Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:01 PM GMT

PDB ID	:	1N59
Title	:	Crystal structure of the Murine class I Major Histocompatibility Complex of H-2KB, B2-Microglobulin, and A 9-Residue immunodominant peptide epitope gp33 derived from LCMV
Authors	:	Achour, A.; Michaelsson, J.; Harris, R.A.; Odeberg, J.; Grufman, P.; Sandberg, J.K.; Levitsky, V.; Karre, K.; Sandalova, T.; Schneider, G.
Deposited on	:	2002-11-05
Resolution	:	2.95 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

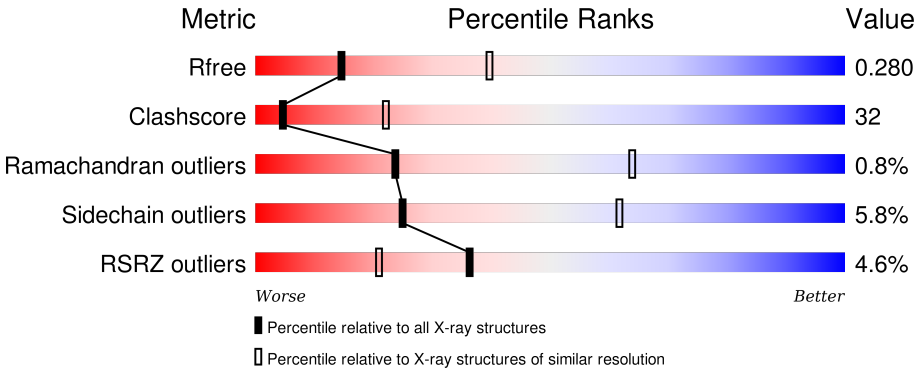
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.95 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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	276	% 52% 42% 6%
1	C	276	8% 50% 45% 5%
2	B	99	57% 40%
2	D	99	8% 58% 38%
3	P	9	44% 33% 11% 11%

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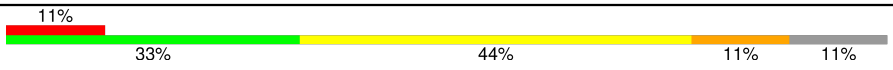
Mol	Chain	Length	Quality of chain
3	Q	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6344 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, K-B alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2247	1418	395	425	9			
1	C	276	Total	C	N	O	S	0	0	0
			2247	1418	395	425	9			

- 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
			820	524	138	151	7			
2	D	99	Total	C	N	O	S	0	0	0
			820	524	138	151	7			

- Molecule 3 is a protein called nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	8	Total	C	N	O	S	0	0	0
			63	42	9	11	1			
3	Q	8	Total	C	N	O	S	0	0	0
			63	42	9	11	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	9	MET	CYS	ENGINEERED	UNP Q9QDK7
Q	9	MET	CYS	ENGINEERED	UNP Q9QDK7

- Molecule 4 is water.

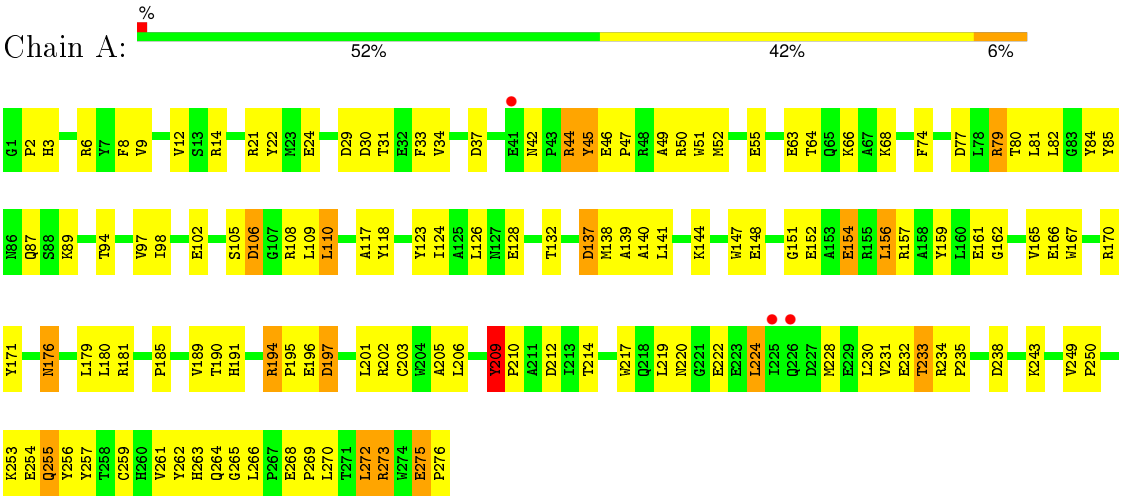
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0
4	B	18	Total O 18 18	0	0
4	C	13	Total O 13 13	0	0
4	D	8	Total O 8 8	0	0
4	P	3	Total O 3 3	0	0
4	Q	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

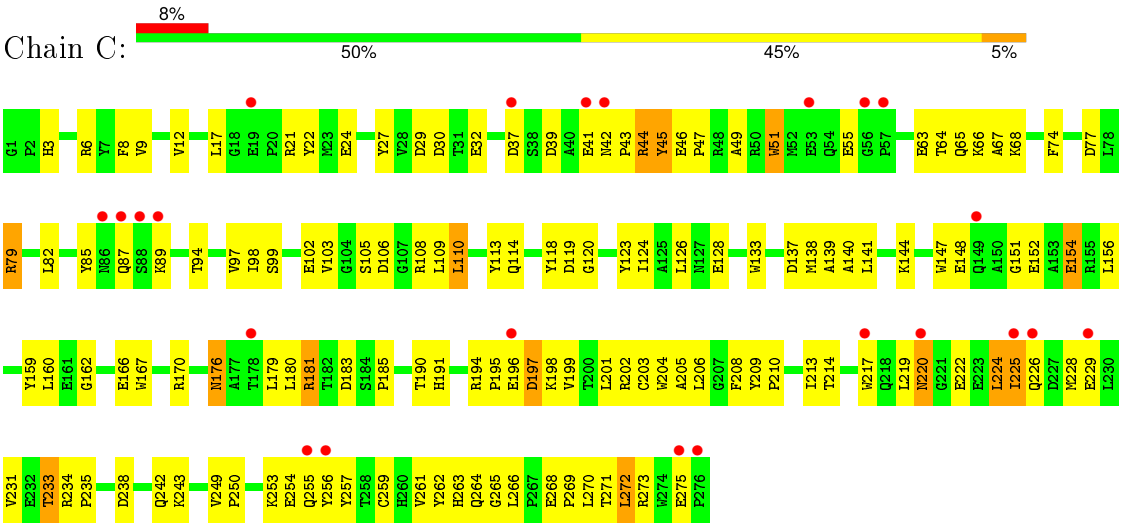
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain A:



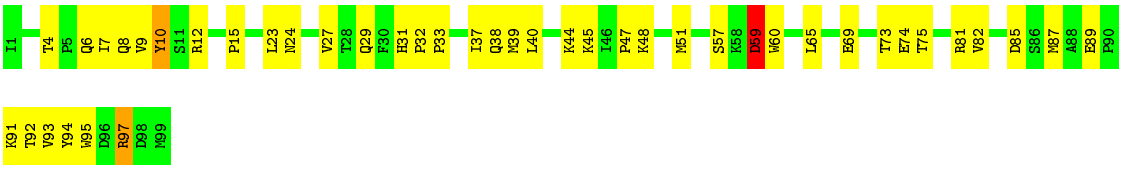
- Molecule 1: H-2 class I histocompatibility antigen, K-B alpha chain

Chain C:

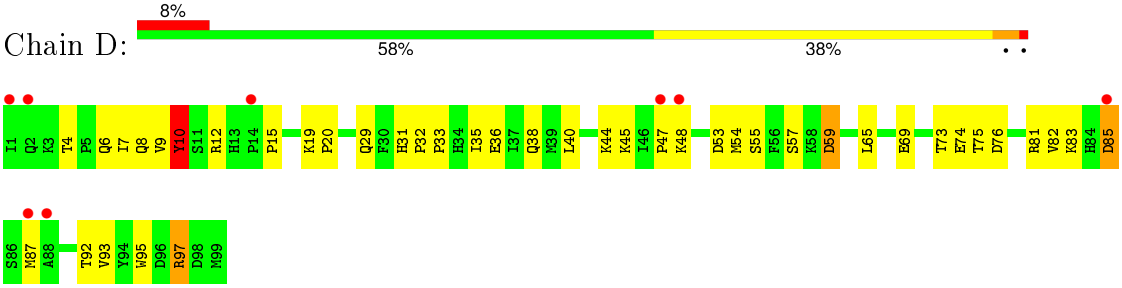


- Molecule 2: Beta-2-microglobulin

Chain B:



• Molecule 2: Beta-2-microglobulin



• Molecule 3: nonameric peptide, gp33 derived from lymphocytic choriomeningitis virus

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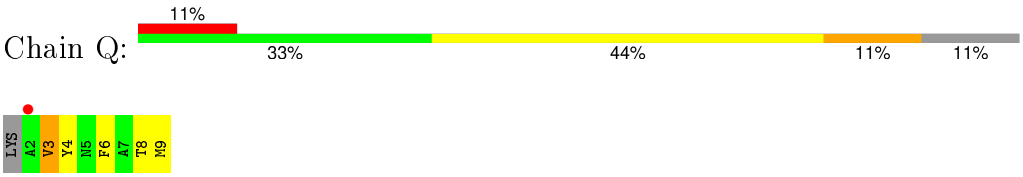

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.55Å 88.57Å 120.09Å 90.00° 93.72° 90.00°	Depositor
Resolution (Å)	19.92 – 2.95 19.91 – 2.92	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-2.95) 85.8 (19.91-2.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.229 , 0.287 0.225 , 0.280	Depositor DCC
R_{free} test set	986 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	37.5	Xtriage
Anisotropy	1.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 19731 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6344	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.96	1/2309 (0.0%)	1.00	7/3137 (0.2%)
1	C	0.63	0/2309	0.86	3/3137 (0.1%)
2	B	1.07	5/846 (0.6%)	1.01	0/1148
2	D	0.84	5/846 (0.6%)	0.86	0/1148
3	P	2.01	6/64 (9.4%)	1.19	0/86
3	Q	1.94	6/64 (9.4%)	1.30	1/86 (1.2%)
All	All	0.89	23/6438 (0.4%)	0.94	11/8742 (0.1%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	TYR	CE1-CZ	-9.08	1.26	1.38
2	D	10	TYR	CE2-CZ	-8.18	1.27	1.38
3	P	6	PHE	CE1-CZ	-7.85	1.22	1.37
3	Q	6	PHE	CE2-CZ	-7.11	1.23	1.37
2	D	85	ASP	CB-CG	-6.94	1.37	1.51
2	B	85	ASP	CB-CG	-6.90	1.37	1.51
2	B	10	TYR	CE2-CZ	-6.75	1.29	1.38
2	D	10	TYR	CG-CD2	-6.42	1.30	1.39
2	D	10	TYR	CG-CD1	-6.25	1.31	1.39
3	Q	6	PHE	CG-CD1	-6.22	1.29	1.38
3	Q	6	PHE	CE1-CZ	-6.10	1.25	1.37
3	P	6	PHE	CG-CD1	-5.95	1.29	1.38
3	P	6	PHE	CG-CD2	-5.75	1.30	1.38
2	B	59	ASP	CB-CG	-5.64	1.40	1.51
3	Q	3	VAL	CB-CG2	-5.56	1.41	1.52
2	B	51	MET	CG-SD	-5.54	1.66	1.81
3	Q	3	VAL	CB-CG1	-5.52	1.41	1.52
3	P	3	VAL	CB-CG1	-5.43	1.41	1.52
3	P	6	PHE	CE2-CZ	-5.33	1.27	1.37
3	Q	6	PHE	CG-CD2	-5.31	1.30	1.38
1	A	159	TYR	CD2-CE2	-5.29	1.31	1.39
2	B	10	TYR	CE1-CZ	-5.21	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	3	VAL	CB-CG2	-5.10	1.42	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	106	ASP	CB-CG-OD2	6.96	124.57	118.30
1	A	197	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	238	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	212	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	209	TYR	C-N-CD	-5.87	107.69	120.60
1	C	197	ASP	CB-CG-OD2	5.80	123.52	118.30
1	A	209	TYR	CA-C-N	5.67	132.98	117.10
1	A	137	ASP	CB-CG-OD2	5.58	123.33	118.30
1	A	37	ASP	CB-CG-OD2	5.52	123.27	118.30
3	Q	3	VAL	CB-CA-C	-5.30	101.33	111.40
1	C	119	ASP	CB-CG-OD2	5.23	123.00	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	2247	0	2136	156	0
1	C	2247	0	2136	154	0
2	B	820	0	796	46	0
2	D	820	0	796	56	0
3	P	63	0	58	14	0
3	Q	63	0	58	8	0
4	A	41	0	0	5	0
4	B	18	0	0	1	0
4	C	13	0	0	1	0
4	D	8	0	0	1	0
4	P	3	0	0	0	0
4	Q	1	0	0	1	0
All	All	6344	0	5980	392	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 32.

