Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:36 PM GMT

PDB ID	:	1UCY
Title	:	THROMBIN COMPLEXED WITH FIBRINOPEPTIDE A ALPHA (RESIDUES 7-19). THREE COMPLEXES, ONE WITH EPSILON-THROMBIN AND TWO WITH ALPHA-THROMBIN
Authors	:	Martin, P.; Edwards, B.
Deposited on	:	1996-08-30
Resolution	:	2.20 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:

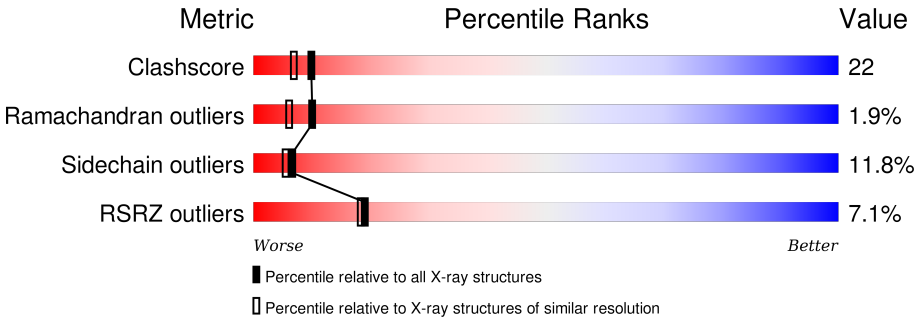
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.20 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))
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	J	49	12% 31% 35% 8% 27%
1	L	49	18% 45% 24% • 27%
1	M	49	16% 41% 24% 8% 27%
2	H	150	2% 60% 32% 7% •
3	E	109	7% 58% 36% 5% •
4	F	13	46% 85% 8% 8%
4	G	13	8% 62% 31% 8%

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Mol	Chain	Length	Quality of chain
4	I	13	8% 54% 46%
5	K	259	4% 56% 37% 7%
5	N	259	5% 58% 36% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8184 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 THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	J	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			
1	M	36	Total	C	N	O	S	0	0	0
			290	181	48	60	1			

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	150	Total	C	N	O	S	0	0	0
			1235	793	222	215	5			

- Molecule 3 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	109	Total	C	N	O	S	0	0	0
			860	544	154	155	7			

- Molecule 4 is a protein called FIBRINOPEPTIDE A-ALPHA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	13	Total	C	N	O	0	0	0
			97	60	18	19			
4	G	12	Total	C	N	O	0	0	0
			85	54	14	17			
4	I	13	Total	C	N	O	0	2	0
			116	71	23	22			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	6	ACE	GLY	CONFLICT	UNP P12803
F	16	OPR	ARG	CONFLICT	UNP P12803
G	6	ACE	GLY	CONFLICT	UNP P12803
G	16	OPR	ARG	CONFLICT	UNP P12803
I	6	ACE	GLY	CONFLICT	UNP P12803
I	16	OPR	ARG	CONFLICT	UNP P12803

- Molecule 5 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	K	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			
5	N	259	Total	C	N	O	S	0	0	0
			2094	1337	376	369	12			

- Molecule 6 is water.

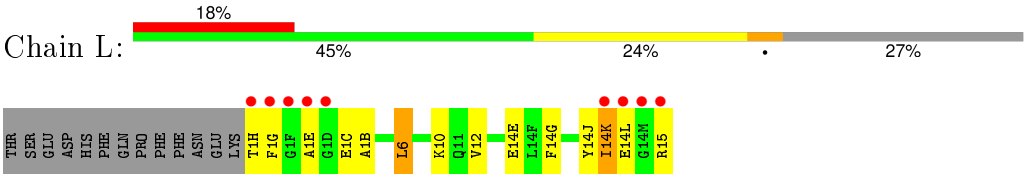
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	74	Total	O	0	0
			74	74		
6	F	8	Total	O	0	0
			8	8		
6	G	5	Total	O	0	0
			5	5		
6	H	99	Total	O	0	0
			99	99		
6	I	10	Total	O	0	0
			10	10		
6	J	42	Total	O	0	0
			42	42		
6	K	226	Total	O	0	0
			226	226		
6	L	49	Total	O	0	0
			49	49		
6	M	17	Total	O	0	0
			17	17		
6	N	203	Total	O	0	0
			203	203		

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.

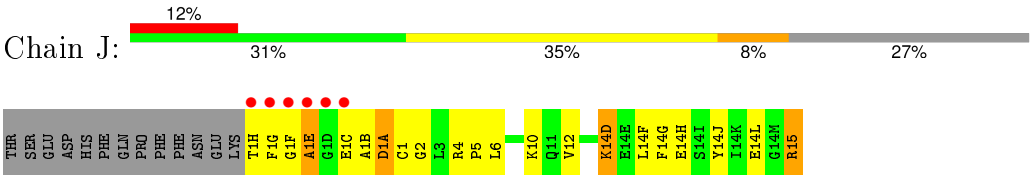
- Molecule 1: THROMBIN

Chain L:



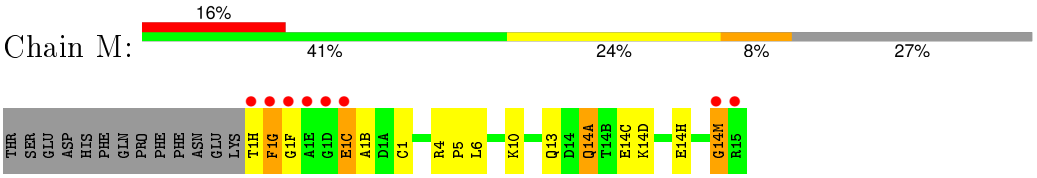
- Molecule 1: THROMBIN

Chain J:



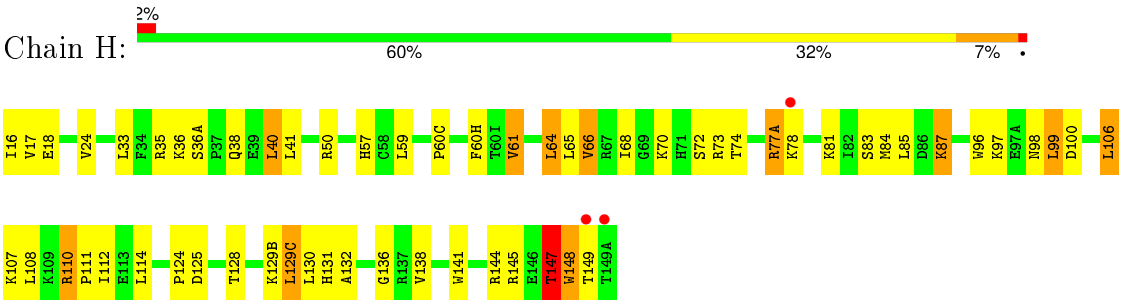
- Molecule 1: THROMBIN

Chain M:



