



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:36 PM UTC

PDB ID : 8EB2 / pdb_00008eb2
Title : Structure of HLA-A*02:01 in complex with NY-ESO-1 peptide and PA2.1 Fab
Authors : Jette, C.A.; West, A.P.
Deposited on : 2022-08-30
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

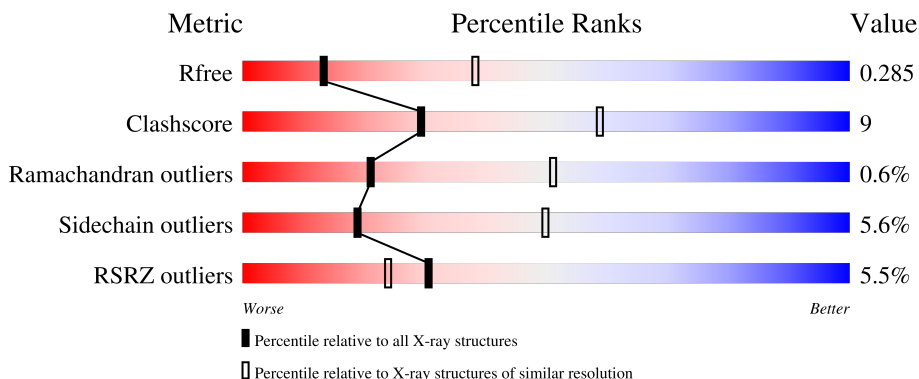
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	275	76% 23% .
1	D	275	77% 23% .
1	G	275	80% 20% .
2	B	100	84% 15% .
2	E	100	86% 14% .

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Mol	Chain	Length	Quality of chain
2	H	100	
3	C	9	
3	F	9	
3	I	9	
4	J	221	
4	K	221	
4	N	221	
5	L	219	
5	M	219	
5	O	219	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 19374 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 HLA-A*02:01 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			
1	D	274	Total	C	N	O	S	0	0	0
			2237	1398	408	422	9			
1	G	275	Total	C	N	O	S	0	0	0
			2246	1403	409	425	9			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	E	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			
2	H	100	Total	C	N	O	S	0	0	0
			836	533	141	158	4			

There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is a protein called NY-ESO-1 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			
3	F	9	Total	C	N	O	S	0	0	0
			75	51	11	12	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	I	9	75	51	11	12	1	0	0	0

- Molecule 4 is a protein called PA2.1 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	J	215	1628	1032	267	323	6	0	0	0
4	K	215	1628	1032	267	323	6	0	0	0
4	N	215	1628	1032	267	323	6	0	0	0

- Molecule 5 is a protein called PA2.1 Fab Light Chain.

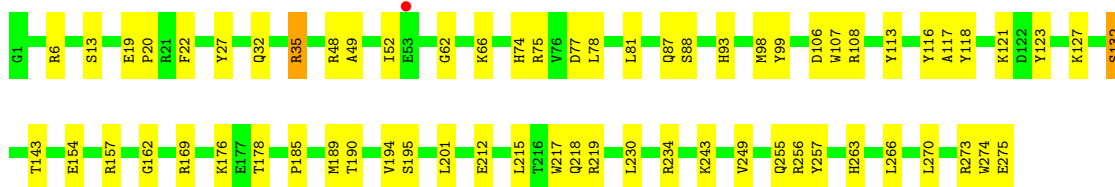
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	L	218	1683	1052	288	338	5	0	0	0
5	M	217	1671	1044	287	335	5	0	0	0
5	O	217	1673	1046	287	335	5	0	0	0

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.