All (392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LYS:HE3	3:P:3:VAL:CG1	1.58	1.34
1:C:209:TYR:CD1	1:C:209:TYR:O	1.81	1.31
1:A:66:LYS:CE	3:P:3:VAL:HG12	1.64	1.27
1:C:205:ALA:C	1:C:206:LEU:HD23	1.74	1.08
1:C:66:LYS:HE3	3:Q:3:VAL:HB	1.36	1.06
1:C:225:ILE:HA	1:C:228:MET:HE3	1.39	1.03
1:A:209:TYR:HD1	1:A:210:PRO:N	1.57	1.02
1:A:209:TYR:HD1	1:A:209:TYR:C	1.63	0.97
2:B:38:GLN:HG2	2:B:45:LYS:HE3	1.47	0.94
1:A:209:TYR:CD1	1:A:209:TYR:C	2.36	0.94
1:C:209:TYR:HD1	1:C:209:TYR:O	1.28	0.93
1:C:44:ARG:HH11	1:C:44:ARG:HB3	1.33	0.92
1:A:66:LYS:HE3	3:P:3:VAL:HG12	0.92	0.90
1:A:63:GLU:OE1	1:A:66:LYS:HE2	1.70	0.90
2:D:38:GLN:HG2	2:D:45:LYS:HE3	1.54	0.88
1:A:196:GLU:O	1:A:196:GLU:HG2	1.72	0.88
1:C:209:TYR:CD1	1:C:209:TYR:C	2.41	0.85
1:C:79:ARG:HG3	1:C:79:ARG:HH11	1.39	0.84
1:A:77:ASP:HB3	3:P:9:MET:HE3	1.60	0.84
2:D:4:THR:CG2	2:D:87:MET:HE3	2.08	0.83
1:C:225:ILE:HA	1:C:228:MET:CE	2.07	0.83
1:C:214:THR:HB	1:C:262:TYR:HB2	1.58	0.83
1:A:263:HIS:CD2	1:A:265:GLY:H	1.95	0.82
1:A:176:ASN:HB2	1:A:180:LEU:HD12	1.60	0.82
2:D:4:THR:CG2	2:D:87:MET:CE	2.58	0.81
1:C:85:TYR:HB2	1:C:87:GLN:HE21	1.44	0.81
1:C:176:ASN:HB2	1:C:180:LEU:HD12	1.63	0.81
1:A:217:TRP:H	1:A:228:MET:HE2	1.45	0.81
1:A:259:CYS:HB3	1:A:272:LEU:CD1	2.11	0.81
1:C:63:GLU:OE1	1:C:66:LYS:HE2	1.82	0.80
1:A:126:LEU:HD22	1:A:156:LEU:HD13	1.60	0.80
2:D:4:THR:HG23	2:D:87:MET:HE3	1.64	0.80
1:A:9:VAL:HG22	1:A:97:VAL:HB	1.64	0.79
1:C:242:GLN:OE1	2:D:10:TYR:CD2	2.36	0.79
1:C:235:PRO:HG2	2:D:65:LEU:HD22	1.64	0.79
1:C:263:HIS:CD2	1:C:265:GLY:H	2.01	0.78
1:A:167:TRP:CE3	1:A:170:ARG:HD3	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:CYS:HB3	1:C:272:LEU:CD1	2.15	0.77
2:B:57:SER:OG	2:B:59:ASP:HB3	1.84	0.77
1:A:214:THR:HB	1:A:262:TYR:HB2	1.66	0.76
1:A:66:LYS:HE3	3:P:3:VAL:HG13	1.66	0.76
2:D:19:LYS:HG2	4:D:105:HOH:O	1.86	0.75
1:A:138:MET:HA	1:A:141:LEU:HB2	1.67	0.75
1:A:209:TYR:CD1	1:A:210:PRO:N	2.48	0.74
1:C:196:GLU:O	1:C:196:GLU:HG2	1.86	0.74
1:C:9:VAL:HG22	1:C:97:VAL:HB	1.70	0.74
1:C:44:ARG:HH11	1:C:44:ARG:CB	1.99	0.74
2:D:48:LYS:HE3	2:D:69:GLU:HB2	1.69	0.74
1:C:77:ASP:HB3	3:Q:9:MET:HE3	1.68	0.73
1:C:261:VAL:HB	1:C:270:LEU:HB2	1.71	0.72
1:A:224:LEU:HD12	1:A:224:LEU:N	2.04	0.72
1:C:196:GLU:OE1	1:C:198:LYS:HE2	1.90	0.72
1:C:128:GLU:HA	1:C:128:GLU:OE1	1.88	0.71
1:C:242:GLN:OE1	2:D:10:TYR:HD2	1.74	0.70
1:A:259:CYS:HB3	1:A:272:LEU:HD12	1.73	0.70
1:C:22:TYR:HE1	1:C:74:PHE:CD2	2.09	0.70
1:A:181:ARG:NH2	1:A:209:TYR:HD2	1.88	0.70
1:A:12:VAL:O	1:A:12:VAL:HG23	1.92	0.70
2:B:38:GLN:NE2	2:B:45:LYS:HD2	2.07	0.69
1:C:123:TYR:CZ	1:C:140:ALA:HA	2.28	0.69
1:C:235:PRO:CG	2:D:65:LEU:HD22	2.23	0.69
1:C:167:TRP:CE3	1:C:170:ARG:HD3	2.26	0.69
1:C:123:TYR:HD2	1:C:124:ILE:HG22	1.57	0.69
1:C:3:HIS:ND1	1:C:29:ASP:OD2	2.26	0.69
1:A:224:LEU:HD12	1:A:224:LEU:H	1.58	0.69
1:A:194:ARG:O	4:A:301:HOH:O	2.11	0.69
1:A:29:ASP:O	1:A:30:ASP:HB2	1.92	0.68
2:B:48:LYS:HE3	2:B:69:GLU:H	1.59	0.68
1:C:259:CYS:HB3	1:C:272:LEU:HD13	1.75	0.68
2:B:48:LYS:HE3	2:B:69:GLU:HB2	1.74	0.68
1:A:66:LYS:HE2	3:P:3:VAL:HG12	1.72	0.67
1:A:44:ARG:NH2	4:A:314:HOH:O	2.28	0.67
1:A:181:ARG:NH1	1:A:209:TYR:CD2	2.63	0.67
1:C:233:THR:OG1	1:C:243:LYS:HE2	1.95	0.66
1:C:79:ARG:NH1	1:C:79:ARG:HG3	2.10	0.66
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.59	0.66
1:A:49:ALA:HB1	1:A:51:TRP:NE1	2.10	0.66
1:A:82:LEU:HD13	1:A:89:LYS:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:LEU:HD23	1:C:206:LEU:N	2.09	0.65
