



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:27 PM UTC

PDB ID : 1FG2 / pdb_00001fg2
Title : CRYSTAL STRUCTURE OF THE LCMV PEPTIDIC EPITOPE GP33 IN
COMPLEX WITH THE MURINE CLASS I MHC MOLECULE H-2DB
Authors : Tissot, A.C.; Ciatto, C.; Mittl, P.R.E.; Gruetter, M.G.; Plueckthun, A.
Deposited on : 2000-07-27
Resolution : 2.75 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:

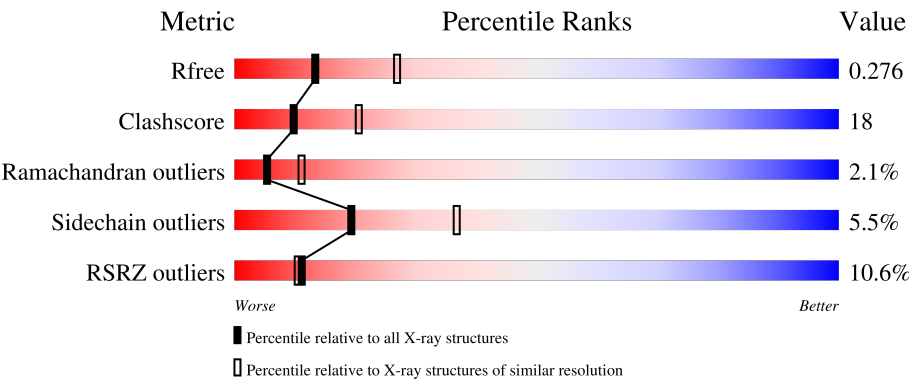
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.75 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.



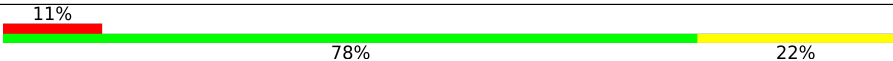
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	281	13% 62% 30% 5%
1	D	281	10% 63% 30%
1	G	281	17% 63% 29% 5%
1	J	281	7% 63% 29% 5%
2	B	100	7% 66% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	E	100	
2	H	100	
2	K	100	
3	C	9	
3	F	9	
3	I	9	
3	L	9	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12656 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 H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	D	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	G	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			
1	J	273	Total	C	N	O	S	0	0	0
			2244	1418	397	420	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P01899
D	0	MET	-	initiating methionine	UNP P01899
G	0	MET	-	initiating methionine	UNP P01899
J	0	MET	-	initiating methionine	UNP P01899

- Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	E	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	H	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			
2	K	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P01887
E	0	MET	-	initiating methionine	UNP P01887
H	0	MET	-	initiating methionine	UNP P01887
K	0	MET	-	initiating methionine	UNP P01887

- Molecule 3 is a protein called LCMV PEPTIDIC EPITOPE GP33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			
3	F	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			
3	I	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			
3	L	9	Total	C	N	O	S	0	0	0
			71	46	11	13	1			

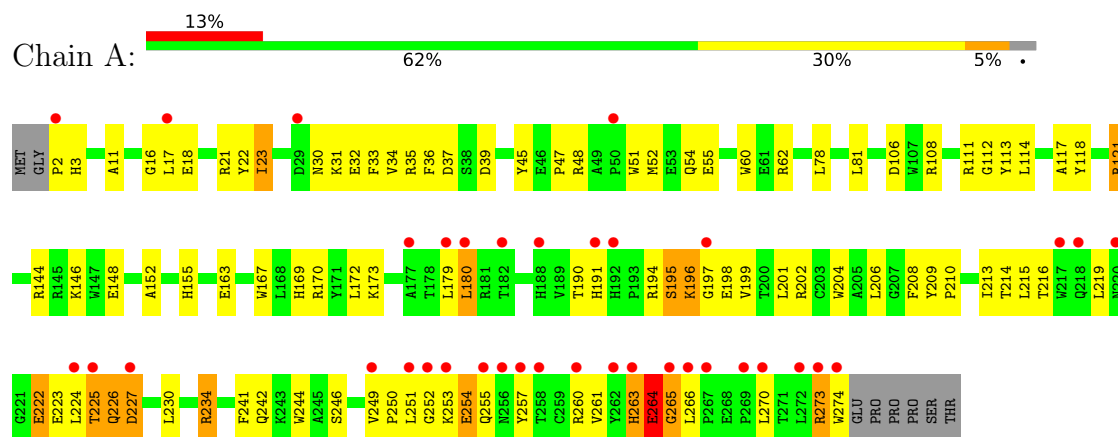
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	14	Total	O	0	0
			14	14		
4	C	2	Total	O	0	0
			2	2		
4	D	14	Total	O	0	0
			14	14		
4	E	13	Total	O	0	0
			13	13		
4	G	15	Total	O	0	0
			15	15		
4	H	8	Total	O	0	0
			8	8		
4	I	1	Total	O	0	0
			1	1		
4	J	18	Total	O	0	0
			18	18		
4	K	9	Total	O	0	0
			9	9		
4	L	2	Total	O	0	0
			2	2		

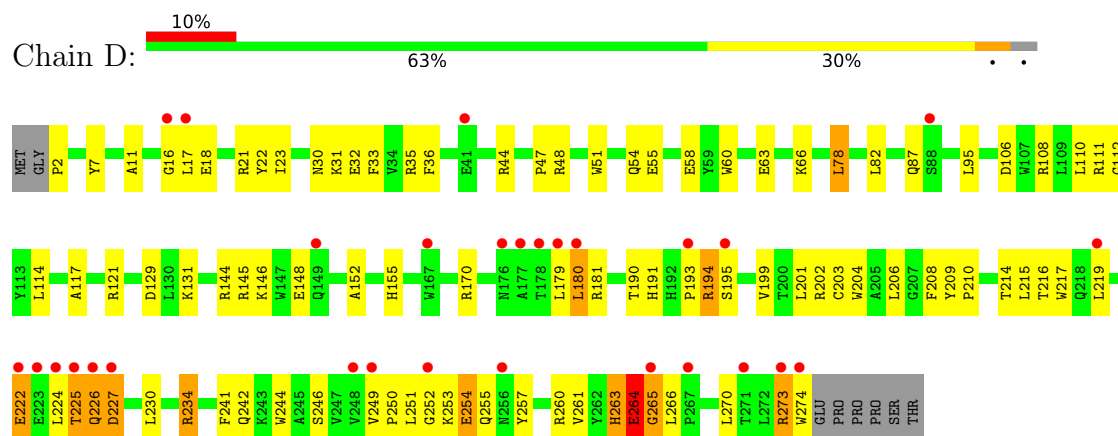
3 Residue-property plots [i](#)

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.

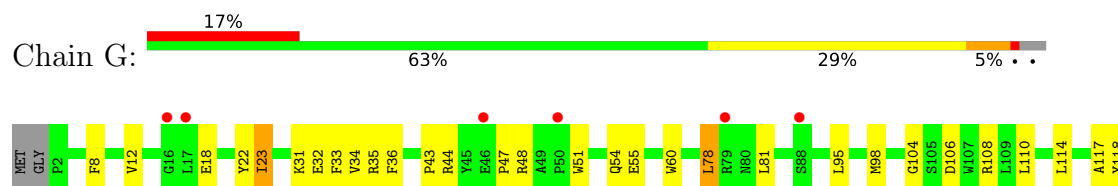
- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN

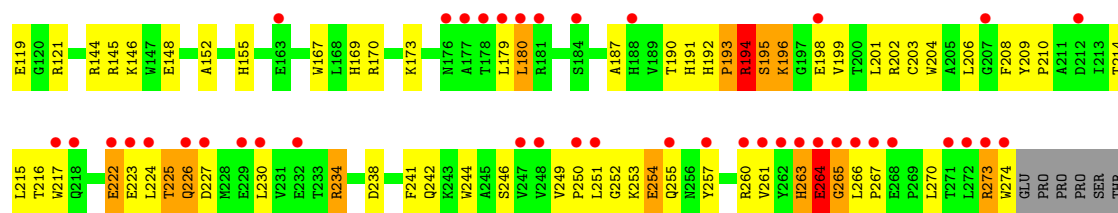


- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN

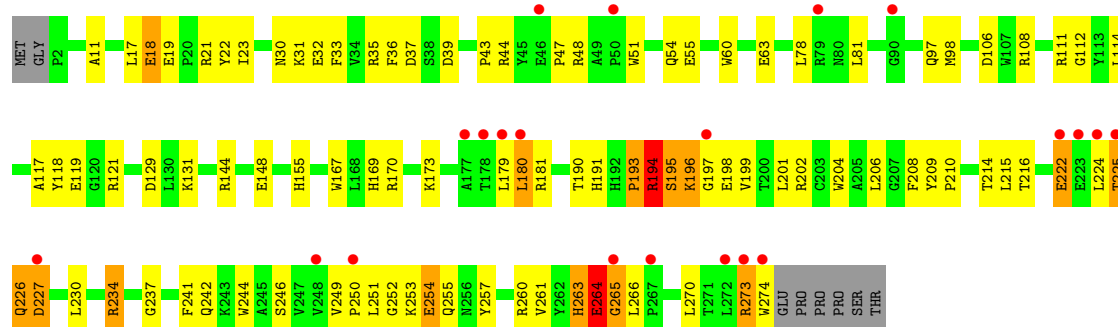


- Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN

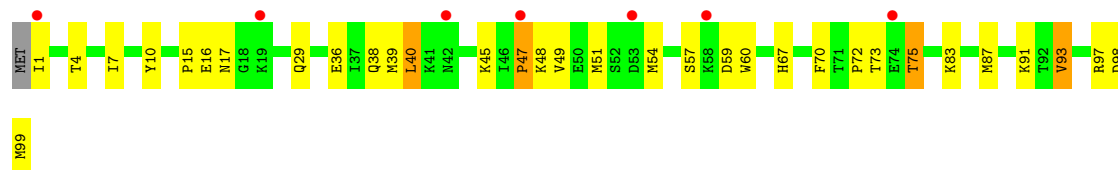




• Molecule 1: H-2 CLASS I HISTOCOMPATIBILITY ANTIGEN, D-B ALPHA CHAIN



• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 2: BETA-2 MICROGLOBULIN



• Molecule 2: BETA-2 MICROGLOBULIN

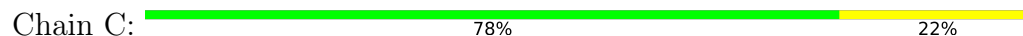


• Molecule 2: BETA-2 MICROGLOBULIN

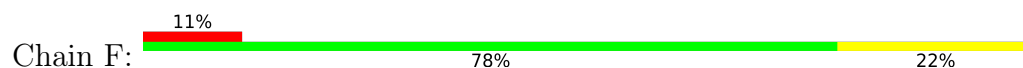




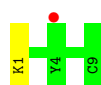
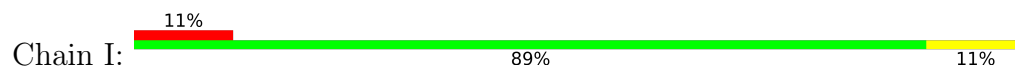
- Molecule 3: LCMV PEPTIDIC EPITOPE GP33



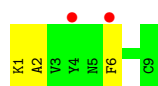
- Molecule 3: LCMV PEPTIDIC EPITOPE GP33



- Molecule 3: LCMV PEPTIDIC EPITOPE GP33



- Molecule 3: LCMV PEPTIDIC EPITOPE GP33



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.53Å 124.77Å 99.56Å 90.00° 103.03° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.75) 90.2 (30.00-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.76Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.236 , 0.276 0.235 , 0.276	Depositor DCC
R_{free} test set	5197 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12656	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% 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	0.55	0/2310	0.91	6/3136 (0.2%)
1	D	0.50	0/2310	0.91	5/3136 (0.2%)
1	G	0.52	0/2310	0.97	8/3136 (0.3%)
1	J	0.55	0/2310	0.96	7/3136 (0.2%)
2	B	0.55	0/847	0.96	2/1148 (0.2%)
2	E	0.56	0/847	0.97	1/1148 (0.1%)
2	H	0.59	0/847	0.98	3/1148 (0.3%)
2	K	0.58	0/847	0.99	2/1148 (0.2%)
3	C	0.77	0/72	1.11	0/95
3	F	0.72	0/72	1.09	0/95
3	I	0.78	0/72	1.05	0/95
3	L	0.72	0/72	0.90	0/95
All	All	0.55	0/12916	0.95	34/17516 (0.2%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	195	SER	N-CA-C	-11.14	96.29	113.89
1	J	195	SER	N-CA-C	-9.11	99.07	111.55
1	J	194	ARG	N-CA-C	7.83	120.86	110.53
1	G	192	HIS	CA-C-N	7.25	128.91	119.84
1	G	192	HIS	C-N-CA	7.25	128.91	119.84
1	A	263	HIS	N-CA-C	5.93	123.44	110.80
1	A	197	GLY	N-CA-C	-5.89	107.04	115.64
1	J	263	HIS	N-CA-C	5.88	123.33	110.80
1	A	264	GLU	N-CA-C	-5.81	98.43	110.80
1	G	194	ARG	N-CA-C	5.74	123.02	110.80
1	G	263	HIS	N-CA-C	5.66	122.86	110.80
1	D	263	HIS	N-CA-C	5.64	122.81	110.80
1	J	264	GLU	N-CA-C	-5.64	98.79	110.80
2	H	73	THR	N-CA-C	-5.63	100.95	109.85
2	K	73	THR	N-CA-C	-5.63	100.96	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	73	THR	N-CA-C	-5.55	101.08	109.85
1	D	264	GLU	N-CA-C	-5.53	99.01	110.80
1	G	264	GLU	N-CA-C	-5.48	99.13	110.80
2	K	40	LEU	N-CA-C	5.39	118.25	109.24
1	J	225	THR	N-CA-C	-5.38	107.02	113.21
2	B	73	THR	N-CA-C	-5.38	101.35	109.85
1	D	30	ASN	N-CA-C	5.38	119.42	112.86
1	G	225	THR	N-CA-C	-5.36	107.04	113.21
1	D	2	PRO	N-CA-CB	5.36	108.89	103.00
1	A	225	THR	N-CA-C	-5.28	107.14	113.21
1	J	30	ASN	N-CA-C	5.27	119.29	112.86
2	H	5	PRO	N-CA-C	5.21	119.36	111.19
2	B	40	LEU	N-CA-C	5.19	117.90	109.24
1	A	30	ASN	N-CA-C	5.16	119.53	113.23
1	A	2	PRO	N-CA-CB	5.11	108.62	103.00
2	H	40	LEU	N-CA-C	5.11	117.77	109.24
1	J	18	GLU	N-CA-C	5.06	117.20	111.02
1	D	225	THR	N-CA-C	-5.04	107.42	113.21
1	G	187	ALA	N-CA-C	5.03	117.94	109.95

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	2244	0	2118	91	0
1	D	2244	0	2118	87	0
1	G	2244	0	2118	81	0
1	J	2244	0	2118	88	0
2	B	821	0	796	37	0
2	E	821	0	796	27	0
2	H	821	0	796	29	0
2	K	821	0	796	27	0
3	C	71	0	70	8	0
3	F	71	0	70	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	71	0	70	1	0
3	L	71	0	70	3	0
4	A	16	0	0	1	0
4	B	14	0	0	4	0
4	C	2	0	0	1	0
4	D	14	0	0	2	0
4	E	13	0	0	1	0
4	G	15	0	0	0	0
4	H	8	0	0	0	0
4	I	1	0	0	0	0
4	J	18	0	0	2	0
4	K	9	0	0	3	0
4	L	2	0	0	1	0
All	All	12656	0	11936	431	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 18.

