306	SER
1	F	311	LEU
1	F	313	LEU
1	F	315	VAL
1	F	316	VAL
1	F	322	VAL
1	F	326	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	176	ASN
1	A	320	HIS
1	B	171	ASN
1	B	216	ASN
1	B	326	ASN
1	C	11	ASN
1	C	174	ASN
1	C	176	ASN
1	C	190	HIS
1	C	326	ASN
1	D	11	ASN
1	D	117	ASN
1	D	153	ASN
1	D	174	ASN
1	D	320	HIS
1	E	216	ASN
1	E	232	ASN
1	F	153	ASN
1	F	171	ASN
1	F	174	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	338	ASN

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	341/349 (97%)	-0.06	4 (1%) 76 71	32, 68, 115, 153	0
1	B	345/349 (98%)	-0.23	2 (0%) 85 82	33, 56, 100, 137	0
1	C	332/349 (95%)	0.16	8 (2%) 59 51	45, 80, 125, 144	0
1	D	337/349 (96%)	0.30	13 (3%) 43 35	37, 85, 145, 171	0
1	E	341/349 (97%)	-0.16	4 (1%) 76 71	39, 62, 99, 136	0
1	F	346/349 (99%)	-0.32	0 100 100	35, 52, 93, 143	0
All	All	2042/2094 (97%)	-0.06	31 (1%) 72 65	32, 67, 118, 171	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	337	ASP	4.5
1	A	172	ILE	4.3
1	D	313	LEU	4.2
1	D	144	GLY	3.7
1	E	172	ILE	3.6
1	D	189	ASP	3.5
1	D	316	VAL	3.4
1	C	340	VAL	3.2
1	C	313	LEU	3.1
1	C	165	VAL	3.1
1	D	340	VAL	2.8
1	A	142	ALA	2.8
1	D	333	LEU	2.7
1	D	320	HIS	2.6
1	C	172	ILE	2.6
1	D	190	HIS	2.5
1	A	236	VAL	2.4
1	C	68	PRO	2.4
1	D	165	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	148	PRO	2.3
1	E	144	GLY	2.3
1	B	346	GLN	2.2
1	A	346	GLN	2.2
1	D	222	PHE	2.1
1	B	95	THR	2.1
1	C	149	ALA	2.1
1	D	236	VAL	2.1
1	D	226	TYR	2.0
1	E	340	VAL	2.0
1	D	142	ALA	2.0
1	E	142	ALA	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.