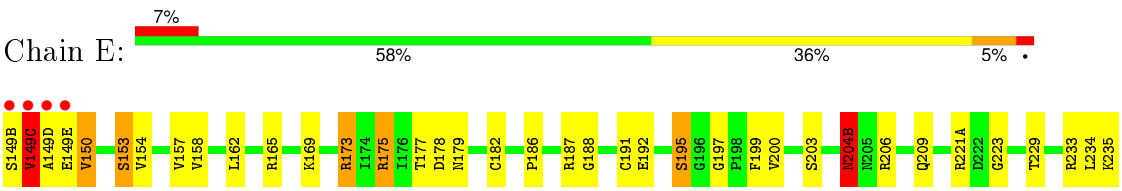
- Molecule 2: THROMBIN

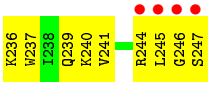
Chain H:



- Molecule 3: THROMBIN

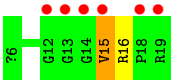
Chain E:





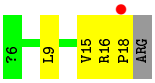
• Molecule 4: FIBRINOPEPTIDE A-ALPHA

Chain F:



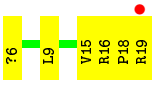
• Molecule 4: FIBRINOPEPTIDE A-ALPHA

Chain G:



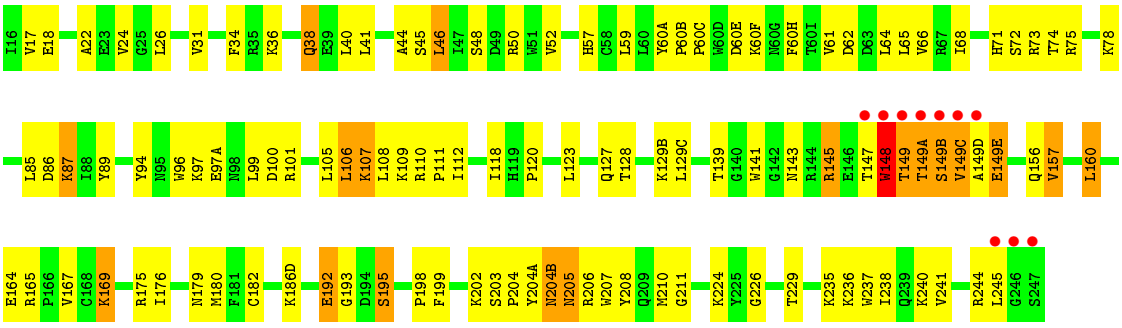
• Molecule 4: FIBRINOPEPTIDE A-ALPHA

Chain I:



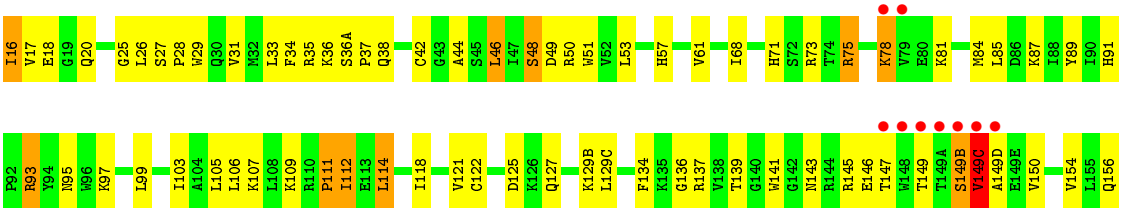
• Molecule 5: THROMBIN

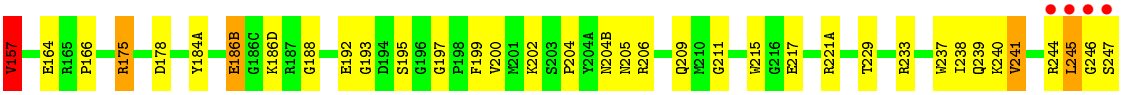
Chain K:



• Molecule 5: THROMBIN

Chain N:




V157
E164
R165
P166
R175
D178
Y184A
E186B
G186C
K186D
R187
G188
E192
G193
D194
S195
G196
G197
P198
F199
V200
M201
K202
S203
P204
Y204A
N204B
N205
R206
Q209
M210
G211
W215
G216
E217
R221A
T229
R233
W237
I238
Q239
K240
V241
R244
L245
G246
S247

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.47Å 88.78Å 98.55Å 90.00° 106.21° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 41.38 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.20) 69.3 (41.38-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 2.20Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , (Not available) 0.172 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 120.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 48052 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8184	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ACE, OPR

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	J	0.61	0/294	0.80	0/390
1	L	0.59	0/294	0.81	0/390
1	M	0.47	0/294	0.83	1/390 (0.3%)
2	H	0.52	0/1267	0.84	2/1716 (0.1%)
3	E	0.50	0/881	0.78	1/1186 (0.1%)
4	F	0.56	0/80	0.83	0/103
4	G	0.44	0/68	0.77	0/89
4	I	0.66	0/99	1.06	0/125
5	K	0.57	0/2148	0.87	2/2905 (0.1%)
5	N	0.48	0/2148	0.77	2/2905 (0.1%)
All	All	0.53	0/7573	0.82	8/10199 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	40	LEU	CA-CB-CG	6.89	131.14	115.30
1	M	14(M)	GLY	N-CA-C	6.36	129.01	113.10
5	N	157	VAL	CB-CA-C	-5.69	100.59	111.40
5	K	199	PHE	N-CA-C	-5.62	95.83	111.00
5	K	148	TRP	N-CA-C	5.21	125.07	111.00
3	E	204(B)	ASN	N-CA-C	-5.15	97.10	111.00
2	H	147	THR	N-CA-C	5.09	124.75	111.00
5	N	186(B)	GLU	N-CA-C	5.02	124.56	111.00

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	J	290	0	276	22	0
1	L	290	0	276	12	0
1	M	290	0	276	18	0
2	H	1235	0	1252	67	0
3	E	860	0	844	57	0
4	F	97	0	90	4	0
4	G	85	0	77	8	0
4	I	116	0	110	8	0
5	K	2094	0	2097	113	0
5	N	2094	0	2097	79	0
6	E	74	0	0	8	0
6	F	8	0	0	0	0
6	G	5	0	0	1	0
6	H	99	0	0	7	0
6	I	10	0	0	1	0
6	J	42	0	0	7	0
6	K	226	0	0	26	0
6	L	49	0	0	2	0
6	M	17	0	0	3	0
6	N	203	0	0	6	0
All	All	8184	0	7395	328	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 22.