1:A:230:LEU:HD23	1:A:230:LEU:N	2.12	0.65
1:C:205:ALA:O	1:C:206:LEU:HD23	1.96	0.65
3:Q:3:VAL:HG12	3:Q:4:TYR:N	2.12	0.65
1:C:12:VAL:HG12	1:C:94:THR:HG23	1.78	0.65
2:D:4:THR:HG23	2:D:87:MET:CE	2.27	0.64
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.62	0.64
1:C:138:MET:HA	1:C:141:LEU:HB2	1.80	0.64
1:A:109:LEU:HD12	1:A:110:LEU:H	1.63	0.64
2:B:94:TYR:HE2	4:B:113:HOH:O	1.80	0.64
1:C:224:LEU:H	1:C:224:LEU:CD1	2.11	0.64
1:A:98:ILE:O	1:A:98:ILE:HG23	1.98	0.63
1:A:132:THR:HA	4:A:309:HOH:O	1.97	0.63
1:A:171:TYR:OH	3:P:2:ALA:HB2	1.98	0.63
2:D:4:THR:CG2	2:D:87:MET:HE2	2.27	0.63
1:A:167:TRP:CZ3	1:A:170:ARG:HD3	2.34	0.62
1:C:98:ILE:O	1:C:98:ILE:HG23	2.00	0.62
1:A:181:ARG:CZ	1:A:209:TYR:CD2	2.82	0.61
1:A:22:TYR:HE1	1:A:74:PHE:CD2	2.17	0.61
2:D:38:GLN:NE2	2:D:45:LYS:HD2	2.16	0.61
2:B:87:MET:HE1	2:B:91:LYS:HD2	1.82	0.61
1:C:196:GLU:OE1	1:C:198:LYS:CG	2.49	0.61
2:D:48:LYS:HE3	2:D:69:GLU:H	1.65	0.61
1:A:233:THR:OG1	1:A:243:LYS:HE2	2.01	0.61
1:C:87:GLN:HE22	1:C:118:TYR:HE2	1.49	0.60
1:A:12:VAL:HG12	1:A:94:THR:HG23	1.82	0.60
1:A:275:GLU:O	1:A:275:GLU:HG2	2.01	0.60
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.34	0.60
1:C:22:TYR:CE1	1:C:74:PHE:CD2	2.90	0.60
2:D:57:SER:OG	2:D:59:ASP:HB3	2.02	0.60
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.37	0.59
1:C:201:LEU:HD11	1:C:254:GLU:HB2	1.84	0.59
1:A:201:LEU:HD11	1:A:254:GLU:HB2	1.83	0.59
1:A:181:ARG:NH2	1:A:209:TYR:CD2	2.70	0.59
1:A:9:VAL:CG2	1:A:97:VAL:HB	2.32	0.59
1:A:261:VAL:HB	1:A:270:LEU:HB2	1.85	0.59
1:A:8:PHE:CE1	1:A:98:ILE:HD12	2.38	0.59
1:C:85:TYR:HB2	1:C:87:GLN:NE2	2.18	0.58
1:A:181:ARG:HH22	1:A:209:TYR:HD2	1.50	0.58
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.16	0.58
1:C:12:VAL:O	1:C:12:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HD2	2:B:10:TYR:CE2	2.38	0.58
1:A:259:CYS:HB3	1:A:272:LEU:HD13	1.85	0.58
1:A:123:TYR:CZ	1:A:140:ALA:HA	2.39	0.58
1:A:209:TYR:CD1	1:A:209:TYR:O	2.56	0.58
2:B:7:ILE:HD11	2:B:82:VAL:HB	1.85	0.58
1:A:106:ASP:OD2	1:A:108:ARG:HB2	2.03	0.58
1:C:196:GLU:OE1	1:C:198:LYS:HG3	2.04	0.58
1:A:205:ALA:C	1:A:206:LEU:HD23	2.24	0.57
1:A:190:THR:OG1	1:A:202:ARG:HB3	2.04	0.57
1:A:64:THR:O	1:A:68:LYS:HG3	2.04	0.57
1:A:235:PRO:HG2	2:B:65:LEU:HD22	1.85	0.57
1:A:24:GLU:OE1	3:P:3:VAL:HG21	2.04	0.57
2:B:73:THR:HG22	2:B:74:GLU:N	2.18	0.57
2:D:73:THR:HG22	2:D:75:THR:H	1.70	0.57
1:C:167:TRP:CZ3	1:C:170:ARG:HD3	2.40	0.57
2:B:97:ARG:HH11	2:B:97:ARG:CB	2.18	0.57
1:C:22:TYR:CE1	1:C:74:PHE:HD2	2.23	0.57
1:C:126:LEU:HB2	1:C:133:TRP:CZ3	2.39	0.57
1:C:196:GLU:OE1	1:C:198:LYS:CE	2.53	0.57
2:D:15:PRO:HG3	2:D:95:TRP:HZ2	1.70	0.57
1:C:64:THR:O	1:C:68:LYS:HG3	2.05	0.57
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.40	0.57
1:A:266:LEU:CD1	1:A:270:LEU:HG	2.35	0.56
2:B:6:GLN:HG3	2:B:29:GLN:OE1	2.04	0.56
1:C:162:GLY:O	1:C:166:GLU:HG3	2.05	0.56
2:D:97:ARG:HB3	2:D:97:ARG:HH11	1.68	0.56
1:C:85:TYR:HB2	1:C:87:GLN:HG3	1.88	0.56
2:B:97:ARG:HH11	2:B:97:ARG:HB3	1.69	0.56
1:A:266:LEU:HD13	1:A:270:LEU:HG	1.87	0.56
1:A:22:TYR:CE1	1:A:74:PHE:CD2	2.93	0.56
1:C:82:LEU:HD13	1:C:89:LYS:HD3	1.88	0.56
1:C:190:THR:OG1	1:C:202:ARG:HB3	2.05	0.56
1:A:81:LEU:HD12	1:A:84:TYR:CD2	2.41	0.56
1:A:205:ALA:O	1:A:206:LEU:HD23	2.07	0.55
1:C:109:LEU:HD12	1:C:110:LEU:H	1.70	0.55
1:A:80:THR:HG21	3:P:9:MET:O	2.06	0.55
1:C:266:LEU:CD1	1:C:270:LEU:HG	2.37	0.55
1:A:144:LYS:O	1:A:148:GLU:HG3	2.06	0.55
3:Q:8:THR:HG23	4:Q:52:HOH:O	2.06	0.55
1:C:234:ARG:HB2	2:D:10:TYR:OH	2.07	0.55
