Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2024 – 04:12 pm GMT

PDB ID	:	8RJ5
Title	:	P1-15 T-cell Receptor bound to HLA A*2402-NF9 pMHC complex
Authors	:	Wall, A.; Sewell, A.K.; Motozono, C.; Rizkallah, P.J.; Fuller, A.
Deposited on	:	2023-12-20
Resolution	:	3.02 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:

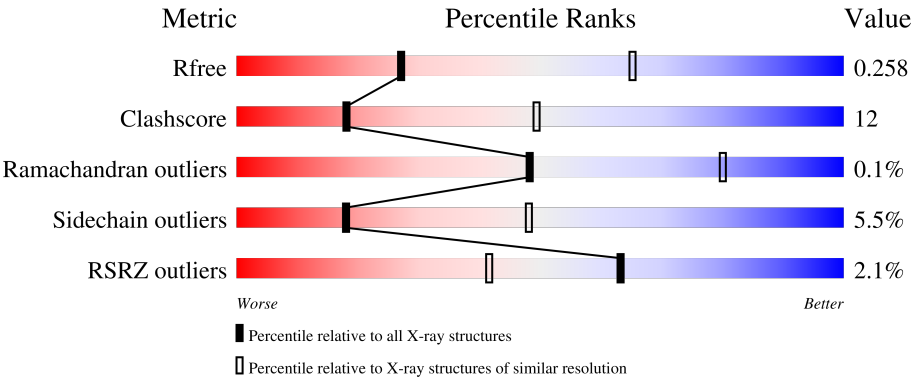
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.02 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}	164625	2927 (3.04-3.00)
Clashscore	180529	3300 (3.04-3.00)
Ramachandran outliers	177936	3188 (3.04-3.00)
Sidechain outliers	177891	3191 (3.04-3.00)
RSRZ outliers	164620	2939 (3.04-3.00)

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 <=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	277	3% 79% 19%
1	F	277	% 82% 17%
2	B	100	3% 72% 26%
2	G	100	3% 79% 20%
3	C	9	22% 78%

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Mol	Chain	Length	Quality of chain
3	H	9	67% 33%
4	D	204	2% 63% 35%
4	I	204	3% 73% 26%
5	E	245	% 67% 30%
5	J	245	2% 66% 34%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13408 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			
1	F	276	Total	C	N	O	S	0	0	0
			2238	1392	405	431	10			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	G	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			91	62	14	15			
3	H	9	Total	C	N	O	0	0	0
			91	62	14	15			

- Molecule 4 is a protein called P1-15 T-cell Receptor Alpha Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	204	Total	C	N	O	S	0	0	0
			1600	998	270	321	11			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	I	204	Total	C	N	O	S	0	0	0
			1600	998	270	321	11			

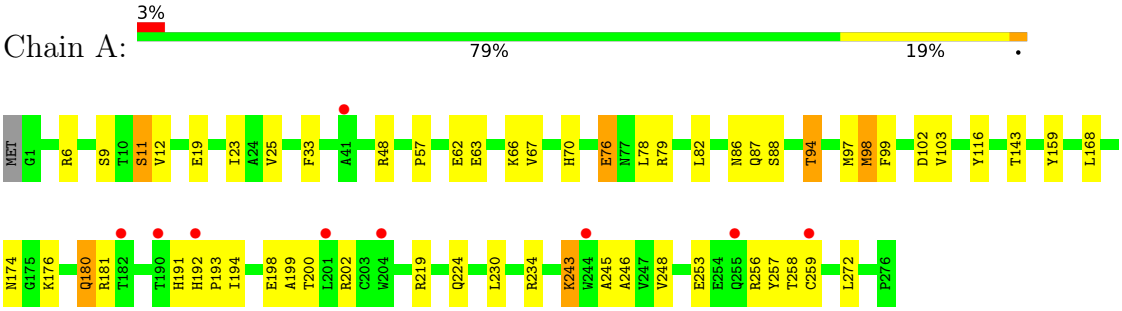
- Molecule 5 is a protein called P1-15 T-cell Receptor Beta Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1938	1212	336	380	10			
5	J	245	Total	C	N	O	S	0	0	0
			1938	1212	336	380	10			

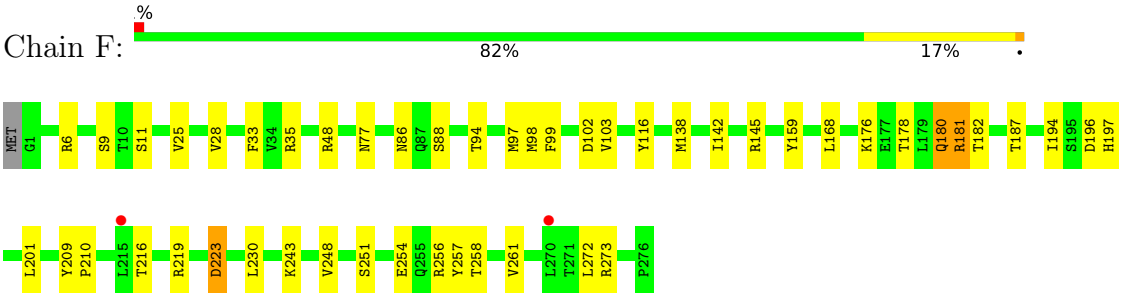
3 Residue-property plots (i)

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.