All (328) 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)
3:E:236:LYS:HZ2	3:E:239:GLN:HG3	1.24	1.03
3:E:149(C):VAL:HG21	3:E:153:SER:HA	1.45	0.99
1:L:15:ARG:HG3	2:H:131:HIS:HB3	1.45	0.97
5:K:99:LEU:HD11	4:G:15:VAL:HG12	1.47	0.94
4:I:19[B]:ARG:OXT	4:I:19[B]:ARG:HD3	1.68	0.93
1:M:1(G):PHE:HB3	5:N:125:ASP:HB3	1.56	0.86
5:N:81:LYS:HD2	5:N:112:ILE:HD11	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:177:THR:HG22	3:E:179:ASN:H	1.45	0.81
5:K:50:ARG:HD2	6:K:290:HOH:O	1.81	0.80
3:E:236:LYS:NZ	3:E:239:GLN:HG3	1.95	0.80
1:L:15:ARG:HG2	2:H:132:ALA:O	1.81	0.80
5:N:147:THR:HG22	5:N:149(B):SER:HB2	1.62	0.79
5:K:160:LEU:HD23	6:K:310:HOH:O	1.84	0.77
1:J:14(G):PHE:HB3	6:J:211:HOH:O	1.85	0.76
5:N:240:LYS:HG3	5:N:245:LEU:HA	1.68	0.76
2:H:73:ARG:HH12	3:E:149(C):VAL:HG22	1.50	0.75
5:K:193:GLY:HA2	4:G:18:PRO:HG3	1.68	0.75
1:M:1(C):GLU:HB3	1:M:1:CYS:HB3	1.68	0.75
5:K:73:ARG:HB3	5:K:73:ARG:HH11	1.49	0.75
5:K:46:LEU:HD22	5:K:48:SER:O	1.87	0.74
5:K:164:GLU:HG2	5:K:167:VAL:HG13	1.70	0.74
2:H:148:TRP:HD1	5:K:149(D):ALA:N	1.85	0.74
5:K:127:GLN:O	5:K:129(B):LYS:HD3	1.87	0.73
5:K:149:THR:HG22	5:K:149(A):THR:H	1.51	0.73
2:H:130:LEU:HD23	3:E:162:LEU:HD21	1.70	0.73
1:J:1(G):PHE:HB2	1:J:1(C):GLU:OE1	1.88	0.73
5:K:210:MET:SD	6:K:331:HOH:O	2.47	0.73
5:K:50:ARG:NE	5:K:111:PRO:HG3	2.05	0.72
5:N:46:LEU:HD22	5:N:48:SER:O	1.89	0.71
5:K:165:ARG:HG2	5:K:169:LYS:NZ	2.05	0.71
1:L:14(K):ILE:HG13	6:L:206:HOH:O	1.91	0.71
5:K:129(B):LYS:HG2	5:K:204(A):TYR:CE2	2.26	0.70
5:K:169:LYS:NZ	5:K:169:LYS:HB2	2.06	0.70
2:H:68:ILE:HD13	2:H:112:ILE:HD13	1.74	0.70
1:L:15:ARG:CG	2:H:131:HIS:HB3	2.21	0.70
2:H:77(A):ARG:HA	6:H:165:HOH:O	1.92	0.69
3:E:195:SER:HB2	4:F:16:OPR:O	1.93	0.69
5:K:78:LYS:HG2	6:K:341:HOH:O	1.92	0.68
5:K:36:LYS:HD2	6:K:415:HOH:O	1.93	0.68
5:N:50:ARG:HD3	6:N:381:HOH:O	1.93	0.67
1:L:1(E):ALA:HB2	3:E:206:ARG:CZ	2.24	0.67
2:H:18:GLU:HB2	3:E:188:GLY:HA2	1.76	0.67
5:K:204(B):ASN:ND2	5:K:206:ARG:HB2	2.10	0.67
3:E:165:ARG:HH21	3:E:233:ARG:HH12	1.43	0.67
5:K:147:THR:OG1	5:K:149(C):VAL:HG21	1.96	0.66
5:N:129(C):LEU:HD11	5:N:204:PRO:HD2	1.78	0.66
5:N:149(C):VAL:HA	6:N:344:HOH:O	1.97	0.65
3:E:239:GLN:HB3	3:E:247:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:14(M):GLY:HA2	6:M:465:HOH:O	1.95	0.65
3:E:197:GLY:HA3	6:E:251:HOH:O	1.97	0.65
5:K:45:SER:HB3	5:K:198:PRO:HG3	1.78	0.65
5:K:204(B):ASN:ND2	5:K:204(B):ASN:O	2.31	0.64
1:L:14(G):PHE:O	1:L:14(J):TYR:HB2	1.97	0.64
1:J:1(B):ALA:HA	5:K:206:ARG:HH22	1.64	0.63
2:H:35:ARG:HB2	2:H:41:LEU:HD11	1.80	0.63
5:K:105:LEU:HD13	5:K:241:VAL:HG21	1.79	0.63
3:E:149(C):VAL:HG21	3:E:153:SER:CA	2.22	0.63
1:J:1(H):THR:N	6:J:276:HOH:O	2.31	0.63
5:K:73:ARG:HB2	5:K:141:TRP:CD1	2.34	0.63
6:K:473:HOH:O	4:G:18:PRO:HB3	1.99	0.62
5:N:84:MET:HB2	5:N:109:LYS:HE3	1.81	0.62
5:N:178:ASP:HB3	5:N:233:ARG:NH2	2.15	0.62
2:H:18:GLU:HG3	3:E:187:ARG:HB2	1.81	0.62
4:I:6:ACE:H1	6:I:24:HOH:O	1.99	0.62
2:H:96:TRP:HA	2:H:99:LEU:HD23	1.80	0.61
5:K:145:ARG:HH21	5:K:149(C):VAL:HG11	1.65	0.61
3:E:240:LYS:HG2	6:E:292:HOH:O	1.99	0.61
5:N:145:ARG:HG2	5:N:146:GLU:N	2.16	0.61
1:J:15:ARG:NH1	1:J:15:ARG:HB3	2.15	0.61
5:N:204(B):ASN:O	5:N:206:ARG:N	2.30	0.60
1:L:1(H):THR:O	2:H:125:ASP:HB3	2.00	0.60
5:K:86:ASP:HB3	5:K:107:LYS:HG3	1.82	0.60
5:N:239:GLN:NE2	5:N:247:SER:HB3	2.16	0.60
5:K:160:LEU:HB3	6:K:310:HOH:O	2.00	0.60
5:K:128:THR:HG23	6:K:379:HOH:O	2.01	0.59
2:H:85:LEU:HD22	2:H:106:LEU:HB3	1.84	0.59
3:E:223:GLY:HA2	6:E:302:HOH:O	2.02	0.59
5:K:85:LEU:HD22	5:K:106:LEU:HB3	1.84	0.59
5:N:240:LYS:HB2	5:N:246:GLY:H	1.68	0.59
5:K:17:VAL:HG12	5:K:18:GLU:HG2	1.83	0.59
2:H:110:ARG:HH11	2:H:110:ARG:HG3	1.67	0.58
5:N:87:LYS:HD2	5:N:89:TYR:OH	2.03	0.58
5:K:22:ALA:O	5:K:71:HIS:HE1	1.87	0.58
2:H:148:TRP:CD1	5:K:149(C):VAL:HA	2.39	0.58
2:H:77(A):ARG:HG2	6:H:165:HOH:O	2.02	0.58
2:H:107:LYS:NZ	3:E:244:ARG:HH22	2.03	0.57
2:H:73:ARG:NH1	3:E:149(C):VAL:HG22	2.17	0.57
1:J:15:ARG:HH11	1:J:15:ARG:HB3	1.69	0.57
2:H:148:TRP:HA	6:H:170:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:141:TRP:HE3	6:K:325:HOH:O	1.87	0.57
5:N:149(D):ALA:C	5:N:150:VAL:H	2.06	0.57
5:N:215:TRP:HA	4:I:16:OPR:HG2	1.87	0.57
1:J:14(H):GLU:O	1:J:14(L):GLU:HG3	2.04	0.57
2:H:70:LYS:HE3	2:H:72:SER:O	2.05	0.56
2:H:147:THR:HB	3:E:192:GLU:OE2	2.05	0.56
5:N:35:ARG:O	5:N:38:GLN:HA	2.05	0.56
5:N:139:THR:HA	5:N:156:GLN:O	2.06	0.56
2:H:17:VAL:O	3:E:188:GLY:HA2	2.06	0.56
5:K:145:ARG:HE	5:K:147:THR:HG23	1.71	0.56
5:K:149:THR:O	5:K:149(B):SER:N	2.38	0.56
1:J:1(C):GLU:HG2	1:J:1:CYS:SG	2.46	0.56
5:N:73:ARG:HB2	5:N:141:TRP:CD1	2.41	0.56
5:N:127:GLN:O	5:N:129(B):LYS:HD2	2.06	0.56
2:H:149:THR:HG21	3:E:150:VAL:HG21	1.88	0.56
5:K:204(B):ASN:HD21	5:K:206:ARG:HB2	1.71	0.56
2:H:100:ASP:OD1	3:E:177:THR:HG21	2.06	0.55
5:K:176:ILE:HB	6:K:257:HOH:O	2.06	0.55
5:K:240:LYS:HD2	6:K:334:HOH:O	2.06	0.55
5:K:149(A):THR:HA	5:K:149(D):ALA:HA	1.88	0.55
5:K:105:LEU:HD13	5:K:241:VAL:CG2	2.37	0.55
5:N:61:VAL:HG13	5:N:85:LEU:HB2	1.88	0.55
5:N:193:GLY:HA2	4:I:18[B]:PRO:HG3	1.89	0.55