1:C:259:CYS:HB3	1:C:272:LEU:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:PRO:O	1:C:196:GLU:HB3	2.07	0.54
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.23	0.54
1:C:228:MET:HG2	1:C:229:GLU:H	1.72	0.54
1:C:24:GLU:OE1	1:C:45:TYR:OH	2.23	0.54
2:D:97:ARG:CB	2:D:97:ARG:HH11	2.21	0.54
2:B:73:THR:HG22	2:B:75:THR:H	1.73	0.54
1:A:209:TYR:CD1	1:A:210:PRO:CA	2.91	0.54
1:C:147:TRP:HB3	1:C:152:GLU:HB3	1.89	0.54
1:A:77:ASP:CB	3:P:9:MET:HE3	2.35	0.54
1:A:263:HIS:HD2	1:A:265:GLY:H	1.51	0.54
1:A:224:LEU:H	1:A:224:LEU:CD1	2.20	0.53
2:B:23:LEU:HG	2:B:39:MET:HE1	1.91	0.53
1:A:255:GLN:O	1:A:273:ARG:NH2	2.36	0.53
1:C:151:GLY:O	1:C:154:GLU:HG2	2.09	0.53
1:C:126:LEU:HD22	1:C:156:LEU:HD13	1.90	0.53
1:C:263:HIS:HD2	1:C:265:GLY:H	1.55	0.52
1:A:275:GLU:O	1:A:276:PRO:O	2.27	0.52
1:C:49:ALA:HB1	1:C:51:TRP:NE1	2.24	0.52
1:C:42:ASN:HB3	1:C:44:ARG:HH22	1.74	0.52
1:C:8:PHE:CE1	1:C:98:ILE:HD12	2.45	0.52
1:A:106:ASP:OD1	1:A:106:ASP:N	2.41	0.52
1:A:263:HIS:CG	1:A:264:GLN:N	2.77	0.52
1:C:108:ARG:HG2	1:C:108:ARG:HH11	1.75	0.52
1:C:219:LEU:HD12	1:C:256:TYR:O	2.09	0.52
1:C:204:TRP:HB3	1:C:206:LEU:HD21	1.91	0.52
2:B:40:LEU:HD23	2:B:45:LYS:HA	1.90	0.52
1:A:22:TYR:CE1	1:A:74:PHE:HD2	2.27	0.52
1:C:250:PRO:HG2	1:C:253:LYS:HB2	1.91	0.52
1:C:210:PRO:HD2	1:C:263:HIS:NE2	2.24	0.52
1:A:231:VAL:HG23	1:A:231:VAL:O	2.10	0.52
2:B:59:ASP:C	2:B:59:ASP:OD1	2.48	0.52
1:A:250:PRO:HG2	1:A:253:LYS:HB2	1.92	0.51
1:A:234:ARG:HD2	2:B:10:TYR:HE2	1.74	0.51
1:A:151:GLY:O	1:A:154:GLU:HG2	2.09	0.51
1:A:66:LYS:CE	3:P:3:VAL:CG1	2.47	0.51
1:A:224:LEU:N	1:A:224:LEU:CD1	2.73	0.51
1:C:224:LEU:N	1:C:224:LEU:CD1	2.72	0.51
1:A:46:GLU:HB2	1:A:47:PRO:HD2	1.92	0.51
2:B:40:LEU:HA	2:B:44:LYS:O	2.09	0.51
2:D:4:THR:HG21	2:D:87:MET:HE2	1.93	0.51
1:A:102:GLU:O	1:A:109:LEU:HD12	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:57:SER:C	2:D:59:ASP:N	2.64	0.51
1:C:228:MET:HG2	1:C:229:GLU:N	2.26	0.51
1:C:176:ASN:HB2	1:C:180:LEU:CD1	2.38	0.51
1:A:109:LEU:HD12	1:A:110:LEU:N	2.26	0.51
1:A:85:TYR:HB2	1:A:87:GLN:HG3	1.93	0.51
1:A:108:ARG:HG2	1:A:108:ARG:NH1	2.25	0.50
1:A:147:TRP:HB3	1:A:152:GLU:HB3	1.92	0.50
2:D:6:GLN:HG3	2:D:29:GLN:OE1	2.11	0.50
1:C:167:TRP:CZ3	1:C:170:ARG:CD	2.95	0.50
1:C:219:LEU:O	1:C:222:GLU:HG2	2.12	0.50
1:C:263:HIS:CG	1:C:264:GLN:N	2.80	0.49
1:C:29:ASP:O	1:C:30:ASP:HB2	2.12	0.49
2:D:31:HIS:ND1	2:D:32:PRO:HA	2.27	0.49
1:C:181:ARG:NH1	1:C:209:TYR:CD2	2.81	0.49
2:B:73:THR:CG2	2:B:74:GLU:N	2.75	0.49
1:C:51:TRP:CZ2	1:C:179:LEU:HD11	2.48	0.49
1:C:106:ASP:OD2	1:C:108:ARG:HB2	2.13	0.49
1:C:144:LYS:O	1:C:148:GLU:HG3	2.13	0.49
2:B:10:TYR:CD1	2:B:24:ASN:HB2	2.47	0.49
1:A:6:ARG:NE	4:A:285:HOH:O	2.45	0.49
1:C:225:ILE:CA	1:C:228:MET:HE3	2.26	0.49
1:A:167:TRP:CZ3	1:A:170:ARG:CD	2.95	0.49
1:C:141:LEU:O	1:C:144:LYS:HB3	2.13	0.49
2:D:36:GLU:HB3	2:D:83:LYS:HB3	1.95	0.49
2:D:73:THR:HB	2:D:76:ASP:OD2	2.13	0.49
1:A:82:LEU:HD11	4:A:312:HOH:O	2.12	0.49
2:B:7:ILE:CD1	2:B:82:VAL:HB	2.42	0.49
1:A:79:ARG:NH1	1:A:79:ARG:HG3	2.28	0.48
1:C:109:LEU:HD12	1:C:110:LEU:N	2.28	0.48
1:C:51:TRP:CH2	1:C:179:LEU:HD11	2.48	0.48
1:C:77:ASP:CB	3:Q:9:MET:HE3	2.40	0.48
1:C:12:VAL:HG22	1:C:21:ARG:HB3	1.96	0.48
2:D:97:ARG:NH1	2:D:97:ARG:HB3	2.29	0.48
2:B:59:ASP:OD1	2:B:59:ASP:O	2.32	0.48
1:C:203:CYS:HB2	1:C:217:TRP:CZ2	2.48	0.48
2:B:15:PRO:HG3	2:B:95:TRP:HZ2	1.79	0.48
2:D:35:ILE:HD11	2:D:82:VAL:CG1	2.43	0.48
1:C:217:TRP:O	1:C:224:LEU:HD13	2.13	0.48
1:A:275:GLU:O	1:A:275:GLU:CG	2.62	0.48
1:A:31:THR:HG21	1:A:209:TYR:HE2	1.78	0.48