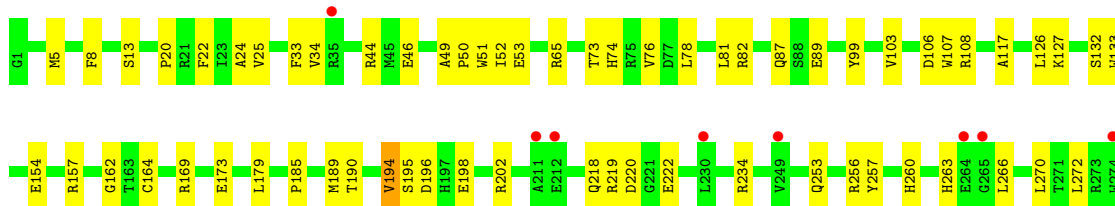
- Molecule 1: HLA-A*02:01 alpha chain

Chain A: 




- Molecule 1: HLA-A*02:01 alpha chain

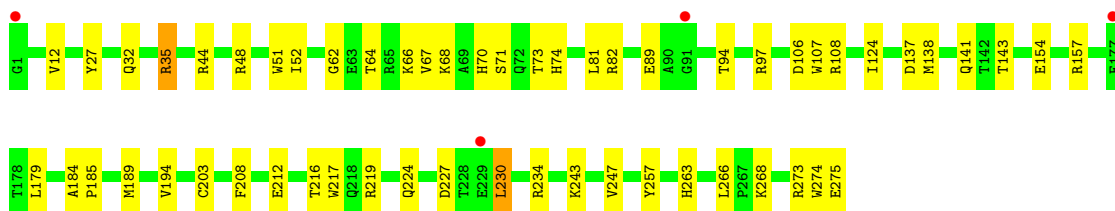
Chain D: 




GLU

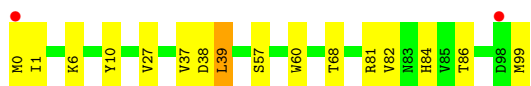
- Molecule 1: HLA-A*02:01 alpha chain

Chain G: 

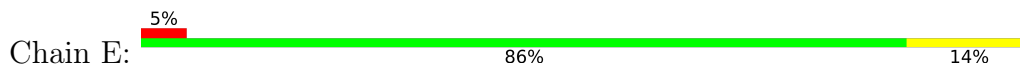


- Molecule 2: Beta-2-microglobulin

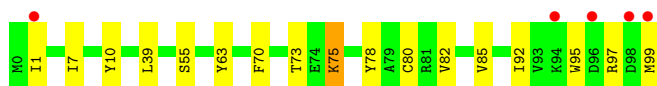
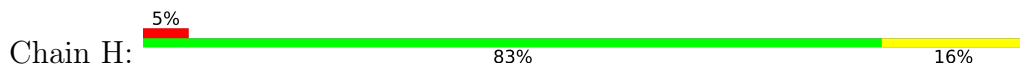
Chain B: 