1:L:10:LYS:HB3	1:L:12:VAL:HG23	1.88	0.55
1:L:1(C):GLU:O	1:L:1(B):ALA:HB3	2.07	0.55
4:I:19[B]:ARG:HH11	4:I:19[B]:ARG:HB2	1.72	0.55
5:K:165:ARG:HG2	5:K:169:LYS:HZ1	1.72	0.55
3:E:195:SER:HB2	4:F:16:OPR:C	2.36	0.54
5:N:147:THR:CG2	5:N:150:VAL:HG11	2.37	0.54
1:J:14(D):LYS:HE2	6:J:644:HOH:O	2.08	0.54
3:E:204(B):ASN:C	3:E:204(B):ASN:HD22	2.10	0.54
5:N:200:VAL:HG12	5:N:209:GLN:HA	1.89	0.54
2:H:87:LYS:HG2	6:H:202:HOH:O	2.08	0.54
6:J:57:HOH:O	5:K:120:PRO:HG2	2.07	0.54
3:E:149(C):VAL:HG11	3:E:153:SER:HB3	1.90	0.53
5:N:239:GLN:HE21	5:N:247:SER:HB3	1.72	0.53
5:K:211:GLY:HA2	5:K:229:THR:O	2.09	0.53
1:J:1(F):GLY:HA3	5:K:123:LEU:HB2	1.91	0.53
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.43	0.53
1:M:1(F):GLY:HA2	6:N:328:HOH:O	2.09	0.52
5:N:81:LYS:HD2	5:N:112:ILE:CD1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:14(D):LYS:O	1:M:14(H):GLU:HG3	2.10	0.52
5:K:205:ASN:N	6:K:278:HOH:O	2.43	0.52
2:H:128:THR:HG23	2:H:129(C):LEU:HD22	1.90	0.52
5:N:95:ASN:O	5:N:99:LEU:HA	2.10	0.52
5:K:208:TYR:HB2	5:K:210:MET:CE	2.40	0.52
5:N:18:GLU:HB2	5:N:188:GLY:HA2	1.91	0.52
5:K:149(A):THR:HA	5:K:149(D):ALA:CA	2.40	0.52
1:M:1(G):PHE:CB	5:N:125:ASP:HB3	2.35	0.51
5:K:97:LYS:HE2	6:K:411:HOH:O	2.09	0.51
5:K:143:ASN:ND2	5:K:192:GLU:HG3	2.26	0.51
5:K:60(A):TYR:CE2	5:K:60(C):PRO:HG2	2.46	0.51
2:H:96:TRP:CZ3	2:H:97:LYS:HG2	2.46	0.51
5:K:60(F):LYS:HZ3	5:K:60(H):PHE:HE2	1.58	0.51
3:E:186:PRO:HB3	6:E:296:HOH:O	2.11	0.51
2:H:61:VAL:HG22	2:H:85:LEU:HB2	1.93	0.50
5:N:49:ASP:OD2	5:N:111:PRO:HB3	2.11	0.50
5:K:176:ILE:CB	6:K:257:HOH:O	2.60	0.50
3:E:149(E):GLU:O	3:E:150:VAL:HB	2.11	0.50
1:J:1(C):GLU:C	1:J:1(A):ASP:H	2.13	0.49
1:J:1(F):GLY:HA2	6:J:174:HOH:O	2.12	0.49
3:E:236:LYS:HZ2	3:E:236:LYS:HA	1.77	0.49
5:K:208:TYR:HB2	5:K:210:MET:HE2	1.94	0.49
5:N:237:TRP:O	5:N:241:VAL:HG13	2.13	0.49
5:K:34:PHE:CZ	5:K:38:GLN:O	2.65	0.49
5:K:31:VAL:HB	5:K:44:ALA:HB3	1.95	0.49
2:H:148:TRP:HB2	5:K:149(A):THR:O	2.12	0.49
1:M:13:GLN:NE2	6:M:674:HOH:O	2.45	0.49
1:J:5:PRO:O	1:J:10:LYS:HE2	2.11	0.49
2:H:98:ASN:ND2	3:E:175:ARG:NH1	2.60	0.49
5:N:95:ASN:OD1	5:N:97:LYS:HG3	2.13	0.49
5:N:17:VAL:O	5:N:188:GLY:HA2	2.12	0.49
1:M:4:ARG:NH1	5:N:26:LEU:HD12	2.28	0.49
5:N:114:LEU:N	5:N:114:LEU:HD13	2.28	0.49
5:K:22:ALA:HB2	5:K:157:VAL:HG22	1.93	0.49
5:K:176:ILE:HG21	6:K:257:HOH:O	2.13	0.49
5:N:105:LEU:HD11	5:N:238:ILE:HG23	1.95	0.48
5:N:136:GLY:HA3	5:N:199:PHE:CE1	2.48	0.48
5:K:208:TYR:CB	5:K:210:MET:CE	2.91	0.48
3:E:165:ARG:NH2	3:E:233:ARG:HH12	2.11	0.48
3:E:149(C):VAL:HG13	3:E:149(D):ALA:N	2.28	0.48
5:K:145:ARG:NH2	5:K:147:THR:HG21	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:149(C):VAL:CG1	3:E:149(D):ALA:N	2.76	0.48
1:J:1(F):GLY:O	1:J:1(E):ALA:HB2	2.14	0.48
2:H:145:ARG:HD2	5:K:149(A):THR:HG21	1.96	0.48
2:H:60(H):PHE:HB3	2:H:64:LEU:HD21	1.95	0.48
5:N:195:SER:OG	4:I:16:OPR:C	2.62	0.48
1:M:14(C):GLU:OE2	5:N:202:LYS:NZ	2.46	0.47
5:K:87:LYS:HB3	5:K:89:TYR:CE2	2.49	0.47
1:M:1(G):PHE:HB3	5:N:125:ASP:CB	2.37	0.47
5:K:145:ARG:HH21	5:K:147:THR:HG21	1.78	0.47
5:N:175:ARG:O	5:N:175:ARG:HG3	2.12	0.47
2:H:129(B):LYS:HG3	6:H:224:HOH:O	2.14	0.47
1:J:1(C):GLU:C	1:J:1(A):ASP:N	2.68	0.47
5:K:85:LEU:CD2	5:K:106:LEU:HB3	2.44	0.47
5:N:53:LEU:HD11	5:N:103:ILE:HD11	1.97	0.47
1:M:4:ARG:HD3	5:N:26:LEU:O	2.15	0.47
3:E:165:ARG:NH2	6:E:283:HOH:O	2.46	0.47
5:N:204:PRO:HA	6:N:330:HOH:O	2.14	0.47
5:N:61:VAL:HG23	6:N:316:HOH:O	2.14	0.47
5:K:73:ARG:HB3	5:K:73:ARG:NH1	2.26	0.47
1:L:1(H):THR:HA	6:E:276:HOH:O	2.15	0.47
5:K:139:THR:HA	5:K:156:GLN:O	2.15	0.47
5:N:71:HIS:CD2	5:N:154:VAL:HG23	2.50	0.46
2:H:128:THR:HG23	2:H:129(C):LEU:CD2	2.46	0.46
5:N:68:ILE:CD1	5:N:112:ILE:HD13	2.45	0.46
2:H:18:GLU:HG3	3:E:187:ARG:CB	2.43	0.46
3:E:203:SER:HB3	3:E:204(B):ASN:ND2	2.30	0.46
5:N:184(A):TYR:CZ	5:N:186(D):LYS:HD3	2.51	0.46
2:H:124:PRO:HD3	3:E:209:GLN:O	2.16	0.46
5:K:108:LEU:CD1	5:K:112:ILE:HG12	2.46	0.46
1:M:1:CYS:O	5:N:122:CYS:SG	2.74	0.46
2:H:68:ILE:HD13	2:H:112:ILE:CD1	2.42	0.46
5:K:68:ILE:HD12	5:K:112:ILE:HG13	1.96	0.46
5:K:149(E):GLU:HG2	6:K:417:HOH:O	2.15	0.46
1:M:4:ARG:HH12	5:N:26:LEU:HD12	1.80	0.46
3:E:200:VAL:HG12	3:E:209:GLN:HA	1.97	0.46
3:E:221(A):ARG:NH2	5:K:148:TRP:CE3	2.83	0.46
5:N:91:HIS:CE1	5:N:93:ARG:HB2	2.51	0.46
3:E:236:LYS:HA	3:E:236:LYS:NZ	2.30	0.46
2:H:57:HIS:CD2	4:F:15:VAL:HG13	2.51	0.46
1:J:14(J):TYR:HB3	6:K:447:HOH:O	2.16	0.46
5:K:57:HIS:CD2	4:G:15:VAL:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:147:THR:HA	5:N:149(B):SER:OG	2.15	0.46
5:K:108:LEU:HD13	5:K:112:ILE:HG12	1.98	0.45
3:E:157:VAL:HG12	3:E:158:VAL:N	2.32	0.45
5:K:208:TYR:CB	5:K:210:MET:HE2	2.46	0.45
5:K:224:LYS:HD3	5:K:224:LYS:HA	1.73	0.45
5:K:235:LYS:HA	5:K:238:ILE:HD12	1.99	0.45
5:K:176:ILE:CG2	6:K:257:HOH:O	2.64	0.45
5:N:105:LEU:HD13	5:N:241:VAL:CG2	2.46	0.45
5:K:60(B):PRO:N	5:K:60(C):PRO:HD2	2.31	0.45
2:H:50:ARG:HD3	6:H:160:HOH:O	2.17	0.45
3:E:240:LYS:HG3	3:E:246:GLY:N	2.32	0.45
2:H:107:LYS:HZ1	3:E:244:ARG:HH22	1.65	0.45
5:N:75:ARG:HE	5:N:75:ARG:HB2	1.68	0.45