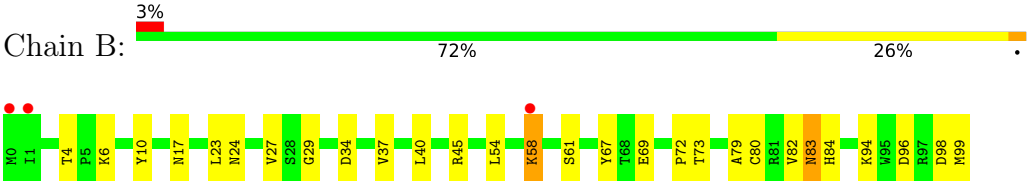
• Molecule 1: MHC class I antigen



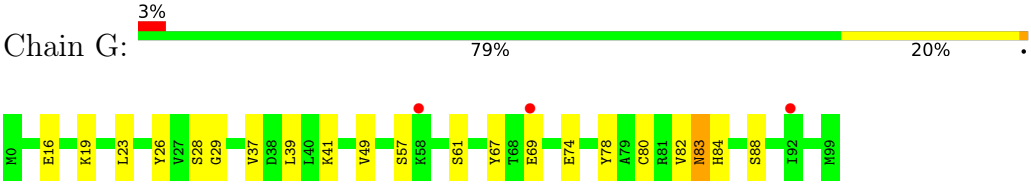
• Molecule 1: MHC class I antigen



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin

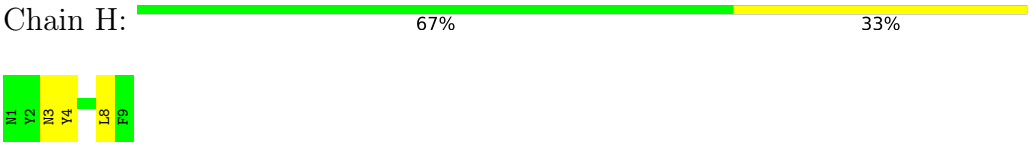


• Molecule 3: Spike protein S1

Chain C:

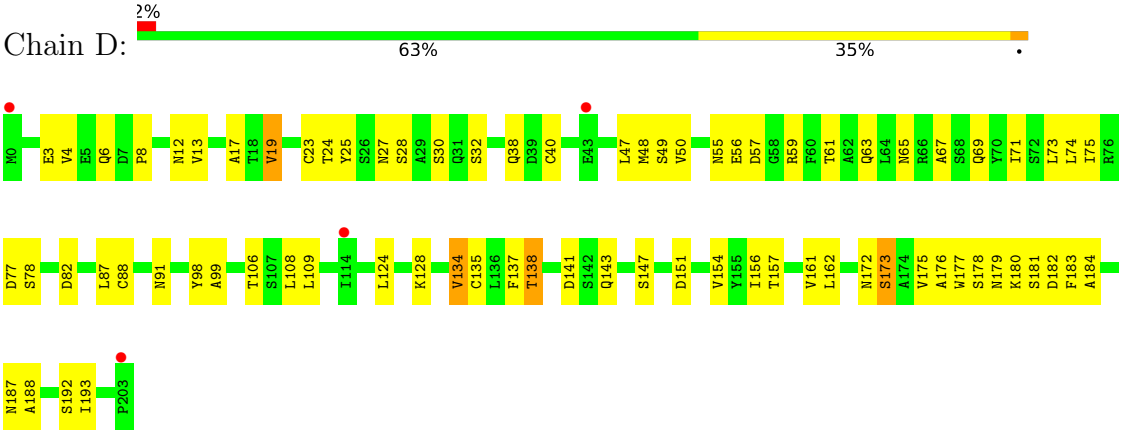
• Molecule 3: Spike protein S1

Chain H:



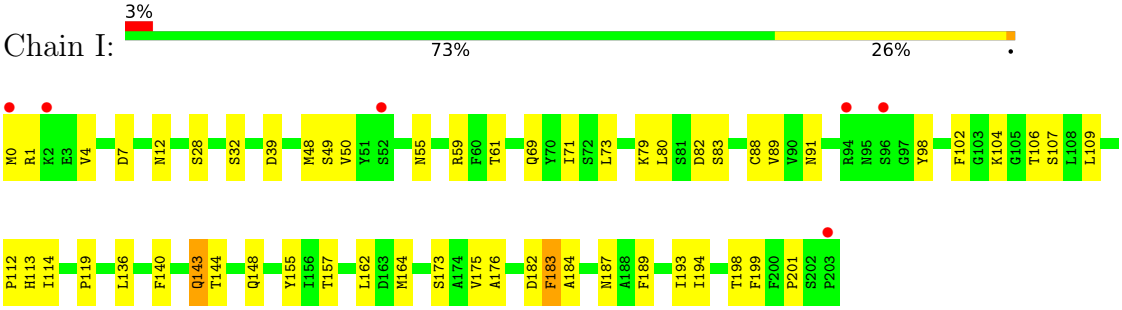
• Molecule 4: P1-15 T-cell Receptor Alpha Chain

Chain D:



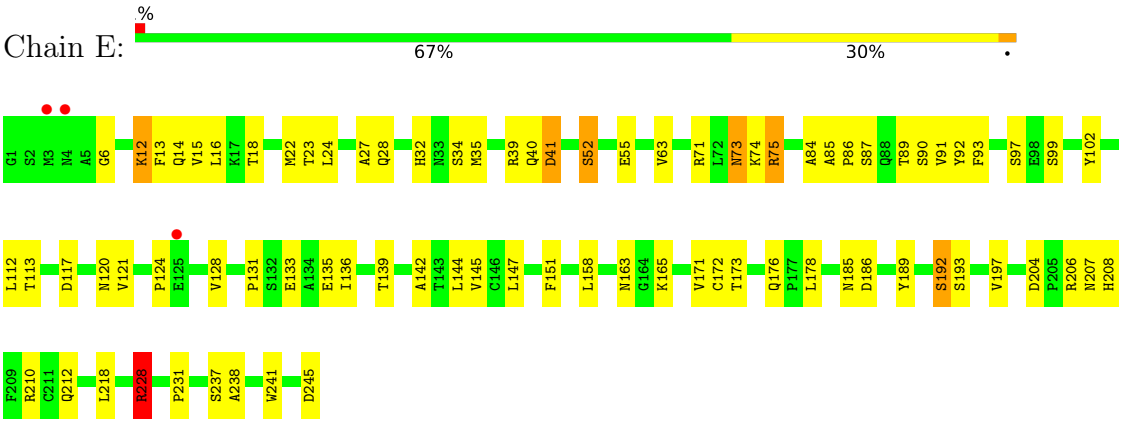
• Molecule 4: P1-15 T-cell Receptor Alpha Chain

Chain I:



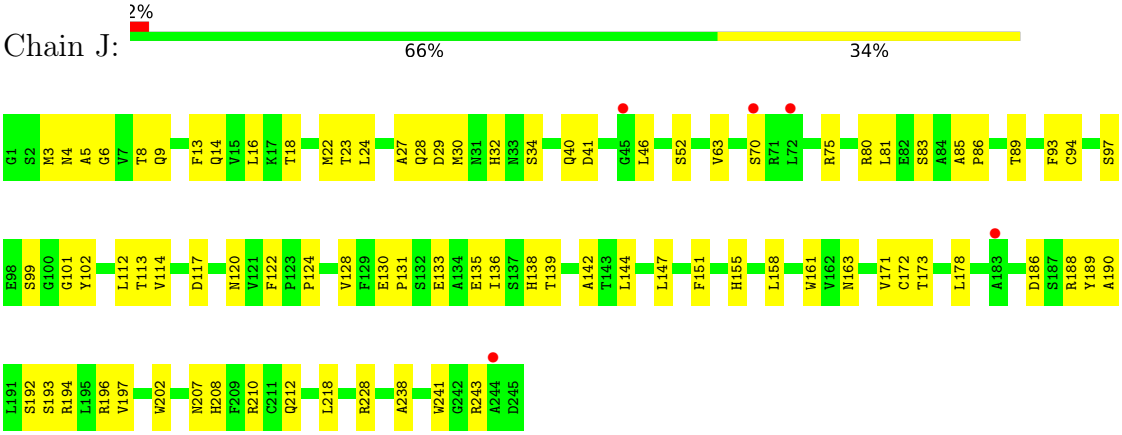
• Molecule 5: P1-15 T-cell Receptor Beta Chain

Chain E:



• Molecule 5: P1-15 T-cell Receptor Beta Chain

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.44Å 200.44Å 156.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	61.62 – 3.02 61.62 – 3.02	Depositor EDS
% Data completeness (in resolution range)	97.5 (61.62-3.02) 97.7 (61.62-3.02)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.97 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.260 0.221 , 0.258	Depositor DCC
R_{free} test set	3529 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	103.1	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 101.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.043 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13408	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, 0.333 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	0.79	2/2299 (0.1%)	0.80	1/3116 (0.0%)
1	F	0.76	0/2299	0.76	0/3116
2	B	0.77	0/860	0.79	0/1162
2	G	0.73	0/860	0.74	0/1162
3	C	0.86	0/94	0.76	0/125
3	H	0.58	0/94	0.76	0/125
4	D	0.77	0/1635	0.87	0/2215
4	I	0.76	0/1635	0.81	0/2215
5	E	0.83	2/1989 (0.1%)	0.84	0/2703
5	J	0.75	1/1989 (0.1%)	0.82	0/2703
All	All	0.77	5/13754 (0.0%)	0.81	1/18642 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
5	E	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	192	SER	CA-CB	-5.71	1.44	1.52
5	J	101	GLY	C-O	5.35	1.32	1.23
1	A	19	GLU	CD-OE1	5.10	1.31	1.25
5	E	237	SER	CA-CB	-5.03	1.45	1.52
1	A	76	GLU	CD-OE2	5.01	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	LYS	CB-CA-C	5.03	120.46	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	228	ARG	Sidechain
1	F	181	ARG	Sidechain

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	2238	0	2095	45	0
1	F	2238	0	2095	25	0
2	B	837	0	803	17	0
2	G	837	0	803	13	0
3	C	91	0	85	17	0
3	H	91	0	85	6	0
4	D	1600	0	1522	59	0
4	I	1600	0	1522	37	0
5	E	1938	0	1827	61	0
5	J	1938	0	1827	65	0
All	All	13408	0	12664	312	0