All (431) 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:G:194:ARG:HB2	1:G:196:LYS:H	1.26	0.99
2:B:75:THR:O	4:B:100:HOH:O	1.83	0.97
1:D:263:HIS:O	1:D:264:GLU:HB2	1.66	0.94
1:G:263:HIS:O	1:G:264:GLU:HB2	1.68	0.92
2:H:39:MET:HE3	2:H:49:VAL:HG13	1.52	0.92
1:A:263:HIS:O	1:A:264:GLU:HB2	1.71	0.91
1:J:263:HIS:O	1:J:264:GLU:HB2	1.69	0.88
1:G:255:GLN:HE22	1:G:274:TRP:HB3	1.38	0.87
1:A:255:GLN:HE22	1:A:274:TRP:HB3	1.39	0.86
1:J:255:GLN:HE22	1:J:274:TRP:HB3	1.38	0.86
1:D:255:GLN:HE22	1:D:274:TRP:HB3	1.41	0.85
2:E:39:MET:HE3	2:E:49:VAL:HG13	1.58	0.85
1:G:119:GLU:HB3	2:H:1:ILE:HD13	1.57	0.84
1:D:66:LYS:HZ1	3:F:1:LYS:HG2	1.40	0.83
2:K:39:MET:HE3	2:K:49:VAL:HG13	1.59	0.83
1:G:119:GLU:HB3	2:H:1:ILE:CD1	2.08	0.82
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.17	0.80
2:B:39:MET:HE3	2:B:49:VAL:HG13	1.65	0.78
1:G:194:ARG:HA	1:G:198:GLU:O	1.83	0.78
1:J:155:HIS:HB3	3:L:6:PHE:CZ	2.19	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:ARG:CD	1:J:194:ARG:H	1.95	0.77
1:J:194:ARG:H	1:J:194:ARG:HD2	1.49	0.76
2:H:1:ILE:HG23	2:H:1:ILE:O	1.89	0.73
2:K:39:MET:HE1	2:K:67:HIS:CA	2.19	0.73
1:D:16:GLY:C	1:D:18:GLU:H	1.97	0.73
2:B:39:MET:HE1	2:B:67:HIS:CA	2.19	0.73
2:B:87:MET:HE1	2:B:91:LYS:HB2	1.71	0.73
1:A:234:ARG:HD3	2:B:10:TYR:CE2	2.24	0.72
1:A:273:ARG:H	1:A:273:ARG:HD3	1.54	0.72
2:H:87:MET:HE1	2:H:91:LYS:HB2	1.70	0.71
2:K:3:LYS:HE3	4:K:106:HOH:O	1.90	0.71
1:A:194:ARG:HG3	1:A:198:GLU:O	1.90	0.71
1:D:66:LYS:HZ1	3:F:1:LYS:CG	2.03	0.71
2:E:87:MET:HE1	2:E:91:LYS:HB2	1.72	0.71
2:E:1:ILE:HG23	2:E:1:ILE:O	1.89	0.71
1:G:273:ARG:H	1:G:273:ARG:HD3	1.56	0.71
2:B:1:ILE:HG23	2:B:1:ILE:O	1.91	0.71
1:D:263:HIS:O	1:D:264:GLU:CB	2.38	0.71
1:A:254:GLU:HG3	1:A:255:GLN:HE21	1.55	0.70
2:E:39:MET:HE1	2:E:67:HIS:CA	2.21	0.70
1:G:263:HIS:O	1:G:264:GLU:CB	2.40	0.69
1:J:263:HIS:O	1:J:264:GLU:CB	2.41	0.69
1:J:273:ARG:HD3	1:J:273:ARG:H	1.56	0.69
2:K:87:MET:HE1	2:K:91:LYS:HB2	1.75	0.69
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.28	0.69
2:B:75:THR:HG23	4:B:100:HOH:O	1.92	0.68
2:K:1:ILE:HG23	2:K:1:ILE:O	1.92	0.68
1:A:62:ARG:NH1	3:C:1:LYS:HD2	2.09	0.68
1:G:254:GLU:HG3	1:G:255:GLN:HE21	1.59	0.68
1:A:251:LEU:HD23	1:A:252:GLY:N	2.09	0.68
1:A:121:ARG:NH1	2:B:1:ILE:HG13	2.08	0.68
1:J:254:GLU:HG3	1:J:255:GLN:HE21	1.59	0.68
1:D:58:GLU:CD	1:D:58:GLU:H	2.01	0.68
1:D:251:LEU:HD23	1:D:252:GLY:N	2.09	0.67
1:D:254:GLU:HG3	1:D:255:GLN:HE21	1.58	0.67
2:H:39:MET:HE1	2:H:67:HIS:CA	2.23	0.67
1:D:193:PRO:O	1:D:194:ARG:HG3	1.95	0.67
1:J:251:LEU:HD23	1:J:252:GLY:N	2.09	0.67
1:G:35:ARG:NH2	2:H:54:MET:O	2.23	0.67
1:D:32:GLU:OE2	1:D:48:ARG:HD2	1.95	0.66
1:A:263:HIS:O	1:A:264:GLU:CB	2.43	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ARG:HD3	2:E:10:TYR:CE2	2.31	0.66
1:G:32:GLU:OE2	1:G:48:ARG:HD2	1.95	0.66
1:J:234:ARG:HD3	2:K:10:TYR:CE2	2.31	0.66
1:D:273:ARG:H	1:D:273:ARG:HD3	1.59	0.66
1:G:251:LEU:HD23	1:G:252:GLY:N	2.09	0.66
1:D:202:ARG:HG2	1:D:204:TRP:NE1	2.11	0.66
1:J:117:ALA:HB2	2:K:60:TRP:CE2	2.32	0.65
1:A:121:ARG:CZ	2:B:1:ILE:CD1	2.75	0.65
2:B:16:GLU:HG3	2:K:88:ALA:HB3	1.77	0.65
1:J:222:GLU:CD	1:J:222:GLU:H	2.05	0.64
1:D:63:GLU:OE2	3:F:1:LYS:HG3	1.98	0.64
1:D:222:GLU:H	1:D:222:GLU:CD	2.05	0.64
1:G:119:GLU:CB	2:H:1:ILE:CD1	2.75	0.64
1:A:222:GLU:CD	1:A:222:GLU:H	2.06	0.63
1:D:66:LYS:NZ	3:F:1:LYS:HG2	2.11	0.63
1:J:43:PRO:O	1:J:44:ARG:HG3	1.97	0.63
1:A:23:ILE:N	1:A:23:ILE:HD12	2.13	0.63
1:A:202:ARG:HG2	1:A:204:TRP:NE1	2.13	0.62
1:J:194:ARG:HG3	1:J:199:VAL:CG1	2.29	0.62
1:J:201:LEU:HD12	1:J:249:VAL:HG21	1.80	0.62
1:A:31:LYS:HD3	1:A:179:LEU:CD2	2.30	0.62
1:G:222:GLU:CD	1:G:222:GLU:H	2.08	0.62
1:G:47:PRO:HG3	1:G:60:TRP:CZ2	2.34	0.62
1:G:264:GLU:O	1:G:266:LEU:N	2.32	0.62
1:G:23:ILE:N	1:G:23:ILE:HD12	2.15	0.62
1:A:31:LYS:HD3	1:A:179:LEU:HD21	1.81	0.61
1:J:23:ILE:HD12	1:J:23:ILE:N	2.14	0.61
1:A:214:THR:C	1:A:215:LEU:HD12	2.26	0.61
1:D:23:ILE:N	1:D:23:ILE:HD12	2.16	0.61
2:E:36:GLU:HB2	2:E:83:LYS:HB3	1.82	0.61
1:J:32:GLU:OE2	1:J:48:ARG:HD2	2.00	0.61
1:J:194:ARG:HD2	1:J:194:ARG:N	2.13	0.61
1:J:202:ARG:HG2	1:J:204:TRP:NE1	2.15	0.61
1:A:201:LEU:HD12	1:A:249:VAL:HG21	1.83	0.61
1:G:234:ARG:HD3	2:H:10:TYR:CE2	2.36	0.61
1:G:202:ARG:HG2	1:G:204:TRP:NE1	2.16	0.61
1:G:264:GLU:C	1:G:266:LEU:N	2.59	0.61
1:G:144:ARG:O	1:G:148:GLU:HG3	2.01	0.60
1:G:201:LEU:HD12	1:G:249:VAL:HG21	1.83	0.60
1:J:214:THR:C	1:J:215:LEU:HD12	2.27	0.60
1:A:32:GLU:OE2	1:A:48:ARG:HD2	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:GLU:HB2	2:H:83:LYS:HB3	1.83	0.60
1:D:117:ALA:HB2	2:E:60:TRP:CZ2	2.37	0.59
2:K:36:GLU:HB2	2:K:83:LYS:HB3	1.84	0.59
1:J:18:GLU:HG2	1:J:19:GLU:HG2	1.84	0.59
1:G:264:GLU:C	1:G:266:LEU:H	2.09	0.59
2:B:36:GLU:HB2	2:B:83:LYS:HB3	1.83	0.59
2:K:54:MET:HA	4:K:102:HOH:O	2.02	0.59
1:D:31:LYS:HD3	1:D:179:LEU:CD2	2.33	0.59
1:A:202:ARG:HD2	1:A:244:TRP:CD2	2.37	0.59
1:D:266:LEU:HD21	1:D:270:LEU:HG	1.84	0.59
1:J:31:LYS:HD3	1:J:179:LEU:CD2	2.32	0.59
1:J:31:LYS:HD3	1:J:179:LEU:HD21	1.83	0.59