2:H:50:ARG:NE	2:H:111:PRO:HB3	2.31	0.45
5:K:165:ARG:NH1	6:K:398:HOH:O	2.49	0.45
2:H:148:TRP:CD1	5:K:149(C):VAL:CA	2.99	0.44
5:K:169:LYS:HZ2	5:K:169:LYS:HB2	1.79	0.44
2:H:36:LYS:O	2:H:38:GLN:HG3	2.17	0.44
5:K:34:PHE:CE2	5:K:38:GLN:O	2.70	0.44
5:K:94:TYR:CZ	5:K:96:TRP:HB3	2.53	0.44
5:N:129(C):LEU:O	5:N:134:PHE:HD2	2.00	0.44
5:N:197:GLY:HA3	6:N:275:HOH:O	2.18	0.44
1:J:1(B):ALA:CA	5:K:206:ARG:HH22	2.29	0.44
2:H:17:VAL:O	2:H:18:GLU:HB2	2.18	0.44
3:E:177:THR:HG22	3:E:178:ASP:N	2.32	0.44
5:N:204(B):ASN:O	5:N:204(B):ASN:ND2	2.51	0.44
3:E:149(B):SER:O	3:E:149(C):VAL:HG23	2.18	0.44
5:K:203:SER:HB2	6:K:379:HOH:O	2.17	0.43
5:N:192:GLU:OE1	4:I:19[A]:ARG:HD2	2.18	0.43
5:K:203:SER:HA	5:K:204:PRO:HD3	1.89	0.43
1:J:10:LYS:HE3	6:J:518:HOH:O	2.18	0.43
5:N:20:GLN:CG	5:N:157:VAL:HG23	2.48	0.43
1:M:1(H):THR:HG22	1:M:1(G):PHE:N	2.33	0.43
2:H:148:TRP:HD1	5:K:149(C):VAL:C	2.21	0.43
3:E:165:ARG:HD3	6:E:262:HOH:O	2.18	0.43
5:N:36:LYS:O	5:N:38:GLN:HG3	2.19	0.43
5:K:97(A):GLU:OE2	5:K:175:ARG:HD3	2.18	0.43
2:H:99:LEU:HD23	2:H:99:LEU:HA	1.87	0.43
5:K:72:SER:OG	5:K:75:ARG:HG2	2.19	0.43
2:H:81:LYS:HB3	2:H:112:ILE:HD11	2.00	0.43
5:K:86:ASP:HB2	5:K:109:LYS:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:85:LEU:HD23	2:H:108:LEU:HD23	2.01	0.43
3:E:173:ARG:HG3	6:E:266:HOH:O	2.19	0.43
5:N:149(B):SER:O	5:N:149(C):VAL:HG13	2.18	0.43
2:H:148:TRP:CD1	5:K:149(D):ALA:N	2.75	0.43
3:E:237:TRP:O	3:E:241:VAL:HG13	2.19	0.43
2:H:145:ARG:HH21	2:H:149:THR:HB	1.83	0.43
3:E:244:ARG:HD3	3:E:244:ARG:HA	1.68	0.43
1:J:2:GLY:O	5:K:207:TRP:HD1	2.02	0.43
3:E:149(E):GLU:O	3:E:150:VAL:CB	2.67	0.42
5:N:129(C):LEU:HD11	5:N:204:PRO:CD	2.48	0.42
1:M:4:ARG:HG2	5:N:28:PRO:HG3	2.01	0.42
2:H:36:LYS:HG2	2:H:65:LEU:HG	2.01	0.42
5:K:236:LYS:HD2	6:K:449:HOH:O	2.19	0.42
1:J:4:ARG:NH1	5:K:26:LEU:O	2.41	0.42
2:H:50:ARG:HE	2:H:111:PRO:HB3	1.83	0.42
5:K:226:GLY:HA3	6:K:280:HOH:O	2.18	0.42
5:N:68:ILE:HG22	5:N:118:ILE:HG12	2.01	0.42
5:N:184(A):TYR:CE2	5:N:186(D):LYS:HB3	2.54	0.42
5:N:51:TRP:CZ2	5:N:107:LYS:HD3	2.55	0.42
2:H:145:ARG:CD	5:K:149(A):THR:HG21	2.49	0.42
5:K:202:LYS:HD2	5:K:207:TRP:CZ2	2.55	0.42
5:N:57:HIS:CD2	4:I:15:VAL:HB	2.54	0.42
3:E:235:LYS:O	3:E:239:GLN:HG2	2.18	0.42
2:H:136:GLY:HA3	3:E:199:PHE:CZ	2.54	0.42
2:H:60(H):PHE:CB	2:H:64:LEU:HD21	2.50	0.42
5:K:59:LEU:HD11	5:K:106:LEU:HD11	2.00	0.42
5:K:60(F):LYS:NZ	5:K:60(H):PHE:HE2	2.17	0.42
2:H:77(A):ARG:HD3	6:H:214:HOH:O	2.20	0.42
2:H:99:LEU:HD11	4:F:15:VAL:CG2	2.50	0.42
6:K:388:HOH:O	4:G:16:OPR:H21	2.18	0.42
5:K:41:LEU:O	4:G:18:PRO:CD	2.68	0.41
2:H:130:LEU:HA	2:H:130:LEU:HD23	1.90	0.41
5:N:149(D):ALA:C	5:N:150:VAL:N	2.74	0.41
3:E:165:ARG:O	3:E:169:LYS:HG3	2.21	0.41
5:K:44:ALA:HB1	5:K:52:VAL:CG1	2.50	0.41
1:L:14(E):GLU:HG3	6:L:43:HOH:O	2.20	0.41
5:K:107:LYS:HE3	5:K:107:LYS:HB2	1.79	0.41
1:M:14(D):LYS:HA	6:M:327:HOH:O	2.19	0.41
5:N:164:GLU:HB3	5:N:166:PRO:HD2	2.02	0.41
2:H:57:HIS:NE2	3:E:195:SER:OG	2.43	0.41
5:K:68:ILE:HG22	5:K:118:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:195:SER:HB2	4:G:16:OPR:O	2.20	0.41
5:K:40:LEU:C	5:K:40:LEU:HD23	2.40	0.41
5:N:29:TRP:CG	5:N:121:VAL:HB	2.56	0.41
5:K:100:ASP:O	5:K:101:ARG:HB2	2.21	0.41
1:M:10:LYS:NZ	1:M:10:LYS:HB3	2.34	0.41
2:H:16:ILE:O	2:H:144:ARG:HA	2.20	0.41
2:H:59:LEU:HD11	2:H:106:LEU:HD11	2.02	0.41
3:E:239:GLN:CB	3:E:247:SER:HB3	2.48	0.41
2:H:17:VAL:HG23	3:E:191:CYS:HB2	2.03	0.41
3:E:177:THR:CG2	3:E:178:ASP:N	2.84	0.41
5:K:169:LYS:HZ3	5:K:169:LYS:HB2	1.78	0.41
2:H:17:VAL:HG22	2:H:144:ARG:O	2.20	0.41
5:K:237:TRP:O	5:K:241:VAL:HG13	2.20	0.41
5:K:61:VAL:HG13	5:K:85:LEU:O	2.21	0.41
1:J:1(F):GLY:HA2	6:J:173:HOH:O	2.20	0.41
5:N:36(A):SER:HA	5:N:37:PRO:HA	1.88	0.41
5:N:31:VAL:HB	5:N:44:ALA:HB3	2.02	0.41
1:L:6:LEU:HA	1:L:6:LEU:HD12	1.83	0.41
5:K:179:ASN:CB	6:K:320:HOH:O	2.69	0.41
5:N:93:ARG:HH11	5:N:93:ARG:HG2	1.86	0.41
5:N:16:ILE:N	5:N:143:ASN:O	2.54	0.41
2:H:16:ILE:HD11	2:H:138:VAL:HG12	2.03	0.40
1:J:10:LYS:HB3	1:J:12:VAL:HG23	2.04	0.40
3:E:229:THR:CG2	3:E:234:LEU:HD12	2.50	0.40
5:N:217:GLU:O	5:N:221(A):ARG:HD2	2.20	0.40
5:N:78:LYS:HE3	5:N:78:LYS:HB3	1.97	0.40
5:K:208:TYR:HB3	5:K:210:MET:HE1	2.04	0.40
5:N:211:GLY:HA2	5:N:229:THR:O	2.20	0.40
1:M:6:LEU:HD22	5:N:25:GLY:HA3	2.03	0.40
5:K:179:ASN:HB3	6:K:320:HOH:O	2.21	0.40
2:H:66:VAL:HG12	2:H:83:SER:HB3	2.04	0.40
4:G:15:VAL:HG22	6:G:372:HOH:O	2.21	0.40
5:K:17:VAL:O	5:K:18:GLU:HB2	2.20	0.40
5:K:60(F):LYS:NZ	6:K:396:HOH:O	2.54	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	J	34/49 (69%)	27 (79%)	6 (18%)	1 (3%)	6 2
1	L	34/49 (69%)	26 (76%)	5 (15%)	3 (9%)	1 0
1	M	34/49 (69%)	29 (85%)	3 (9%)	2 (6%)	2 1
2	H	148/150 (99%)	136 (92%)	11 (7%)	1 (1%)	26 25
3	E	107/109 (98%)	94 (88%)	11 (10%)	2 (2%)	10 6
4	F	9/13 (69%)	7 (78%)	2 (22%)	0	100 100
4	G	9/13 (69%)	9 (100%)	0	0	100 100
4	I	9/13 (69%)	9 (100%)	0	0	100 100
5	K	257/259 (99%)	231 (90%)	21 (8%)	5 (2%)	10 6
5	N	257/259 (99%)	227 (88%)	27 (10%)	3 (1%)	16 12
All	All	898/963 (93%)	795 (88%)	86 (10%)	17 (2%)	10 6