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

All (312) 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:192:HIS:HB2	1:A:200:THR:HB	1.40	1.02
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.45	0.99
1:A:230:LEU:HD13	1:A:245:ALA:HB2	1.60	0.83
5:J:135:GLU:O	5:J:139:THR:HG22	1.79	0.82
4:I:71:ILE:HD11	4:I:88:CYS:SG	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:135:GLU:O	5:E:139:THR:HG22	1.82	0.80
4:D:38:GLN:HE22	5:E:40:GLN:HE22	1.29	0.78
2:B:29:GLY:HA2	2:B:61:SER:HB2	1.66	0.77
5:J:23:THR:CG2	5:J:80:ARG:HH11	1.98	0.76
5:J:5:ALA:O	5:J:29:ASP:HB2	1.85	0.75
4:I:114:ILE:HD12	4:I:140:PHE:O	1.87	0.74
4:D:71:ILE:HD11	4:D:88:CYS:SG	2.31	0.70
5:E:128:VAL:HG23	5:E:238:ALA:HB3	1.73	0.70
5:J:89:THR:HG23	5:J:113:THR:HA	1.74	0.69
4:D:138:THR:HG22	4:D:173:SER:HB3	1.75	0.69
5:E:228:ARG:HH22	5:E:231:PRO:HB3	1.55	0.69
1:A:97:MET:HE3	3:C:5:LEU:HD11	1.75	0.69
1:A:67:VAL:HG23	3:C:2:TYR:CZ	2.28	0.69
5:E:52:SER:HB3	5:E:71:ARG:HD2	1.74	0.68
2:G:29:GLY:HA2	2:G:61:SER:HB2	1.75	0.67
5:J:23:THR:CG2	5:J:80:ARG:NH1	2.58	0.67
1:F:258:THR:HA	1:F:272:LEU:O	1.95	0.67
2:B:23:LEU:O	2:B:67:TYR:HA	1.95	0.66
4:D:28:SER:HA	4:D:69:GLN:HE21	1.59	0.66
4:D:28:SER:HA	4:D:69:GLN:NE2	2.11	0.66
5:E:89:THR:HG23	5:E:113:THR:HA	1.78	0.66
5:E:52:SER:CB	5:E:71:ARG:HD2	2.26	0.66
5:J:131:PRO:HD3	5:J:144:LEU:HD23	1.78	0.66
4:I:49:SER:O	4:I:55:ASN:ND2	2.28	0.65
5:J:128:VAL:HG23	5:J:238:ALA:HB3	1.77	0.65
4:I:59:ARG:NH2	4:I:82:ASP:OD2	2.27	0.65
2:G:23:LEU:O	2:G:67:TYR:HA	1.97	0.65
4:D:183:PHE:CE1	4:D:188:ALA:HB2	2.30	0.65
4:D:49:SER:O	4:D:55:ASN:ND2	2.29	0.65
4:D:156:ILE:HG22	4:D:176:ALA:CB	2.27	0.65
5:E:73:ASN:OD1	5:E:74:LYS:N	2.30	0.64
1:A:99:PHE:CE2	3:C:3:ASN:HB2	2.33	0.64
4:D:179:ASN:OD1	4:D:179:ASN:C	2.36	0.64
1:A:258:THR:HA	1:A:272:LEU:O	1.98	0.64
4:D:19:VAL:HG13	4:D:75:ILE:HB	1.80	0.63
3:C:6:TYR:OH	4:D:32:SER:OG	2.16	0.62
4:D:63:GLN:N	4:D:63:GLN:OE1	2.32	0.61
1:A:99:PHE:CD2	3:C:3:ASN:HB2	2.35	0.61
4:I:162:LEU:C	4:I:162:LEU:HD23	2.20	0.61
1:F:219:ARG:HB2	1:F:257:TYR:CE2	2.36	0.61
5:J:6:GLY:HA2	5:J:30:MET:HE1	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:MET:HE3	3:C:5:LEU:CD1	2.32	0.60
5:J:133:GLU:O	5:J:136:ILE:HG13	2.02	0.60
4:D:59:ARG:NH2	4:D:82:ASP:OD2	2.24	0.60
4:D:13:VAL:HG11	4:D:108:LEU:HD11	1.84	0.59
5:J:3:MET:HG2	5:J:4:ASN:N	2.18	0.59
4:I:199:PHE:CE2	5:J:138:HIS:HD2	2.20	0.59
5:J:9:GLN:NE2	5:J:94:CYS:H	2.01	0.59
5:J:23:THR:HG21	5:J:80:ARG:HH11	1.67	0.59
4:I:199:PHE:CE2	4:I:201:PRO:HB3	2.37	0.59
5:J:158:LEU:HD23	5:J:158:LEU:C	2.23	0.59
5:E:131:PRO:CG	5:E:142:ALA:HB1	2.33	0.58
4:I:28:SER:HB3	4:I:69:GLN:NE2	2.18	0.58
3:C:6:TYR:HB3	4:D:98:TYR:CD2	2.39	0.58
5:E:117:ASP:O	5:E:120:ASN:ND2	2.37	0.58
5:J:6:GLY:HA2	5:J:30:MET:CE	2.34	0.58
5:J:40:GLN:HB2	5:J:46:LEU:HD23	1.86	0.58
5:J:131:PRO:CG	5:J:142:ALA:HB1	2.34	0.58
5:E:55:GLU:HA	5:E:71:ARG:NH1	2.19	0.57
5:E:158:LEU:HD23	5:E:158:LEU:C	2.23	0.57
1:F:33:PHE:O	1:F:48:ARG:N	2.37	0.57
2:G:83:ASN:HD22	2:G:84:HIS:N	2.03	0.57
2:G:37:VAL:HG22	2:G:82:VAL:HG22	1.85	0.57
4:D:157:THR:HG22	4:D:175:VAL:H	1.70	0.57
5:E:133:GLU:O	5:E:136:ILE:HG13	2.05	0.57
1:A:33:PHE:O	1:A:48:ARG:N	2.37	0.57
4:I:199:PHE:CD2	5:J:138:HIS:HD2	2.23	0.57
5:E:63:VAL:O	5:E:63:VAL:HG22	2.04	0.57
4:I:48:MET:HE1	4:I:73:LEU:HD13	1.87	0.57
4:D:162:LEU:HB3	5:E:172:CYS:HB2	1.87	0.56
1:A:143:THR:HG23	3:C:9:PHE:HA	1.88	0.56
5:J:210:ARG:HH22	5:J:212:GLN:HG3	1.69	0.56
1:A:234:ARG:HD2	2:B:10:TYR:CE2	2.40	0.56
4:D:4:VAL:HG13	4:D:23:CYS:SG	2.46	0.56
4:D:40:CYS:SG	5:E:176:GLN:NE2	2.70	0.55
5:J:63:VAL:O	5:J:63:VAL:HG22	2.06	0.55
1:F:219:ARG:HD2	1:F:256:ARG:HH22	1.71	0.55
4:I:119:PRO:HB2	4:I:198:THR:HA	1.87	0.55
5:J:124:PRO:CA	5:J:151:PHE:HB3	2.37	0.55
4:D:183:PHE:HE1	4:D:188:ALA:HB2	1.72	0.55
2:B:29:GLY:HA2	2:B:61:SER:CB	2.35	0.54
4:D:13:VAL:CG1	4:D:108:LEU:HD11	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:28:GLN:OE1	5:J:32:HIS:HB2	2.07	0.54
4:D:179:ASN:OD1	4:D:180:LYS:N	2.41	0.54
4:D:135:CYS:HB2	4:D:176:ALA:HB3	1.90	0.54
4:I:0:MET:HG2	4:I:1:ARG:H	1.73	0.54
4:D:124:LEU:HB2	4:D:134:VAL:CG1	2.38	0.54
4:I:184:ALA:O	4:I:187:ASN:HB3	2.08	0.54
1:A:82:LEU:HD23	1:A:87:GLN:HB2	1.90	0.54
5:E:18:THR:O	5:E:84:ALA:O	2.25	0.54
5:E:163:ASN:HD21	5:E:207:ASN:HD22	1.55	0.53
1:F:182:THR:HG23	1:F:182:THR:O	2.08	0.53
5:J:161:TRP:HB2	5:J:210:ARG:HG3	1.91	0.53
1:A:97:MET:CE	3:C:5:LEU:CD1	2.86	0.53
5:E:131:PRO:HD3	5:E:144:LEU:HG	1.90	0.53
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.91	0.52
1:F:230:LEU:HD11	1:F:243:LYS:HE3	1.90	0.52
1:A:67:VAL:HA	3:C:2:TYR:CE2	2.44	0.52
4:I:7:ASP:O	4:I:106:THR:HG23	2.09	0.52
5:E:218:LEU:HD12	5:E:218:LEU:N	2.24	0.52
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.22	0.52
1:F:194:ILE:HD11	1:F:248:VAL:HG12	1.92	0.52
5:J:3:MET:HG2	5:J:4:ASN:H	1.75	0.52
5:J:34:SER:HA	5:J:52:SER:O	2.09	0.52
4:D:138:THR:CG2	4:D:173:SER:HB3	2.39	0.51