2:D:7:ILE:HD11	2:D:82:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:TYR:N	2:D:10:TYR:CD1	2.81	0.48
1:C:213:ILE:HG13	1:C:263:HIS:HB2	1.96	0.47
1:C:181:ARG:CZ	1:C:209:TYR:CD2	2.98	0.47
1:A:110:LEU:HD12	1:A:110:LEU:O	2.14	0.47
2:D:57:SER:C	2:D:59:ASP:H	2.18	0.47
1:A:123:TYR:HD2	1:A:124:ILE:HG22	1.79	0.47
2:D:73:THR:HG22	2:D:74:GLU:N	2.28	0.47
2:D:4:THR:HG22	2:D:87:MET:HE3	1.93	0.47
2:D:7:ILE:CD1	2:D:82:VAL:HB	2.45	0.47
1:A:29:ASP:O	1:A:30:ASP:CB	2.58	0.47
1:C:99:SER:CB	1:C:114:GLN:OE1	2.62	0.47
2:B:97:ARG:NH1	2:B:97:ARG:HB3	2.29	0.47
1:C:55:GLU:HA	1:C:55:GLU:OE1	2.14	0.47
2:D:81:ARG:HG3	2:D:92:THR:OG1	2.15	0.47
1:C:37:ASP:OD1	1:C:39:ASP:HB2	2.15	0.47
1:C:266:LEU:HD13	1:C:270:LEU:HG	1.97	0.47
1:A:231:VAL:O	1:A:232:GLU:C	2.53	0.47
1:C:27:TYR:OH	2:D:53:ASP:HA	2.14	0.47
2:D:40:LEU:HD23	2:D:45:LYS:HA	1.97	0.46
1:A:176:ASN:HB2	1:A:180:LEU:CD1	2.39	0.46
1:C:123:TYR:OH	1:C:140:ALA:HA	2.15	0.46
2:D:40:LEU:HA	2:D:44:LYS:O	2.14	0.46
2:D:59:ASP:C	2:D:59:ASP:OD1	2.54	0.46
2:D:85:ASP:O	2:D:85:ASP:CG	2.54	0.46
1:A:49:ALA:HB1	1:A:51:TRP:CD1	2.51	0.46
2:B:48:LYS:CE	2:B:69:GLU:H	2.26	0.46
2:B:9:VAL:CG2	2:B:93:VAL:HG12	2.45	0.46
1:A:63:GLU:CD	1:A:66:LYS:HE2	2.34	0.46
1:A:31:THR:CG2	1:A:209:TYR:HE2	2.29	0.46
1:A:138:MET:O	1:A:141:LEU:HB3	2.16	0.46
1:C:224:LEU:HD12	1:C:224:LEU:N	2.31	0.46
1:A:234:ARG:CD	2:B:10:TYR:CE2	2.98	0.46
1:A:77:ASP:CG	3:P:9:MET:HE2	2.36	0.46
1:C:272:LEU:HD12	1:C:272:LEU:H	1.80	0.46
1:C:124:ILE:HD13	1:C:147:TRP:CZ3	2.51	0.46
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.51	0.46
1:C:22:TYR:CE2	1:C:24:GLU:HG3	2.51	0.46
1:C:268:GLU:O	1:C:269:PRO:C	2.54	0.46
1:A:12:VAL:O	1:A:12:VAL:CG2	2.61	0.46
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.51	0.45
2:D:59:ASP:O	2:D:59:ASP:OD1	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:VAL:HB	1:C:257:TYR:CE1	2.51	0.45
1:A:33:PHE:C	1:A:34:VAL:HG13	2.36	0.45
1:A:31:THR:CG2	1:A:209:TYR:CE2	2.99	0.45
1:C:44:ARG:NH1	1:C:44:ARG:CG	2.78	0.45
1:A:171:TYR:OH	3:P:2:ALA:CB	2.63	0.45
1:A:22:TYR:CE2	1:A:24:GLU:HG3	2.52	0.45
2:B:48:LYS:HD3	2:B:48:LYS:O	2.16	0.45
1:C:224:LEU:HD21	1:C:257:TYR:HE2	1.81	0.45
2:B:81:ARG:HG3	2:B:92:THR:OG1	2.16	0.45
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.98	0.45
1:C:65:GLN:C	1:C:67:ALA:N	2.69	0.45
1:C:231:VAL:HG23	1:C:231:VAL:O	2.15	0.45
2:B:59:ASP:O	2:B:60:TRP:HB2	2.16	0.45
2:B:10:TYR:CE1	2:B:24:ASN:HB2	2.52	0.45
1:A:268:GLU:O	1:A:269:PRO:C	2.54	0.45
2:D:48:LYS:O	2:D:48:LYS:HD3	2.16	0.45
1:C:185:PRO:HD3	1:C:263:HIS:CD2	2.52	0.45
1:A:98:ILE:CG2	1:A:98:ILE:O	2.65	0.45
1:A:235:PRO:CG	2:B:65:LEU:HD22	2.46	0.45
2:B:74:GLU:OE1	2:B:74:GLU:HA	2.17	0.45
1:C:156:LEU:O	1:C:159:TYR:HB3	2.17	0.45
1:C:6:ARG:HG2	1:C:113:TYR:OH	2.17	0.45
1:A:108:ARG:HE	1:C:214:THR:HG21	1.82	0.44
1:C:79:ARG:CG	1:C:79:ARG:NH1	2.76	0.44
1:C:224:LEU:H	1:C:224:LEU:HD12	1.83	0.44
1:A:234:ARG:CZ	2:B:10:TYR:CD2	2.99	0.44
1:A:154:GLU:HG2	1:A:154:GLU:H	1.32	0.44
1:A:219:LEU:O	1:A:222:GLU:HG2	2.17	0.44
1:A:219:LEU:HD12	1:A:256:TYR:O	2.18	0.44
1:C:44:ARG:NH1	1:C:44:ARG:HB3	2.16	0.44
1:A:249:VAL:HB	1:A:257:TYR:CE1	2.53	0.44
1:C:120:GLY:HA2	2:D:31:HIS:HE2	1.82	0.44
1:A:128:GLU:OE1	1:A:128:GLU:HA	2.17	0.44
1:A:264:GLN:HG3	1:C:105:SER:HB2	1.99	0.44
1:A:185:PRO:HD3	1:A:263:HIS:CD2	2.52	0.44
1:A:105:SER:HB2	1:C:264:GLN:HG3	1.99	0.43
1:C:255:GLN:O	1:C:273:ARG:NH2	2.38	0.43
1:A:275:GLU:O	1:A:276:PRO:C	2.55	0.43
2:D:54:MET:HG2	2:D:55:SER:N	2.33	0.43