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	150	VAL
1	J	1(E)	ALA
5	K	148	TRP
5	K	149	THR
5	K	149(A)	THR
5	K	245	LEU
5	N	149(C)	VAL
5	N	205	ASN
1	L	1(G)	PHE
1	L	14(K)	ILE
2	H	77(A)	ARG
3	E	149(C)	VAL
5	K	205	ASN
1	M	1(B)	ALA

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Mol	Chain	Res	Type
5	N	186(B)	GLU
1	L	14(L)	GLU
1	M	14(A)	GLN

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	J	30/43 (70%)	25 (83%)	5 (17%)	3 2
1	L	30/43 (70%)	29 (97%)	1 (3%)	45 56
1	M	30/43 (70%)	26 (87%)	4 (13%)	5 4
2	H	134/134 (100%)	115 (86%)	19 (14%)	4 3
3	E	92/92 (100%)	83 (90%)	9 (10%)	10 9
4	F	7/7 (100%)	6 (86%)	1 (14%)	4 3
4	G	6/7 (86%)	5 (83%)	1 (17%)	3 2
4	I	9/7 (129%)	8 (89%)	1 (11%)	8 6
5	K	226/226 (100%)	197 (87%)	29 (13%)	5 4
5	N	226/226 (100%)	203 (90%)	23 (10%)	9 8
All	All	790/828 (95%)	697 (88%)	93 (12%)	6 5