1:F:98:MET:SD	1:F:98:MET:C	2.89	0.51
4:D:134:VAL:HG23	4:D:177:TRP:HB3	1.92	0.51
5:E:12:LYS:HD3	5:E:13:PHE:HD1	1.76	0.51
5:E:34:SER:HA	5:E:52:SER:O	2.10	0.51
4:I:157:THR:HG22	4:I:175:VAL:H	1.76	0.51
5:J:124:PRO:HA	5:J:151:PHE:HB3	1.93	0.51
5:E:6:GLY:O	5:E:28:GLN:HA	2.11	0.51
5:E:210:ARG:HE	5:E:212:GLN:HG3	1.74	0.51
4:I:12:ASN:OD1	4:I:109:LEU:HD12	2.11	0.51
4:D:32:SER:HB2	4:D:91:ASN:OD1	2.11	0.51
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.44	0.51
1:A:57:PRO:HB3	2:G:69:GLU:OE1	2.10	0.51
3:H:4:TYR:HA	4:I:98:TYR:OH	2.11	0.51
3:H:8:LEU:HD12	3:H:8:LEU:N	2.26	0.51
4:I:59:ARG:NH2	4:I:79:LYS:HE2	2.26	0.51
5:E:28:GLN:O	5:E:75:ARG:HG3	2.11	0.50
5:J:16:LEU:HD12	5:J:112:LEU:HD11	1.93	0.50
5:J:131:PRO:HD3	5:J:144:LEU:CD2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:GLN:N	4:D:143:GLN:OE1	2.44	0.50
5:J:163:ASN:HD21	5:J:207:ASN:HD22	1.59	0.50
1:A:103:VAL:HG22	1:A:168:LEU:HD21	1.93	0.50
2:B:83:ASN:HD22	2:B:84:HIS:N	2.08	0.50
4:D:27:ASN:O	4:D:30:SER:OG	2.30	0.50
5:E:52:SER:HB3	5:E:71:ARG:CD	2.42	0.50
1:F:209:TYR:CD1	1:F:210:PRO:HA	2.47	0.50
2:G:39:LEU:HB2	2:G:49:VAL:HG21	1.93	0.50
4:I:143:GLN:OE1	4:I:143:GLN:N	2.45	0.50
4:D:65:ASN:OD1	4:D:67:ALA:HB3	2.12	0.49
2:G:83:ASN:HD22	2:G:84:HIS:H	1.60	0.49
4:D:56:GLU:HG3	4:D:57:ASP:N	2.28	0.49
5:J:218:LEU:HD12	5:J:218:LEU:N	2.27	0.49
4:D:147:SER:H	4:D:192:SER:HB3	1.77	0.49
5:E:24:LEU:N	5:E:24:LEU:HD12	2.27	0.49
1:F:216:THR:CG2	1:F:223:ASP:OD1	2.61	0.49
1:A:230:LEU:CD1	1:A:245:ALA:HB2	2.36	0.49
1:A:176:LYS:HA	1:A:180:GLN:HG3	1.94	0.49
1:F:6:ARG:NH2	1:F:102:ASP:OD1	2.46	0.48
4:I:183:PHE:HB2	4:I:187:ASN:ND2	2.28	0.48
1:A:194:ILE:O	1:A:198:GLU:HB3	2.13	0.48
5:J:130:GLU:OE2	5:J:243:ARG:NH2	2.43	0.48
2:B:96:ASP:HB3	2:B:99:MET:HG3	1.95	0.48
1:A:97:MET:HE2	3:C:5:LEU:HD13	1.96	0.48
2:G:29:GLY:HA2	2:G:61:SER:CB	2.44	0.48
1:A:70:HIS:CE1	1:A:97:MET:HG2	2.48	0.48
4:D:141:ASP:OD2	4:D:143:GLN:HB2	2.13	0.48
1:F:176:LYS:HA	1:F:180:GLN:HG3	1.96	0.48
5:J:27:ALA:HA	5:J:75:ARG:O	2.13	0.48
4:I:83:SER:OG	4:I:109:LEU:HA	2.14	0.48
1:A:12:VAL:HG22	1:A:94:THR:HG23	1.96	0.48
3:C:3:ASN:HB3	3:C:5:LEU:HG	1.96	0.48
4:D:184:ALA:O	4:D:187:ASN:HB3	2.14	0.48
5:E:185:ASN:O	5:E:186:ASP:HB2	2.14	0.48
5:J:117:ASP:O	5:J:120:ASN:ND2	2.39	0.48
1:A:97:MET:CE	3:C:5:LEU:HD13	2.44	0.47
2:B:29:GLY:CA	2:B:61:SER:HB2	2.41	0.47
1:A:219:ARG:HG3	1:A:257:TYR:CE1	2.48	0.47
2:B:96:ASP:HB3	2:B:99:MET:CG	2.43	0.47
4:D:6:GLN:HG2	4:D:106:THR:OG1	2.14	0.47
4:D:32:SER:N	4:D:91:ASN:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:VAL:HA	4:D:178:SER:HB2	1.95	0.47
4:I:157:THR:CG2	4:I:175:VAL:H	2.27	0.47
5:E:131:PRO:CB	5:E:142:ALA:HB1	2.45	0.47
1:A:253:GLU:HG2	1:A:256:ARG:NH1	2.29	0.47
5:E:15:VAL:O	5:E:16:LEU:HD23	2.14	0.47
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.97	0.47
4:D:161:VAL:HG22	4:D:172:ASN:ND2	2.29	0.47
5:E:55:GLU:HA	5:E:71:ARG:HH11	1.79	0.47
5:E:158:LEU:HD23	5:E:158:LEU:O	2.15	0.47
5:E:121:VAL:O	5:E:228:ARG:NH1	2.48	0.47
2:G:41:LYS:HD3	2:G:78:TYR:CE2	2.49	0.47
4:D:91:ASN:HA	4:D:99:ALA:O	2.14	0.46
5:J:28:GLN:O	5:J:28:GLN:HG3	2.15	0.46
1:A:23:ILE:HG21	2:B:54:LEU:HB3	1.97	0.46
5:E:173:THR:HG23	5:E:193:SER:HB2	1.97	0.46
5:E:204:ASP:OD1	5:E:206:ARG:HG3	2.15	0.46
4:I:162:LEU:HD11	5:J:196:ARG:HB2	1.97	0.46
1:A:98:MET:SD	1:A:98:MET:C	2.93	0.46
5:E:12:LYS:HD2	5:E:13:PHE:H	1.79	0.46
5:J:85:ALA:O	5:J:86:PRO:C	2.51	0.46
4:D:6:GLN:HE22	4:D:88:CYS:H	1.63	0.46
5:E:85:ALA:O	5:E:86:PRO:C	2.54	0.46
1:F:159:TYR:CE1	3:H:3:ASN:HA	2.50	0.46
1:F:187:THR:HG21	1:F:261:VAL:HG21	1.97	0.46
1:F:187:THR:OG1	1:F:272:LEU:HD11	2.15	0.45
2:G:57:SER:HG	2:G:61:SER:HG	1.64	0.45
5:E:124:PRO:CA	5:E:151:PHE:HB3	2.46	0.45
5:J:210:ARG:NH2	5:J:212:GLN:HG3	2.31	0.45
5:J:81:LEU:N	5:J:81:LEU:HD12	2.31	0.45
3:C:4:TYR:HA	4:D:98:TYR:OH	2.16	0.45
4:D:3:GLU:O	4:D:25:TYR:HA	2.16	0.45
4:D:134:VAL:CG1	4:D:134:VAL:O	2.64	0.45
2:G:16:GLU:HB2	2:G:19:LYS:HE2	1.98	0.45
5:E:18:THR:HG22	5:E:86:PRO:HD3	1.98	0.45
1:F:97:MET:HG3	1:F:116:TYR:CZ	2.52	0.45
1:A:97:MET:CE	3:C:5:LEU:HD11	2.43	0.45
1:A:11:SER:HB3	1:A:78:LEU:HD11	1.99	0.45
2:B:6:LYS:O	2:B:27:VAL:HA	2.16	0.45
4:I:155:TYR:O	4:I:176:ALA:HA	2.16	0.45
2:B:58:LYS:HD2	2:B:58:LYS:HA	1.71	0.44
4:D:17:ALA:O	4:D:78:SER:OG	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:LEU:CD1	5:E:145:VAL:HB	2.47	0.44
5:J:122:PHE:CE1	5:J:228:ARG:CZ	2.99	0.44
5:J:218:LEU:N	5:J:218:LEU:CD1	2.80	0.44
5:E:27:ALA:HA	5:E:75:ARG:O	2.17	0.44
5:J:18:THR:HG22	5:J:114:VAL:HG12	1.98	0.44
1:A:199:ALA:O	1:A:248:VAL:HA	2.17	0.44
2:B:17:ASN:HA	2:B:72:PRO:O	2.18	0.44
5:J:208:HIS:HB2	5:J:241:TRP:CZ3	2.53	0.44
4:D:87:LEU:HD12	4:D:87:LEU:N	2.33	0.44
5:J:13:PHE:CD2	5:J:155:HIS:HB3	2.52	0.44
5:J:122:PHE:CZ	5:J:188:ARG:NH2	2.86	0.44
2:G:41:LYS:HD3	2:G:78:TYR:HE2	1.83	0.43
5:J:178:LEU:HD12	5:J:190:ALA:O	2.18	0.43
1:A:103:VAL:HG13	1:A:168:LEU:HD23	1.99	0.43
5:E:218:LEU:HD13	5:E:231:PRO:HG2	1.99	0.43