3:Q:3:VAL:CG1	3:Q:4:TYR:N	2.80	0.43
1:A:238:ASP:C	1:A:238:ASP:OD1	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:VAL:HG23	2:B:93:VAL:CG1	2.48	0.43
1:A:50:ARG:O	1:A:52:MET:N	2.52	0.43
1:A:24:GLU:OE1	1:A:45:TYR:OH	2.24	0.43
2:B:4:THR:HG23	2:B:87:MET:HE2	2.00	0.43
2:D:32:PRO:HB2	2:D:33:PRO:HD2	2.01	0.43
1:C:156:LEU:CD2	1:C:160:LEU:HG	2.48	0.43
1:C:46:GLU:HB2	1:C:47:PRO:HD2	2.00	0.43
1:C:42:ASN:HA	1:C:43:PRO:HD3	1.70	0.43
2:B:9:VAL:HG23	2:B:93:VAL:HG12	2.00	0.43
2:D:74:GLU:OE1	2:D:74:GLU:HA	2.19	0.43
2:D:9:VAL:HG23	2:D:93:VAL:HG12	2.01	0.43
1:C:66:LYS:CE	3:Q:3:VAL:HB	2.27	0.42
1:A:255:GLN:H	1:A:255:GLN:CD	2.19	0.42
1:C:137:ASP:OD1	1:C:139:ALA:HB3	2.19	0.42
2:B:4:THR:CG2	2:B:87:MET:HE2	2.50	0.42
1:C:235:PRO:HB2	2:D:65:LEU:HD22	2.02	0.42
1:C:266:LEU:HD11	1:C:270:LEU:HG	2.01	0.42
1:C:65:GLN:C	1:C:67:ALA:H	2.23	0.42
2:B:27:VAL:HG21	2:B:37:ILE:HD13	2.00	0.42
1:A:181:ARG:NH1	1:A:209:TYR:CE2	2.88	0.42
1:C:102:GLU:O	1:C:109:LEU:HD12	2.20	0.42
1:A:189:VAL:HA	1:A:202:ARG:O	2.18	0.42
1:A:74:PHE:HA	1:A:77:ASP:OD2	2.20	0.42
1:C:235:PRO:CB	2:D:65:LEU:HD22	2.50	0.42
2:D:35:ILE:HD11	2:D:82:VAL:HG13	2.02	0.42
1:A:234:ARG:HB2	2:B:10:TYR:OH	2.20	0.42
1:A:55:GLU:HA	1:A:55:GLU:OE1	2.20	0.41
1:A:137:ASP:OD1	1:A:139:ALA:HB3	2.19	0.41
1:C:183:ASP:HB2	1:C:209:TYR:N	2.35	0.41
1:A:191:HIS:NE2	1:A:254:GLU:OE2	2.52	0.41
2:D:83:LYS:HB2	2:D:83:LYS:HE3	1.93	0.41
1:C:220:ASN:ND2	1:C:220:ASN:N	2.68	0.41
1:C:226:GLN:HB2	1:C:226:GLN:HE21	1.67	0.41
1:A:157:ARG:O	1:A:161:GLU:HG3	2.21	0.41
1:C:191:HIS:NE2	1:C:199:VAL:HG11	2.35	0.41
1:C:185:PRO:HB3	1:C:208:PHE:HB3	2.03	0.41
1:C:259:CYS:O	1:C:271:THR:HA	2.19	0.41
1:A:81:LEU:HD23	1:A:118:TYR:CG	2.56	0.41
1:A:249:VAL:HB	1:A:250:PRO:HD2	2.03	0.41
1:A:194:ARG:HG2	1:A:195:PRO:HD2	2.02	0.41
1:A:14:ARG:HG3	1:A:14:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ASP:CG	3:P:9:MET:CE	2.89	0.41
1:C:108:ARG:HG2	1:C:108:ARG:NH1	2.36	0.41
1:C:103:VAL:HB	1:C:108:ARG:O	2.21	0.41
1:A:231:VAL:HB	2:B:8:GLN:HE22	1.85	0.41
2:D:48:LYS:CE	2:D:69:GLU:H	2.30	0.41
1:A:2:PRO:O	1:A:3:HIS:ND1	2.54	0.41
1:A:51:TRP:CH2	1:A:179:LEU:HD11	2.56	0.41
1:A:109:LEU:HD13	1:A:165:VAL:CG1	2.50	0.41
1:C:224:LEU:H	1:C:224:LEU:HD13	1.82	0.41
1:C:98:ILE:O	1:C:114:GLN:HA	2.21	0.41
1:C:120:GLY:CA	2:D:31:HIS:NE2	2.84	0.41
1:C:27:TYR:CE2	1:C:32:GLU:HB2	2.56	0.41
1:C:231:VAL:HB	2:D:8:GLN:HE22	1.86	0.41
2:D:19:LYS:HA	2:D:20:PRO:HD3	1.97	0.41
1:A:224:LEU:HD21	1:A:257:TYR:HE2	1.84	0.41
1:C:249:VAL:HB	1:C:250:PRO:HD2	2.03	0.41
2:D:9:VAL:CG2	2:D:93:VAL:HG12	2.51	0.41
1:C:17:LEU:HA	1:C:17:LEU:HD23	1.90	0.41
1:C:12:VAL:O	1:C:12:VAL:CG2	2.68	0.40
1:A:81:LEU:HD12	1:A:84:TYR:CE2	2.56	0.40
1:C:268:GLU:HB3	4:C:284:HOH:O	2.20	0.40
1:C:85:TYR:CD2	1:C:87:GLN:NE2	2.90	0.40
1:A:12:VAL:HG22	1:A:21:ARG:HB3	2.02	0.40
1:A:9:VAL:HG12	1:A:24:GLU:HG2	2.03	0.40
1:C:209:TYR:O	1:C:210:PRO:C	2.51	0.40
1:C:77:ASP:CG	3:Q:9:MET:CE	2.90	0.40
1:A:162:GLY:O	1:A:166:GLU:HG3	2.22	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	274/276 (99%)	255 (93%)	18 (7%)	1 (0%)	39 78
1	C	274/276 (99%)	255 (93%)	16 (6%)	3 (1%)	17 56
2	B	97/99 (98%)	94 (97%)	2 (2%)	1 (1%)	19 58
2	D	97/99 (98%)	93 (96%)	3 (3%)	1 (1%)	19 58
3	P	6/9 (67%)	6 (100%)	0	0	100 100
3	Q	6/9 (67%)	5 (83%)	1 (17%)	0	100 100
All	All	754/768 (98%)	708 (94%)	40 (5%)	6 (1%)	24 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	51	TRP
1	C	233	THR
1	A	233	THR
1	C	41	GLU
2	D	47	PRO
2	B	47	PRO