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
2	H	24	VAL
2	H	33	LEU
2	H	36(A)	SER
2	H	40	LEU
2	H	60(C)	PRO
2	H	61	VAL
2	H	64	LEU
2	H	66	VAL
2	H	74	THR

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Mol	Chain	Res	Type
2	H	78	LYS
2	H	84	MET
2	H	87	LYS
2	H	99	LEU
2	H	106	LEU
2	H	110	ARG
2	H	114	LEU
2	H	129(C)	LEU
2	H	147	THR
2	H	148	TRP
3	E	149(C)	VAL
3	E	153	SER
3	E	154	VAL
3	E	173	ARG
3	E	175	ARG
3	E	182	CYS
3	E	195	SER
3	E	204(B)	ASN
3	E	245	LEU
4	F	15	VAL
1	J	1(A)	ASP
1	J	6	LEU
1	J	14(D)	LYS
1	J	14(F)	LEU
1	J	15	ARG
5	K	24	VAL
5	K	38	GLN
5	K	46	LEU
5	K	60(E)	ASP
5	K	62	ASP
5	K	64	LEU
5	K	65	LEU
5	K	66	VAL
5	K	74	THR
5	K	87	LYS
5	K	106	LEU
5	K	107	LYS
5	K	110	ARG
5	K	129(C)	LEU
5	K	145	ARG
5	K	148	TRP
5	K	149(B)	SER