1:J:202:ARG:HD2	1:J:244:TRP:CD2	2.38	0.58
1:G:31:LYS:HD3	1:G:179:LEU:CD2	2.33	0.58
2:B:39:MET:HE1	2:B:67:HIS:HA	1.84	0.58
1:D:201:LEU:HD12	1:D:249:VAL:HG21	1.86	0.58
1:A:250:PRO:HG2	1:A:253:LYS:HB2	1.85	0.58
1:G:202:ARG:HD2	1:G:244:TRP:CD2	2.39	0.57
1:J:250:PRO:HG2	1:J:253:LYS:HB2	1.86	0.57
1:D:31:LYS:HD3	1:D:179:LEU:HD21	1.86	0.57
1:D:191:HIS:NE2	1:D:199:VAL:HG21	2.19	0.57
1:G:250:PRO:HG2	1:G:253:LYS:HB2	1.87	0.57
1:J:194:ARG:HE	1:J:251:LEU:HD12	1.68	0.57
1:G:194:ARG:HB2	1:G:196:LYS:N	2.09	0.57
1:A:266:LEU:HD21	1:A:270:LEU:HG	1.87	0.57
1:G:119:GLU:CB	2:H:1:ILE:HD11	2.34	0.57
1:G:98:MET:HE2	2:H:60:TRP:CH2	2.40	0.57
1:J:264:GLU:O	1:J:266:LEU:N	2.37	0.57
1:A:264:GLU:O	1:A:266:LEU:N	2.36	0.57
1:A:264:GLU:C	1:A:266:LEU:N	2.62	0.56
1:D:214:THR:C	1:D:215:LEU:HD12	2.29	0.56
1:D:264:GLU:O	1:D:266:LEU:N	2.38	0.56
2:H:39:MET:HE3	2:H:49:VAL:CG1	2.32	0.56
1:G:266:LEU:HD21	1:G:270:LEU:HG	1.87	0.56
2:K:39:MET:HE1	2:K:67:HIS:HA	1.87	0.56
1:D:47:PRO:HG3	1:D:60:TRP:CZ2	2.41	0.56
1:A:32:GLU:OE2	1:A:35:ARG:HD2	2.06	0.56
1:A:273:ARG:HD3	1:A:273:ARG:N	2.19	0.56
1:D:264:GLU:C	1:D:266:LEU:N	2.62	0.56
1:G:31:LYS:HD3	1:G:179:LEU:HD21	1.86	0.56
1:J:194:ARG:HA	1:J:198:GLU:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:NH2	2:E:54:MET:O	2.38	0.56
1:G:191:HIS:NE2	1:G:199:VAL:HG21	2.20	0.56
1:D:44:ARG:HH11	1:D:44:ARG:HG3	1.71	0.55
1:D:202:ARG:HD2	1:D:244:TRP:CD2	2.42	0.55
1:J:35:ARG:NH2	2:K:54:MET:O	2.38	0.55
1:J:264:GLU:C	1:J:266:LEU:N	2.62	0.55
1:A:121:ARG:NH2	2:B:1:ILE:HD12	2.21	0.55
1:D:250:PRO:HG2	1:D:253:LYS:HB2	1.88	0.55
2:E:3:LYS:HE3	4:E:107:HOH:O	2.06	0.55
1:A:167:TRP:CE2	3:C:1:LYS:HG3	2.41	0.55
1:J:264:GLU:C	1:J:266:LEU:H	2.15	0.55
1:A:16:GLY:O	1:A:17:LEU:C	2.49	0.55
1:J:266:LEU:HD21	1:J:270:LEU:HG	1.88	0.55
1:G:117:ALA:HB2	2:H:60:TRP:CE2	2.42	0.55
2:B:75:THR:C	4:B:100:HOH:O	2.40	0.54
2:H:40:LEU:HD23	2:H:45:LYS:HA	1.88	0.54
1:D:264:GLU:C	1:D:266:LEU:H	2.13	0.54
1:J:194:ARG:HG3	1:J:199:VAL:HG12	1.89	0.54
1:A:191:HIS:NE2	1:A:199:VAL:HG21	2.23	0.54
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.90	0.54
1:G:214:THR:C	1:G:215:LEU:HD12	2.32	0.54
1:D:32:GLU:OE2	1:D:35:ARG:HD2	2.08	0.54
1:D:58:GLU:CD	1:D:58:GLU:N	2.66	0.54
2:K:39:MET:HE1	2:K:67:HIS:C	2.33	0.54
2:E:40:LEU:HD23	2:E:45:LYS:HA	1.90	0.53
1:J:47:PRO:HG3	1:J:60:TRP:CZ2	2.43	0.53
2:K:40:LEU:HD23	2:K:45:LYS:HA	1.90	0.53
2:K:47:PRO:HG2	2:K:48:LYS:H	1.72	0.53
1:A:47:PRO:HG3	1:A:60:TRP:CZ2	2.44	0.53
1:A:202:ARG:HH12	2:B:99:MET:HE3	1.73	0.53
1:A:264:GLU:C	1:A:266:LEU:H	2.14	0.53
1:G:179:LEU:O	1:G:180:LEU:HB2	2.09	0.53
1:J:237:GLY:HA3	4:K:100:HOH:O	2.07	0.53
1:J:97:GLN:HG2	4:J:285:HOH:O	2.08	0.53
1:G:32:GLU:OE2	1:G:35:ARG:HD2	2.09	0.52
2:B:47:PRO:HG2	2:B:48:LYS:H	1.74	0.52
1:J:119:GLU:HB3	2:K:1:ILE:HD13	1.92	0.52
1:J:195:SER:O	1:J:196:LYS:HB2	2.10	0.52
1:A:121:ARG:CZ	2:B:1:ILE:HD12	2.38	0.52
1:A:213:ILE:HG22	4:A:296:HOH:O	2.09	0.52
1:G:119:GLU:CB	2:H:1:ILE:HD13	2.32	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:191:HIS:NE2	1:J:199:VAL:HG21	2.24	0.52
1:G:273:ARG:HD3	1:G:273:ARG:N	2.20	0.52
1:A:18:GLU:OE2	1:A:18:GLU:HA	2.10	0.52
1:A:179:LEU:O	1:A:180:LEU:HB2	2.10	0.52
1:G:119:GLU:HB2	2:H:1:ILE:HD11	1.92	0.52
1:D:16:GLY:C	1:D:18:GLU:N	2.62	0.52
1:A:152:ALA:O	1:A:155:HIS:HB3	2.10	0.51
1:J:194:ARG:HB3	1:J:198:GLU:C	2.35	0.51
1:J:224:LEU:C	1:J:226:GLN:H	2.19	0.51
1:G:33:PHE:C	1:G:48:ARG:HB2	2.34	0.51
1:J:167:TRP:CZ2	3:L:1:LYS:HE3	2.46	0.51
1:D:16:GLY:O	1:D:18:GLU:N	2.43	0.51
1:D:51:TRP:O	1:D:54:GLN:HG3	2.11	0.51
1:A:244:TRP:CH2	2:B:99:MET:HE2	2.46	0.51
2:H:47:PRO:HG2	2:H:48:LYS:H	1.75	0.51
2:E:39:MET:HE1	2:E:67:HIS:HA	1.91	0.50
1:J:179:LEU:O	1:J:180:LEU:HB2	2.11	0.50
1:G:43:PRO:O	1:G:44:ARG:HG3	2.11	0.50
1:D:33:PHE:C	1:D:48:ARG:HB2	2.36	0.50
1:G:195:SER:O	1:G:196:LYS:HB2	2.11	0.50
2:E:47:PRO:HG2	2:E:48:LYS:H	1.76	0.50
1:G:224:LEU:C	1:G:226:GLN:H	2.19	0.50
2:H:39:MET:HE1	2:H:67:HIS:C	2.36	0.50
1:A:55:GLU:CD	1:A:170:ARG:HH21	2.20	0.50
1:A:224:LEU:C	1:A:226:GLN:H	2.19	0.50
1:A:33:PHE:C	1:A:48:ARG:HB2	2.37	0.49
1:A:195:SER:O	1:A:196:LYS:C	2.55	0.49
1:A:121:ARG:NE	2:B:1:ILE:HD11	2.26	0.49
1:D:255:GLN:C	1:D:257:TYR:H	2.20	0.49
1:D:273:ARG:HD3	1:D:273:ARG:N	2.23	0.49
2:E:39:MET:HE1	2:E:67:HIS:N	2.28	0.49
2:H:10:TYR:CD1	2:H:10:TYR:N	2.81	0.49
1:J:33:PHE:C	1:J:48:ARG:HB2	2.37	0.49
2:B:39:MET:HE1	2:B:67:HIS:C	2.36	0.49
1:D:179:LEU:O	1:D:180:LEU:HB2	2.11	0.49
1:D:216:THR:OG1	1:D:260:ARG:HB2	2.13	0.49
1:A:62:ARG:HH12	3:C:1:LYS:HD2	1.76	0.49
2:E:10:TYR:N	2:E:10:TYR:CD1	2.79	0.49
2:E:39:MET:HE1	2:E:67:HIS:C	2.37	0.49
2:H:39:MET:HE1	2:H:67:HIS:HA	1.93	0.49
1:D:224:LEU:C	1:D:226:GLN:H	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:8:PHE:HB3	2:H:56:PHE:CE2	2.47	0.49
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.13	0.49
1:A:230:LEU:C	1:A:230:LEU:HD12	2.37	0.49
2:B:54:MET:HA	4:B:108:HOH:O	2.13	0.49
1:J:255:GLN:C	1:J:257:TYR:H	2.21	0.49
1:J:194:ARG:HG3	1:J:199:VAL:HG13	1.93	0.49