5:E:99:SER:O	5:E:102:TYR:HB2	2.18	0.43
1:F:197:HIS:HA	1:F:251:SER:HB3	1.99	0.43
1:A:200:THR:HG23	1:A:246:ALA:HB1	2.01	0.43
5:E:32:HIS:HB3	5:E:97:SER:O	2.18	0.43
4:I:32:SER:HB2	4:I:91:ASN:HB3	2.00	0.43
5:E:40:GLN:HE21	5:E:93:PHE:HE2	1.66	0.43
1:A:97:MET:HB2	1:A:116:TYR:CE1	2.53	0.43
1:F:103:VAL:HG22	1:F:168:LEU:CD2	2.49	0.43
4:I:164:MET:CE	5:J:196:ARG:HB3	2.49	0.43
1:A:159:TYR:CE1	3:C:3:ASN:HA	2.54	0.43
4:D:32:SER:CB	4:D:91:ASN:OD1	2.67	0.43
4:D:48:MET:CE	4:D:73:LEU:HD13	2.49	0.43
1:F:77:ASN:OD1	3:H:8:LEU:HA	2.19	0.43
1:F:99:PHE:CD1	3:H:3:ASN:HB2	2.54	0.43
1:F:103:VAL:HG22	1:F:168:LEU:HD21	2.01	0.43
5:J:178:LEU:O	5:J:189:TYR:HA	2.19	0.43
1:A:6:ARG:HD2	1:A:98:MET:HE2	2.00	0.42
4:I:80:LEU:HD21	4:I:112:PRO:HD3	2.02	0.42
5:J:23:THR:HG22	5:J:80:ARG:HG3	2.01	0.42
4:D:109:LEU:HD12	4:D:109:LEU:HA	1.84	0.42
1:F:142:ILE:HA	1:F:145:ARG:NH2	2.34	0.42
5:J:178:LEU:CD1	5:J:190:ALA:O	2.67	0.42
4:D:124:LEU:HD13	5:E:145:VAL:HB	2.02	0.42
4:I:89:VAL:HG22	4:I:102:PHE:CD2	2.53	0.42
5:E:92:TYR:HE2	5:E:112:LEU:HD22	1.84	0.42
5:E:208:HIS:HB2	5:E:241:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:0:MET:CG	4:I:1:ARG:H	2.32	0.42
4:I:91:ASN:HD21	4:I:98:TYR:HB3	1.82	0.42
5:E:39:ARG:HG2	5:E:41:ASP:OD1	2.20	0.42
5:E:163:ASN:HD21	5:E:207:ASN:ND2	2.17	0.42
5:J:131:PRO:HG2	5:J:142:ALA:HB1	2.02	0.42
5:J:158:LEU:HD23	5:J:158:LEU:O	2.19	0.42
1:A:259:CYS:HB3	1:A:272:LEU:HB2	2.00	0.42
5:E:171:VAL:HG12	5:E:172:CYS:N	2.34	0.42
5:E:218:LEU:N	5:E:218:LEU:CD1	2.82	0.42
5:J:24:LEU:N	5:J:24:LEU:CD1	2.82	0.42
4:D:151:ASP:OD2	4:D:180:LYS:HD3	2.20	0.42
5:E:178:LEU:O	5:E:189:TYR:HA	2.20	0.42
5:J:24:LEU:N	5:J:24:LEU:HD12	2.35	0.42
5:J:171:VAL:HG12	5:J:172:CYS:N	2.35	0.42
4:D:73:LEU:HD12	4:D:74:LEU:N	2.34	0.42
4:D:156:ILE:HG22	4:D:176:ALA:HB1	1.99	0.42
4:I:189:PHE:HB3	4:I:194:ILE:HD11	2.01	0.42
5:J:194:ARG:HG3	5:J:194:ARG:HH11	1.85	0.42
5:E:12:LYS:HD2	5:E:13:PHE:N	2.35	0.41
5:E:90:SER:OG	5:E:91:VAL:N	2.53	0.41
4:I:193:ILE:O	4:I:193:ILE:HG23	2.19	0.41
5:J:32:HIS:HB3	5:J:97:SER:O	2.19	0.41
1:A:76:GLU:OE1	1:A:79:ARG:HD3	2.19	0.41
4:D:147:SER:N	4:D:192:SER:HB3	2.35	0.41
2:B:96:ASP:CG	2:B:99:MET:HG2	2.40	0.41
4:I:80:LEU:HD21	4:I:112:PRO:HG3	2.03	0.41
5:J:3:MET:CG	5:J:4:ASN:N	2.82	0.41
5:J:99:SER:O	5:J:102:TYR:HB2	2.19	0.41
1:A:191:HIS:ND1	1:A:193:PRO:HD3	2.35	0.41
3:C:6:TYR:HB3	4:D:98:TYR:CE2	2.55	0.41
4:I:136:LEU:HD23	4:I:175:VAL:HG22	2.02	0.41
5:J:131:PRO:HD2	5:J:202:TRP:CZ2	2.56	0.41
1:A:219:ARG:HH21	1:A:256:ARG:HD2	1.85	0.41
1:F:178:THR:O	1:F:181:ARG:HG2	2.20	0.41
1:F:201:LEU:HD11	1:F:254:GLU:HG3	2.02	0.41
2:G:26:TYR:CE1	2:G:28:SER:HB3	2.55	0.41
4:I:164:MET:CE	5:J:196:ARG:HD3	2.50	0.41
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.90	0.41
1:A:192:HIS:NE2	1:A:202:ARG:HB2	2.36	0.41
4:D:193:ILE:HG22	4:D:193:ILE:O	2.21	0.41
5:E:18:THR:CG2	5:E:86:PRO:HD3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:131:PRO:HB3	5:E:142:ALA:HB1	2.02	0.41
5:J:22:MET:HA	5:J:22:MET:HE2	2.03	0.41
5:J:173:THR:HG23	5:J:193:SER:HB2	2.03	0.41
2:B:79:ALA:HB2	2:B:94:LYS:HD3	2.03	0.40
4:D:137:PHE:O	4:D:173:SER:HA	2.19	0.40
3:H:8:LEU:N	3:H:8:LEU:CD1	2.84	0.40
4:D:25:TYR:CZ	4:D:69:GLN:HA	2.55	0.40
4:D:181:SER:O	4:D:182:ASP:HB2	2.21	0.40
4:I:148:GLN:OE1	4:I:148:GLN:HA	2.22	0.40
5:J:14:GLN:HB3	5:J:112:LEU:HD13	2.03	0.40
5:J:40:GLN:NE2	5:J:93:PHE:HE2	2.19	0.40
5:J:241:TRP:HB2	5:J:243:ARG:HH12	1.86	0.40
2:B:10:TYR:CE1	2:B:24:ASN:CB	3.05	0.40
5:E:14:GLN:HG2	5:E:22:MET:CE	2.52	0.40
5:E:124:PRO:HA	5:E:151:PHE:HB3	2.03	0.40
5:E:71:ARG:HH12	5:E:74:LYS:HA	1.86	0.40
1:F:35:ARG:NH1	1:F:48:ARG:NH1	2.70	0.40
1:A:219:ARG:HB2	1:A:257:TYR:CE2	2.56	0.40
5:E:35:MET:HG3	5:E:71:ARG:HH21	1.86	0.40
4:I:140:PHE:CD2	4:I:144:THR:HB	2.57	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	274/277 (99%)	256 (93%)	18 (7%)	0	100	100
1	F	274/277 (99%)	253 (92%)	21 (8%)	0	100	100
2	B	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
2	G	98/100 (98%)	88 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100 100
4	D	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	25 59
4	I	202/204 (99%)	187 (93%)	15 (7%)	0	100 100
5	E	243/245 (99%)	224 (92%)	19 (8%)	0	100 100
5	J	243/245 (99%)	222 (91%)	21 (9%)	0	100 100
All	All	1648/1670 (99%)	1521 (92%)	126 (8%)	1 (0%)	48 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	8	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	232/233 (100%)	220 (95%)	12 (5%)	19 50
1	F	232/233 (100%)	220 (95%)	12 (5%)	19 50
2	B	95/95 (100%)	87 (92%)	8 (8%)	9 31
2	G	95/95 (100%)	91 (96%)	4 (4%)	25 58
3	C	9/9 (100%)	8 (89%)	1 (11%)	5 20
3	H	9/9 (100%)	9 (100%)	0	100 100
4	D	184/184 (100%)	173 (94%)	11 (6%)	16 45
4	I	184/184 (100%)	173 (94%)	11 (6%)	16 45
5	E	211/211 (100%)	198 (94%)	13 (6%)	15 44
5	J	211/211 (100%)	203 (96%)	8 (4%)	28 61
All	All	1462/1464 (100%)	1382 (94%)	80 (6%)	18 48