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Mol	Chain	Res	Type
5	K	149(C)	VAL
5	K	149(E)	GLU
5	K	157	VAL
5	K	160	LEU
5	K	169	LYS
5	K	180	MET
5	K	182	CYS
5	K	186(D)	LYS
5	K	192	GLU
5	K	195	SER
5	K	204(B)	ASN
5	K	244	ARG
4	G	9	LEU
1	M	1(G)	PHE
1	M	1(C)	GLU
1	M	5	PRO
1	M	14(A)	GLN
5	N	16	ILE
5	N	27	SER
5	N	33	LEU
5	N	34	PHE
5	N	42	CYS
5	N	46	LEU
5	N	48	SER
5	N	75	ARG
5	N	78	LYS
5	N	93	ARG
5	N	106	LEU
5	N	111	PRO
5	N	112	ILE
5	N	114	LEU
5	N	137	ARG
5	N	149	THR
5	N	149(B)	SER
5	N	149(C)	VAL
5	N	157	VAL
5	N	175	ARG
5	N	241	VAL
5	N	244	ARG
5	N	245	LEU
4	I	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	L	13	GLN
2	H	60(G)	ASN
2	H	71	HIS
3	E	204(B)	ASN
5	K	204(B)	ASN
1	M	13	GLN
5	N	127	GLN
5	N	204(B)	ASN
5	N	239	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	OPR	F	16	4	10,14,15	0.58	0	6,16,18	0.61	0
4	OPR	G	16	4	10,14,15	0.94	0	6,16,18	0.65	0
4	OPR	I	16	4	10,14,15	0.93	1 (10%)	6,16,18	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	OPR	F	16	4	-	0/11/15/16	0/0/0/0
4	OPR	G	16	4	-	0/11/15/16	0/0/0/0
4	OPR	I	16	4	-	0/11/15/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	16	OPR	O-C	2.02	1.25	1.21

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	16	OPR	2	0
4	G	16	OPR	2	0
4	I	16	OPR	2	0

5.5 Carbohydrates (i)

There are no carbohydrates 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, 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	J	36/49 (73%)	0.74	6 (16%)	2	2	13, 30, 90, 100	0
1	L	36/49 (73%)	1.38	9 (25%)	1	1	16, 33, 101, 109	0
1	M	36/49 (73%)	1.68	8 (22%)	1	1	32, 50, 120, 126	0
2	H	150/150 (100%)	-0.53	3 (2%)	68	67	8, 25, 55, 90	0
3	E	109/109 (100%)	0.14	8 (7%)	18	17	8, 27, 92, 114	0
4	F	11/13 (84%)	2.24	6 (54%)	0	0	12, 29, 38, 43	11 (100%)
4	G	10/13 (76%)	0.98	1 (10%)	9	8	20, 35, 45, 54	10 (100%)
4	I	11/13 (84%)	-0.60	1 (9%)	11	11	11, 19, 35, 56	2 (18%)
5	K	259/259 (100%)	-0.34	10 (3%)	43	42	6, 19, 56, 106	0
5	N	259/259 (100%)	-0.08	13 (5%)	32	32	11, 31, 75, 120	0
All	All	917/963 (95%)	-0.01	65 (7%)	19	18	6, 26, 85, 126	23 (2%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	247	SER	20.6
1	M	1(F)	GLY	18.3
5	N	246	GLY	15.3
1	M	1(G)	PHE	15.1
1	J	1(F)	GLY	12.9
5	K	148	TRP	12.5
5	N	149	THR	11.9
5	N	149(B)	SER	11.9
3	E	246	GLY	11.6
3	E	149(C)	VAL	10.9
5	N	245	LEU	10.4
3	E	245	LEU	9.8
5	N	247	SER	9.7

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Mol	Chain	Res	Type	RSRZ
5	K	247	SER	9.4
1	L	14(K)	ILE	9.2
1	M	1(H)	THR	9.1
1	L	1(G)	PHE	9.0
1	L	1(H)	THR	9.0
3	E	149(D)	ALA	8.8
1	M	1(E)	ALA	8.4
5	K	149(C)	VAL	8.3
1	L	15	ARG	8.0
1	J	1(E)	ALA	7.9
1	L	1(F)	GLY	7.7
5	K	149(D)	ALA	7.5
5	K	149(A)	THR	7.4
5	K	149(B)	SER	7.3
1	L	1(E)	ALA	7.1
5	N	149(A)	THR	7.1
5	K	149	THR	6.9
5	N	148	TRP	6.7
3	E	149(B)	SER	6.7
1	L	14(M)	GLY	6.6
5	N	149(C)	VAL	6.1
1	J	1(D)	GLY	5.5
1	M	14(M)	GLY	5.4
5	K	246	GLY	5.4
1	J	1(G)	PHE	5.3
1	L	1(D)	GLY	5.1
2	H	149(A)	THR	4.5
4	F	12	GLY	4.4
5	N	244	ARG	4.2
4	F	19	ARG	4.2
1	L	14(L)	GLU	4.0
5	N	147	THR	3.9
4	G	18	PRO	3.8
1	M	15	ARG	3.8
2	H	149	THR	3.7
1	M	1(D)	GLY	3.4
1	J	1(H)	THR	3.4
4	F	14	GLY	3.1
3	E	244	ARG	3.0
4	F	18	PRO	3.0
5	N	149(D)	ALA	2.8
5	N	78	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
5	K	147	THR	2.7
2	H	78	LYS	2.7
4	F	13	GLY	2.6
4	F	15	VAL	2.5
5	K	245	LEU	2.5
1	M	1(C)	GLU	2.5
5	N	79	VAL	2.4
4	I	19[A]	ARG	2.4
3	E	149(E)	GLU	2.4
1	J	1(C)	GLU	2.3

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	OPR	F	16	15/16	0.96	0.26	-	8,13,27,27	15
4	OPR	I	16	15/16	0.98	0.10	-	4,19,31,33	0
4	OPR	G	16	15/16	0.95	0.18	-	6,19,50,52	15

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.