1:A:255:GLN:C	1:A:257:TYR:H	2.20	0.49
2:B:10:TYR:CD1	2:B:10:TYR:N	2.81	0.49
1:D:63:GLU:OE2	1:D:66:LYS:HE2	2.13	0.49
2:K:36:GLU:OE2	2:K:83:LYS:HD3	2.13	0.49
1:J:190:THR:OG1	1:J:202:ARG:HB3	2.12	0.48
1:A:144:ARG:O	1:A:148:GLU:HG3	2.13	0.48
1:D:144:ARG:O	1:D:148:GLU:HG3	2.13	0.48
1:A:216:THR:OG1	1:A:260:ARG:HB2	2.12	0.48
1:D:55:GLU:CD	1:D:170:ARG:HH21	2.21	0.48
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.95	0.48
1:A:111:ARG:HG2	1:A:112:GLY:N	2.28	0.48
1:G:190:THR:OG1	1:G:202:ARG:HB3	2.13	0.48
1:J:206:LEU:HD23	1:J:242:GLN:HB3	1.96	0.48
1:A:206:LEU:HD23	1:A:242:GLN:HB3	1.95	0.48
1:J:32:GLU:OE2	1:J:35:ARG:HD2	2.12	0.48
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.12	0.48
1:D:261:VAL:HB	1:D:270:LEU:HB2	1.96	0.48
2:H:7:ILE:HD12	2:H:7:ILE:N	2.28	0.48
1:D:66:LYS:NZ	3:F:2:ALA:O	2.46	0.48
1:G:255:GLN:C	1:G:257:TYR:H	2.21	0.48
1:J:261:VAL:HB	1:J:270:LEU:HB2	1.95	0.48
2:B:36:GLU:OE2	2:B:83:LYS:HD3	2.13	0.47
1:D:206:LEU:HD23	1:D:242:GLN:HB3	1.95	0.47
1:G:209:TYR:CD1	1:G:210:PRO:HA	2.49	0.47
2:H:36:GLU:OE2	2:H:83:LYS:HD3	2.14	0.47
1:J:63:GLU:OE1	4:J:287:HOH:O	2.20	0.47
3:L:2:ALA:HB1	4:L:11:HOH:O	2.14	0.47
1:D:234:ARG:NH2	2:E:99:MET:OXT	2.47	0.47
1:J:202:ARG:HD2	1:J:244:TRP:CE3	2.49	0.47
1:J:222:GLU:CD	1:J:222:GLU:N	2.72	0.47
1:A:225:THR:HG22	1:A:225:THR:O	2.14	0.47
2:E:36:GLU:OE2	2:E:83:LYS:HD3	2.14	0.47
2:K:10:TYR:CD1	2:K:10:TYR:N	2.81	0.47
1:D:209:TYR:CD1	1:D:210:PRO:HA	2.50	0.47
3:C:1:LYS:NZ	4:C:111:HOH:O	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:ARG:HD3	1:D:246:SER:HB3	1.96	0.47
2:H:1:ILE:O	2:H:1:ILE:CG2	2.61	0.47
1:J:225:THR:HG22	1:J:225:THR:O	2.15	0.47
2:B:87:MET:HE1	2:B:91:LYS:CB	2.45	0.46
1:G:225:THR:HG22	1:G:225:THR:O	2.15	0.46
1:J:230:LEU:HD12	1:J:230:LEU:C	2.40	0.46
2:E:39:MET:CE	2:E:49:VAL:HG13	2.39	0.46
1:D:230:LEU:C	1:D:230:LEU:HD12	2.41	0.46
1:A:163:GLU:OE2	3:C:1:LYS:NZ	2.47	0.46
2:B:7:ILE:N	2:B:7:ILE:HD12	2.30	0.46
2:B:39:MET:HE1	2:B:67:HIS:N	2.31	0.46
1:J:22:TYR:C	1:J:23:ILE:HD12	2.40	0.46
1:D:225:THR:O	1:D:225:THR:HG22	2.14	0.46
2:K:39:MET:HE1	2:K:67:HIS:N	2.31	0.46
1:J:202:ARG:HD3	1:J:246:SER:HB3	1.96	0.46
1:D:22:TYR:C	1:D:23:ILE:HD12	2.41	0.46
1:G:202:ARG:HD3	1:G:246:SER:HB3	1.97	0.46
1:A:163:GLU:OE2	3:C:1:LYS:HD3	2.16	0.46
1:A:22:TYR:C	1:A:23:ILE:HD12	2.41	0.46
1:D:152:ALA:O	1:D:155:HIS:HB3	2.16	0.46
2:K:7:ILE:HD12	2:K:7:ILE:N	2.31	0.46
1:J:36:PHE:CD1	1:J:36:PHE:C	2.93	0.45
1:G:35:ARG:NH2	2:H:53:ASP:HB3	2.32	0.45
1:G:261:VAL:HB	1:G:270:LEU:HB2	1.99	0.45
1:G:106:ASP:OD2	1:G:108:ARG:HB2	2.17	0.45
1:G:216:THR:OG1	1:G:260:ARG:HB2	2.16	0.45
1:J:111:ARG:HG2	1:J:112:GLY:N	2.32	0.45
1:D:145:ARG:O	1:D:146:LYS:C	2.60	0.45
1:D:224:LEU:HG	1:D:226:GLN:HB3	1.99	0.45
1:J:208:PHE:CE1	1:J:241:PHE:HB2	2.51	0.45
1:A:62:ARG:NH1	3:C:1:LYS:CD	2.80	0.45
1:J:216:THR:OG1	1:J:260:ARG:HB2	2.16	0.45
1:G:36:PHE:CD1	1:G:36:PHE:C	2.93	0.45
1:G:169:HIS:O	1:G:173:LYS:HG3	2.17	0.45
1:A:37:ASP:OD1	1:A:39:ASP:HB2	2.16	0.45
1:G:206:LEU:HD23	1:G:242:GLN:HB3	1.99	0.45
1:J:264:GLU:O	1:J:265:GLY:C	2.60	0.45
1:J:273:ARG:HD3	1:J:273:ARG:N	2.20	0.45
1:A:36:PHE:CD1	1:A:36:PHE:C	2.94	0.45
1:D:222:GLU:CD	1:D:222:GLU:N	2.72	0.45
2:E:1:ILE:O	2:E:1:ILE:CG2	2.62	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:35:ARG:NH2	2:K:53:ASP:HB3	2.31	0.45
1:J:191:HIS:NE2	1:J:199:VAL:HG11	2.32	0.45
2:K:41:LYS:HE3	2:K:78:TYR:OH	2.17	0.45
1:A:202:ARG:HD3	1:A:246:SER:HB3	1.98	0.44
1:D:234:ARG:HD3	2:E:10:TYR:CZ	2.52	0.44
1:G:152:ALA:O	1:G:155:HIS:HB3	2.17	0.44
1:J:55:GLU:CD	1:J:170:ARG:HH21	2.25	0.44
1:J:129:ASP:O	1:J:131:LYS:HG3	2.17	0.44
2:E:7:ILE:N	2:E:7:ILE:HD12	2.31	0.44
1:G:224:LEU:HG	1:G:226:GLN:HB3	1.99	0.44
1:J:194:ARG:HB3	1:J:198:GLU:N	2.33	0.44
1:J:144:ARG:O	1:J:148:GLU:HG3	2.17	0.44
1:D:36:PHE:CD1	1:D:36:PHE:C	2.96	0.44
1:D:201:LEU:O	1:D:246:SER:HA	2.17	0.44
1:G:222:GLU:CD	1:G:222:GLU:N	2.74	0.44
1:A:224:LEU:HG	1:A:226:GLN:HB3	2.00	0.44
2:B:87:MET:CE	2:B:91:LYS:HB2	2.45	0.44
1:D:111:ARG:HG2	1:D:112:GLY:N	2.32	0.44
1:A:51:TRP:CZ3	1:A:52:MET:SD	3.11	0.44
1:A:106:ASP:OD2	1:A:108:ARG:HB2	2.18	0.44
2:H:39:MET:CE	2:H:49:VAL:HG13	2.35	0.44
2:K:39:MET:CE	2:K:49:VAL:HG13	2.40	0.44
1:G:167:TRP:CE2	3:I:1:LYS:HD2	2.53	0.44
1:J:81:LEU:HD13	1:J:118:TYR:CD1	2.53	0.44
1:A:234:ARG:NH2	2:B:99:MET:OXT	2.51	0.43
1:D:11:ALA:HA	1:D:21:ARG:O	2.18	0.43
1:G:202:ARG:HD2	1:G:244:TRP:CE3	2.53	0.43
1:J:37:ASP:OD1	1:J:39:ASP:HB2	2.18	0.43
1:D:63:GLU:OE2	1:D:66:LYS:CE	2.66	0.43
1:G:251:LEU:HD23	1:G:251:LEU:C	2.43	0.43
1:A:11:ALA:HA	1:A:21:ARG:O	2.18	0.43
1:A:194:ARG:NH2	1:A:198:GLU:OE1	2.51	0.43
1:D:7:TYR:CE1	3:F:2:ALA:HB2	2.53	0.43
1:J:224:LEU:HG	1:J:226:GLN:HB3	1.99	0.43
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.53	0.43
1:G:145:ARG:O	1:G:146:LYS:C	2.61	0.43
1:G:264:GLU:O	1:G:265:GLY:C	2.60	0.43
1:A:264:GLU:O	1:A:265:GLY:C	2.59	0.43
1:D:181:ARG:HG2	1:D:181:ARG:HH11	1.83	0.43
1:D:193:PRO:O	1:D:194:ARG:CG	2.65	0.43