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	11	SER
1	A	25	VAL
1	A	62	GLU
1	A	86	ASN
1	A	88	SER
1	A	94	THR
1	A	98	MET
1	A	174	ASN
1	A	180	GLN
1	A	181	ARG
1	A	224	GLN
2	B	4	THR
2	B	34	ASP
2	B	58	LYS
2	B	69	GLU
2	B	73	THR
2	B	80	CYS
2	B	83	ASN
2	B	98	ASP
3	C	7	ARG
4	D	12	ASN
4	D	19	VAL
4	D	24	THR
4	D	47	LEU
4	D	50	VAL
4	D	61	THR
4	D	77	ASP
4	D	128	LYS
4	D	134	VAL
4	D	138	THR
4	D	173	SER
5	E	12	LYS
5	E	23	THR
5	E	41	ASP
5	E	52	SER
5	E	73	ASN
5	E	75	ARG
5	E	87	SER
5	E	147	LEU
5	E	165	LYS
5	E	192	SER
5	E	197	VAL

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Mol	Chain	Res	Type
5	E	228	ARG
5	E	245	ASP
1	F	9	SER
1	F	11	SER
1	F	25	VAL
1	F	28	VAL
1	F	86	ASN
1	F	88	SER
1	F	94	THR
1	F	138	MET
1	F	180	GLN
1	F	196	ASP
1	F	223	ASP
1	F	273	ARG
2	G	74	GLU
2	G	80	CYS
2	G	83	ASN
2	G	88	SER
4	I	4	VAL
4	I	39	ASP
4	I	50	VAL
4	I	61	THR
4	I	104	LYS
4	I	107	SER
4	I	113	HIS
4	I	143	GLN
4	I	173	SER
4	I	182	ASP
4	I	183	PHE
5	J	8	THR
5	J	41	ASP
5	J	70	SER
5	J	83	SER
5	J	147	LEU
5	J	186	ASP
5	J	192	SER
5	J	197	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN

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Mol	Chain	Res	Type
1	A	141	GLN
1	A	174	ASN
1	A	180	GLN
1	A	242	GLN
1	A	255	GLN
2	B	83	ASN
4	D	6	GLN
4	D	12	ASN
4	D	69	GLN
4	D	95	ASN
4	D	172	ASN
4	D	187	ASN
5	E	33	ASN
5	E	40	GLN
5	E	68	ASN
5	E	207	ASN
5	E	226	GLN
5	E	234	GLN
1	F	86	ASN
1	F	141	GLN
1	F	174	ASN
1	F	192	HIS
1	F	218	GLN
1	F	242	GLN
2	G	31	HIS
2	G	83	ASN
4	I	27	ASN
4	I	38	GLN
4	I	69	GLN
4	I	91	ASN
4	I	95	ASN
4	I	101	ASN
4	I	116	ASN
4	I	179	ASN
4	I	187	ASN
5	J	4	ASN
5	J	9	GLN
5	J	138	HIS
5	J	207	ASN
5	J	212	GLN
5	J	226	GLN
5	J	234	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 oligosaccharides 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	276/277 (99%)	-0.02	9 (3%) 49 29	80, 126, 200, 231	0
1	F	276/277 (99%)	-0.16	2 (0%) 84 68	99, 146, 252, 289	0
2	B	100/100 (100%)	0.03	3 (3%) 52 32	104, 141, 186, 226	0
2	G	100/100 (100%)	0.11	3 (3%) 52 32	121, 155, 191, 214	0
3	C	9/9 (100%)	-0.31	0 100 100	89, 96, 106, 106	0
3	H	9/9 (100%)	-0.62	0 100 100	107, 109, 118, 124	0
4	D	204/204 (100%)	-0.01	4 (1%) 64 43	74, 103, 141, 204	0
4	I	204/204 (100%)	-0.08	6 (2%) 54 33	81, 114, 170, 207	0
5	E	245/245 (100%)	-0.27	3 (1%) 76 56	70, 98, 138, 225	0
5	J	245/245 (100%)	-0.22	5 (2%) 64 43	82, 109, 160, 198	0
All	All	1668/1670 (99%)	-0.11	35 (2%) 63 41	70, 119, 202, 289	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	58	LYS	4.5
5	J	72	LEU	4.3
4	D	0	MET	4.2
2	B	0	MET	3.9
4	D	203	PRO	3.5
2	B	1	ILE	3.4
1	A	204	TRP	3.4
5	J	45	GLY	3.3
2	G	69	GLU	3.2
2	G	92	ILE	3.2
4	I	2	LYS	3.2
1	A	190	THR	3.1
1	F	270	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	215	LEU	2.9
5	E	4	ASN	2.8
1	A	182	THR	2.8
4	I	94	ARG	2.7
1	A	201	LEU	2.6
1	A	255	GLN	2.6
5	E	3	MET	2.6
1	A	192	HIS	2.6
1	A	259	CYS	2.5
2	G	58	LYS	2.5
5	E	125	GLU	2.4
1	A	41	ALA	2.3
4	I	52	SER	2.3
4	I	0	MET	2.3
4	I	96	SER	2.3
1	A	244	TRP	2.2
5	J	183	ALA	2.2
4	D	43	GLU	2.2
4	D	114	ILE	2.1
5	J	70	SER	2.0
4	I	203	PRO	2.0
5	J	244	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.