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	234/234 (100%)	217 (93%)	17 (7%)	17 50
1	C	234/234 (100%)	220 (94%)	14 (6%)	24 60
2	B	94/94 (100%)	90 (96%)	4 (4%)	35 73
2	D	94/94 (100%)	90 (96%)	4 (4%)	35 73
3	P	6/7 (86%)	6 (100%)	0	100 100
3	Q	6/7 (86%)	6 (100%)	0	100 100
All	All	668/670 (100%)	629 (94%)	39 (6%)	25 62

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	44	ARG
1	A	45	TYR
1	A	79	ARG
1	A	110	LEU
1	A	154	GLU
1	A	156	LEU
1	A	176	ASN
1	A	194	ARG
1	A	197	ASP
1	A	209	TYR
1	A	220	ASN
1	A	224	LEU
1	A	255	GLN
1	A	272	LEU
1	A	273	ARG
1	A	275	GLU
2	B	12	ARG
2	B	59	ASP
2	B	89	GLU
2	B	97	ARG
1	C	44	ARG
1	C	45	TYR
1	C	79	ARG
1	C	110	LEU
1	C	154	GLU
1	C	176	ASN
1	C	181	ARG
1	C	194	ARG
1	C	197	ASP
1	C	220	ASN
1	C	224	LEU
1	C	225	ILE
1	C	272	LEU
1	C	275	GLU
2	D	10	TYR
2	D	12	ARG
2	D	59	ASP
2	D	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	192	HIS
1	A	220	ASN
1	A	226	GLN
1	A	263	HIS
2	B	2	GLN
2	B	8	GLN
2	B	17	ASN
2	B	38	GLN
1	C	87	GLN
1	C	192	HIS
1	C	220	ASN
1	C	226	GLN
1	C	263	HIS
2	D	2	GLN
2	D	17	ASN
2	D	38	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	276/276 (100%)	-0.13	3 (1%) 82 65	8, 25, 48, 71	0
1	C	276/276 (100%)	0.47	23 (8%) 14 7	9, 26, 49, 79	0
2	B	99/99 (100%)	-0.30	0 100 100	9, 20, 35, 39	0
2	D	99/99 (100%)	0.33	8 (8%) 15 7	9, 20, 34, 45	0
3	P	8/9 (88%)	0.31	0 100 100	22, 31, 34, 38	0
3	Q	8/9 (88%)	0.76	1 (12%) 5 2	22, 31, 38, 47	0
All	All	766/768 (99%)	0.14	35 (4%) 36 21	8, 25, 45, 79	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	SER	3.8
1	C	41	GLU	3.7
2	D	47	PRO	3.5
1	C	149	GLN	3.5
1	C	225	ILE	3.5
1	C	87	GLN	3.4
1	C	276	PRO	3.4
2	D	88	ALA	3.4
1	C	196	GLU	3.2
2	D	1	ILE	3.2
1	C	226	GLN	3.1
1	A	225	ILE	2.9
1	C	217	TRP	2.9
2	D	85	ASP	2.9
1	C	42	ASN	2.9
1	C	86	ASN	2.9
3	Q	2	ALA	2.8
2	D	2	GLN	2.7
1	C	275	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	48	LYS	2.5
1	C	89	LYS	2.5
1	C	220	ASN	2.5
1	A	41	GLU	2.5
1	C	53	GLU	2.4
1	C	56	GLY	2.3
1	C	256	TYR	2.3
1	A	226	GLN	2.3
1	C	57	PRO	2.3
1	C	255	GLN	2.2
1	C	37	ASP	2.2
2	D	14	PRO	2.2
2	D	87	MET	2.2
1	C	178	THR	2.1
1	C	229	GLU	2.1
1	C	19	GLU	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 carbohydrates 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.