1:G:238:ASP:OD1	1:G:238:ASP:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:21:ARG:HG2	1:J:23:ILE:HD11	1.99	0.43
1:J:251:LEU:HD23	1:J:251:LEU:C	2.44	0.43
1:A:202:ARG:HD2	1:A:244:TRP:CE3	2.53	0.43
1:D:251:LEU:HD23	1:D:251:LEU:C	2.43	0.43
1:G:230:LEU:C	1:G:230:LEU:HD12	2.44	0.43
2:K:41:LYS:HG3	2:K:78:TYR:CE2	2.53	0.43
1:A:191:HIS:NE2	1:A:199:VAL:HG11	2.34	0.43
1:A:16:GLY:O	1:A:18:GLU:N	2.52	0.43
1:A:51:TRP:O	1:A:54:GLN:HG3	2.18	0.43
1:D:110:LEU:HD13	4:D:288:HOH:O	2.18	0.43
1:D:202:ARG:HD2	1:D:244:TRP:CE3	2.53	0.43
1:G:55:GLU:CD	1:G:170:ARG:HH21	2.26	0.43
1:J:98:MET:HE2	2:K:60:TRP:CH2	2.54	0.43
1:J:209:TYR:CD1	1:J:210:PRO:HA	2.54	0.42
1:D:264:GLU:O	1:D:265:GLY:C	2.61	0.42
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.55	0.42
1:A:202:ARG:NH1	2:B:99:MET:HE3	2.33	0.42
1:A:208:PHE:CE1	1:A:241:PHE:HB2	2.53	0.42
1:A:234:ARG:HD3	2:B:10:TYR:CZ	2.53	0.42
1:A:234:ARG:NH1	1:A:242:GLN:OE1	2.51	0.42
1:D:106:ASP:OD2	1:D:108:ARG:HB2	2.19	0.42
1:D:202:ARG:HG2	1:D:204:TRP:HE1	1.82	0.42
1:G:81:LEU:HD13	1:G:118:TYR:CD1	2.54	0.42
2:H:39:MET:HE1	2:H:67:HIS:N	2.33	0.42
1:A:62:ARG:HE	1:A:62:ARG:HB3	1.76	0.42
1:D:129:ASP:O	1:D:131:LYS:HG3	2.20	0.42
1:J:169:HIS:O	1:J:173:LYS:HG3	2.19	0.42
1:G:78:LEU:CD1	1:G:95:LEU:HB2	2.50	0.42
1:D:214:THR:HA	4:D:287:HOH:O	2.19	0.42
1:G:22:TYR:C	1:G:23:ILE:HD12	2.45	0.42
1:G:43:PRO:O	1:G:44:ARG:CG	2.68	0.42
1:A:111:ARG:HD2	1:A:113:TYR:CZ	2.55	0.42
1:J:194:ARG:HB3	1:J:197:GLY:C	2.45	0.42
1:A:169:HIS:O	1:A:173:LYS:HG3	2.20	0.41
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.55	0.41
1:A:251:LEU:HD23	1:A:251:LEU:C	2.44	0.41
1:D:82:LEU:HD12	1:D:87:GLN:HB2	2.01	0.41
2:E:7:ILE:HB	2:E:93:VAL:HG11	2.02	0.41
2:E:59:ASP:O	2:E:60:TRP:HB2	2.20	0.41
1:G:51:TRP:O	1:G:54:GLN:HG3	2.20	0.41
1:G:208:PHE:CE1	1:G:241:PHE:HB2	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:266:LEU:O	1:G:267:PRO:C	2.62	0.41
1:A:226:GLN:O	1:A:227:ASP:C	2.63	0.41
1:A:254:GLU:H	1:A:254:GLU:HG2	1.73	0.41
1:D:191:HIS:NE2	1:D:199:VAL:HG11	2.34	0.41
1:G:33:PHE:CD2	1:G:34:VAL:HG13	2.55	0.41
1:G:201:LEU:O	1:G:246:SER:HA	2.20	0.41
1:D:203:CYS:HB2	1:D:217:TRP:CZ2	2.55	0.41
1:J:23:ILE:N	1:J:23:ILE:CD1	2.83	0.41
2:K:59:ASP:O	2:K:60:TRP:HB2	2.20	0.41
1:G:191:HIS:NE2	1:G:199:VAL:HG11	2.35	0.41
1:J:255:GLN:HE22	1:J:274:TRP:CB	2.21	0.41
1:D:226:GLN:O	1:D:227:ASP:C	2.62	0.41
2:E:87:MET:HE1	2:E:91:LYS:CB	2.46	0.41
1:A:146:LYS:HE2	3:C:8:THR:O	2.21	0.41
2:B:7:ILE:HB	2:B:93:VAL:HG11	2.03	0.41
1:G:104:GLY:CA	1:G:110:LEU:HD22	2.51	0.41
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.56	0.41
1:J:11:ALA:HA	1:J:21:ARG:O	2.20	0.41
1:J:181:ARG:HH11	1:J:181:ARG:HG2	1.84	0.41
1:D:44:ARG:HG3	1:D:44:ARG:NH1	2.35	0.41
1:D:78:LEU:HD13	1:D:95:LEU:HB2	2.03	0.41
2:E:50:GLU:HB2	2:E:67:HIS:CE1	2.56	0.41
2:H:7:ILE:HB	2:H:93:VAL:HG11	2.03	0.41
1:J:51:TRP:O	1:J:54:GLN:HG3	2.21	0.41
1:J:106:ASP:OD2	1:J:108:ARG:HB2	2.21	0.41
1:J:201:LEU:O	1:J:246:SER:HA	2.21	0.41
1:A:201:LEU:O	1:A:246:SER:HA	2.21	0.40
2:B:15:PRO:HG3	2:B:97:ARG:HB2	2.03	0.40
1:D:208:PHE:CE1	1:D:241:PHE:HB2	2.56	0.40
1:J:234:ARG:HD3	2:K:10:TYR:CZ	2.55	0.40
1:A:3:HIS:CG	1:A:172:LEU:HD11	2.57	0.40
1:A:230:LEU:C	1:A:230:LEU:CD1	2.95	0.40
2:B:17:ASN:HA	2:B:72:PRO:O	2.22	0.40
1:D:219:LEU:HD13	1:D:257:TYR:CZ	2.56	0.40
1:G:23:ILE:N	1:G:23:ILE:CD1	2.84	0.40
1:J:226:GLN:O	1:J:227:ASP:C	2.63	0.40
2:E:21:ASN:HB3	2:E:70:PHE:CE1	2.57	0.40
1:G:12:VAL:O	1:G:12:VAL:HG23	2.22	0.40
1:J:250:PRO:O	1:J:251:LEU:C	2.64	0.40
1:A:219:LEU:HD13	1:A:257:TYR:CZ	2.57	0.40
2:B:57:SER:C	2:B:59:ASP:N	2.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:SER:C	2:B:59:ASP:H	2.30	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	271/281 (96%)	238 (88%)	26 (10%)	7 (3%)	4	7
1	D	271/281 (96%)	239 (88%)	26 (10%)	6 (2%)	5	10
1	G	271/281 (96%)	238 (88%)	25 (9%)	8 (3%)	3	6
1	J	271/281 (96%)	238 (88%)	26 (10%)	7 (3%)	4	7
2	B	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	12	24
2	E	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	12	24
2	H	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	12	24
2	K	97/100 (97%)	93 (96%)	3 (3%)	1 (1%)	12	24
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	F	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	L	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
All	All	1500/1560 (96%)	1349 (90%)	119 (8%)	32 (2%)	5	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	195	SER
1	A	264	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	180	LEU
1	D	264	GLU
1	G	180	LEU
1	G	194	ARG
1	G	264	GLU
1	J	180	LEU
1	J	264	GLU
1	A	196	LYS
2	B	47	PRO
1	D	17	LEU
1	D	194	ARG
1	G	196	LYS
1	J	193	PRO
1	J	196	LYS
2	K	47	PRO
1	A	227	ASP
1	D	227	ASP
2	E	47	PRO
1	G	193	PRO
2	H	47	PRO
1	J	227	ASP
1	G	227	ASP
1	G	265	GLY
1	A	265	GLY
1	D	265	GLY
1	J	17	LEU
1	A	223	GLU
1	G	223	GLU
1	J	265	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	232/239 (97%)	222 (96%)	10 (4%)	26	47
1	D	232/239 (97%)	223 (96%)	9 (4%)	28	51

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	232/239 (97%)	220 (95%)	12 (5%)	21	39
1	J	232/239 (97%)	222 (96%)	10 (4%)	26	47
2	B	94/95 (99%)	86 (92%)	8 (8%)	10	18
2	E	94/95 (99%)	86 (92%)	8 (8%)	10	18
2	H	94/95 (99%)	86 (92%)	8 (8%)	10	18
2	K	94/95 (99%)	86 (92%)	8 (8%)	10	18
3	C	7/7 (100%)	7 (100%)	0	100	100
3	F	7/7 (100%)	7 (100%)	0	100	100
3	I	7/7 (100%)	7 (100%)	0	100	100
3	L	7/7 (100%)	7 (100%)	0	100	100
All	All	1332/1364 (98%)	1259 (94%)	73 (6%)	19	37

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	45	TYR
1	A	78	LEU
1	A	114	LEU
1	A	121	ARG
1	A	222	GLU
1	A	226	GLN
1	A	234	ARG
1	A	254	GLU
1	A	273	ARG
2	B	4	THR
2	B	29	GLN
2	B	38	GLN
2	B	51	MET
2	B	70	PHE
2	B	75	THR
2	B	93	VAL
2	B	98	ASP
1	D	78	LEU
1	D	114	LEU
1	D	121	ARG
1	D	195	SER
1	D	222	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	226	GLN
1	D	234	ARG
1	D	254	GLU
1	D	273	ARG
2	E	4	THR
2	E	29	GLN
2	E	38	GLN
2	E	51	MET
2	E	70	PHE
2	E	75	THR
2	E	93	VAL
2	E	98	ASP
1	G	18	GLU
1	G	23	ILE
1	G	78	LEU
1	G	114	LEU
1	G	121	ARG
1	G	193	PRO
1	G	194	ARG
1	G	222	GLU
1	G	226	GLN
1	G	234	ARG
1	G	254	GLU
1	G	273	ARG
2	H	4	THR
2	H	29	GLN
2	H	38	GLN
2	H	51	MET
2	H	70	PHE
2	H	75	THR
2	H	93	VAL
2	H	98	ASP
1	J	78	LEU
1	J	114	LEU
1	J	121	ARG
1	J	193	PRO
1	J	194	ARG
1	J	222	GLU
1	J	226	GLN
1	J	234	ARG
1	J	254	GLU
1	J	273	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	4	THR
2	K	29	GLN
2	K	38	GLN
2	K	51	MET
2	K	70	PHE
2	K	75	THR
2	K	93	VAL
2	K	98	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	72	GLN
1	A	97	GLN
1	A	220	ASN
1	A	255	GLN
2	B	2	GLN
2	B	13	HIS
2	B	31	HIS
3	C	5	ASN
1	D	54	GLN
1	D	72	GLN
1	D	97	GLN
1	D	220	ASN
1	D	255	GLN
2	E	2	GLN
3	F	5	ASN
1	G	42	ASN
1	G	54	GLN
1	G	72	GLN
1	G	97	GLN
1	G	220	ASN
1	G	255	GLN
2	H	2	GLN
2	H	13	HIS
2	H	31	HIS
2	H	34	HIS
3	I	5	ASN
1	J	54	GLN
1	J	72	GLN
1	J	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	188	HIS
1	J	220	ASN
1	J	255	GLN
2	K	2	GLN
2	K	13	HIS
2	K	31	HIS
3	L	5	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	273/281 (97%)	0.63	37 (13%) 7 5	11, 38, 98, 100	0
1	D	273/281 (97%)	0.47	29 (10%) 11 10	12, 39, 99, 100	0
1	G	273/281 (97%)	0.89	47 (17%) 4 3	12, 43, 100, 100	0
1	J	273/281 (97%)	0.49	21 (7%) 19 19	12, 41, 100, 100	0
2	B	99/100 (99%)	0.37	7 (7%) 22 22	12, 32, 75, 98	0
2	E	99/100 (99%)	0.31	5 (5%) 33 33	15, 38, 72, 85	0
2	H	99/100 (99%)	0.53	9 (9%) 15 14	18, 36, 73, 99	0
2	K	99/100 (99%)	0.22	3 (3%) 52 50	15, 35, 66, 98	0
3	C	9/9 (100%)	0.25	0 100 100	25, 30, 43, 46	0
3	F	9/9 (100%)	0.08	1 (11%) 10 9	18, 24, 51, 54	0
3	I	9/9 (100%)	0.35	1 (11%) 10 9	17, 28, 46, 59	0
3	L	9/9 (100%)	0.33	2 (22%) 2 2	21, 28, 54, 64	0
All	All	1524/1560 (97%)	0.54	162 (10%) 11 10	11, 38, 98, 100	0

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	1	ILE	7.8
1	G	178	THR	6.0
1	G	179	LEU	5.6
2	H	1	ILE	5.6
1	A	265	GLY	5.1
1	J	179	LEU	5.1
1	A	274	TRP	4.8
1	J	178	THR	4.7
2	B	1	ILE	4.7
1	D	17	LEU	4.6
1	D	274	TRP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	272	LEU	4.6
2	E	1	ILE	4.5
1	J	180	LEU	4.4
1	G	88	SER	4.3
1	D	180	LEU	4.2
1	G	17	LEU	4.1
2	B	74	GLU	4.1
1	A	179	LEU	4.1
1	G	274	TRP	4.0
1	G	251	LEU	4.0
1	G	232	GLU	3.9
1	J	274	TRP	3.9
1	G	263	HIS	3.9
1	A	182	THR	3.9
1	G	230	LEU	3.9
1	D	273	ARG	3.8
1	D	178	THR	3.8
1	G	265	GLY	3.8
1	J	265	GLY	3.7
1	G	217	TRP	3.6
1	G	79	ARG	3.5
1	J	225	THR	3.5
1	A	263	HIS	3.5
1	D	177	ALA	3.4
1	D	179	LEU	3.4
1	A	256	ASN	3.4
1	G	248	VAL	3.4
1	D	265	GLY	3.4
1	G	250	PRO	3.4
1	G	268	GLU	3.4
1	J	273	ARG	3.4
1	A	17	LEU	3.3
1	G	180	LEU	3.3
2	H	74	GLU	3.3
1	A	273	ARG	3.3
1	D	88	SER	3.3
1	G	227	ASP	3.3
1	J	224	LEU	3.2
1	J	50	PRO	3.2
2	E	43	GLY	3.2
1	G	267	PRO	3.1
1	D	225	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	176	ASN	3.1
1	J	197	GLY	3.1
1	J	272	LEU	3.1
1	A	217	TRP	3.1
1	G	184	SER	3.1
1	A	270	LEU	3.0
1	D	252	GLY	3.0
2	E	74	GLU	3.0
1	J	250	PRO	3.0
1	G	224	LEU	2.9
2	E	58	LYS	2.9
1	G	255	GLN	2.9
2	H	14	PRO	2.9
1	A	188	HIS	2.9
1	G	271	THR	2.9
1	D	248	VAL	2.9
2	K	98	ASP	2.8
2	K	48	LYS	2.8
1	D	41	GLU	2.8
2	H	98	ASP	2.8
1	A	177	ALA	2.8
1	A	192	HIS	2.8
1	A	257	TYR	2.8
1	J	79	ARG	2.8
1	A	251	LEU	2.7
1	G	177	ALA	2.7
1	G	261	VAL	2.7
1	A	255	GLN	2.7
1	D	16	GLY	2.7
1	D	249	VAL	2.7
1	A	180	LEU	2.7
1	G	229	GLU	2.7
2	H	73	THR	2.6
1	A	252	GLY	2.6
1	A	253	LYS	2.6
1	A	249	VAL	2.6
1	D	176	ASN	2.6
1	G	266	LEU	2.6
1	G	212	ASP	2.6
1	G	16	GLY	2.6
1	J	248	VAL	2.6
1	A	258	THR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	58	LYS	2.5
1	G	262	TYR	2.5
1	G	222	GLU	2.5
1	J	222	GLU	2.5
1	D	149	GLN	2.5
1	A	272	LEU	2.5
1	G	207	GLY	2.5
2	B	47	PRO	2.5
1	G	188	HIS	2.5
1	D	227	ASP	2.4
1	D	219	LEU	2.4
1	J	46	GLU	2.4
1	A	224	LEU	2.4
1	A	266	LEU	2.4
1	G	247	VAL	2.4
3	L	6	PHE	2.4
1	A	2	PRO	2.4
1	D	222	GLU	2.3
2	H	99	MET	2.3
1	G	264	GLU	2.3
1	D	224	LEU	2.3
2	E	34	HIS	2.3
1	J	223	GLU	2.3
1	A	197	GLY	2.3
1	A	262	TYR	2.3
1	G	198	GLU	2.3
1	A	227	ASP	2.3
2	H	97	ARG	2.3
1	G	46	GLU	2.2
1	G	223	GLU	2.2
1	A	260	ARG	2.2
2	H	58	LYS	2.2
1	A	225	THR	2.2
1	G	181	ARG	2.2
1	G	273	ARG	2.2
1	A	269	PRO	2.2
2	B	42	ASN	2.2
1	G	50	PRO	2.2
1	G	218	GLN	2.2
1	D	195	SER	2.2
1	J	227	ASP	2.2
1	A	220	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	256	ASN	2.2
1	G	257	TYR	2.2
2	B	19	LYS	2.1
1	G	163	GLU	2.1
1	G	260	ARG	2.1
1	A	267	PRO	2.1
1	D	193	PRO	2.1
1	D	267	PRO	2.1
2	H	18	GLY	2.1
1	A	29	ASP	2.1
1	A	50	PRO	2.1
1	D	167	TRP	2.1
1	A	191	HIS	2.1
1	J	90	GLY	2.1
3	I	4	TYR	2.1
1	J	177	ALA	2.0
3	F	1	LYS	2.0
1	J	267	PRO	2.0
1	A	218	GLN	2.0
1	D	226	GLN	2.0
1	D	223	GLU	2.0
2	B	53	ASP	2.0
1	D	271	THR	2.0
1	G	226	GLN	2.0
3	L	4	TYR	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.