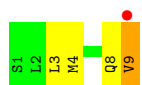
- Molecule 2: Beta-2-microglobulin



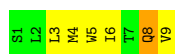
- Molecule 2: Beta-2-microglobulin



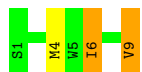
- Molecule 3: NY-ESO-1 peptide



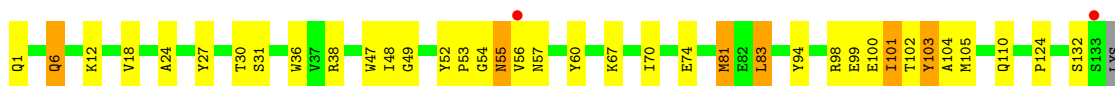
- Molecule 3: NY-ESO-1 peptide




- Molecule 3: NY-ESO-1 peptide

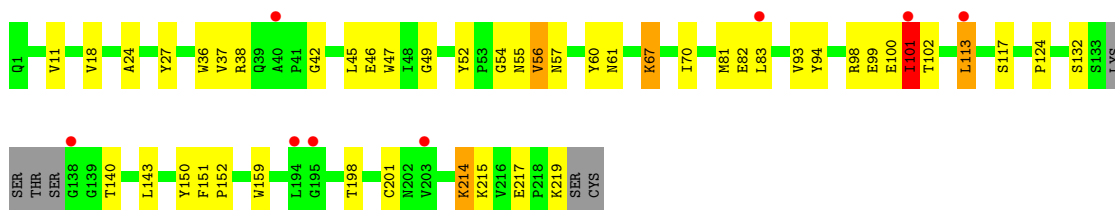


- Molecule 4: PA2.1 Fab Heavy Chain




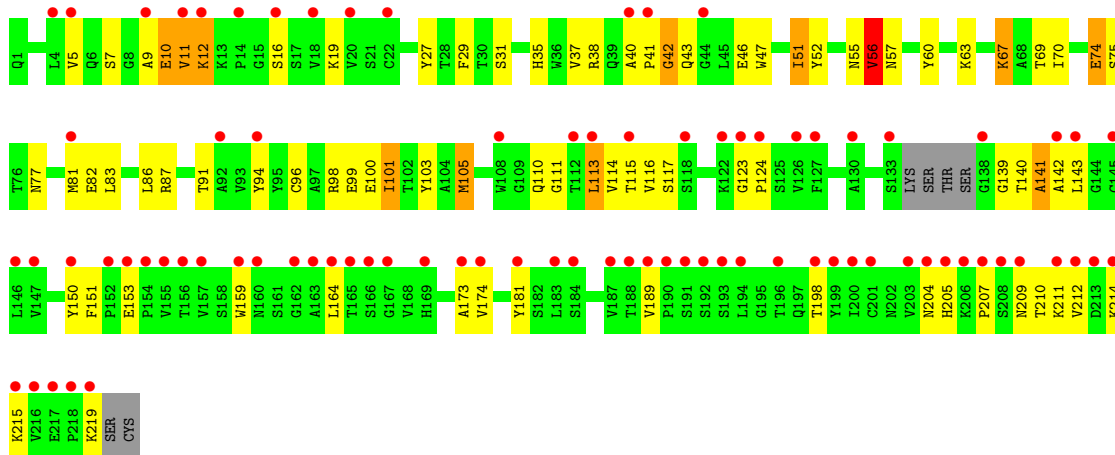
- Molecule 4: PA2.1 Fab Heavy Chain

Chain K:  4% 76% 19% ..



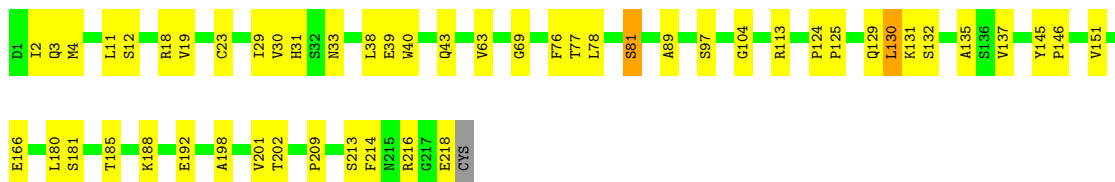
- Molecule 4: PA2.1 Fab Heavy Chain

Chain N:  38% 61% 31% 5% .




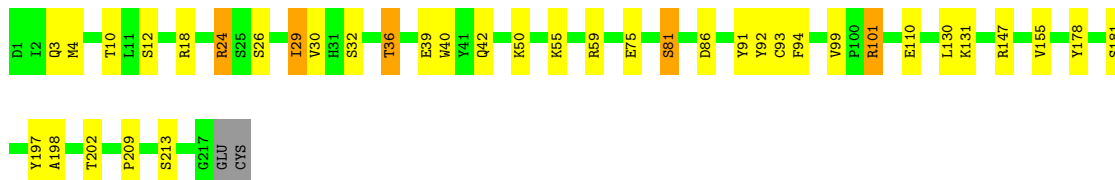
- Molecule 5: PA2.1 Fab Light Chain

Chain L:  76% 22% .



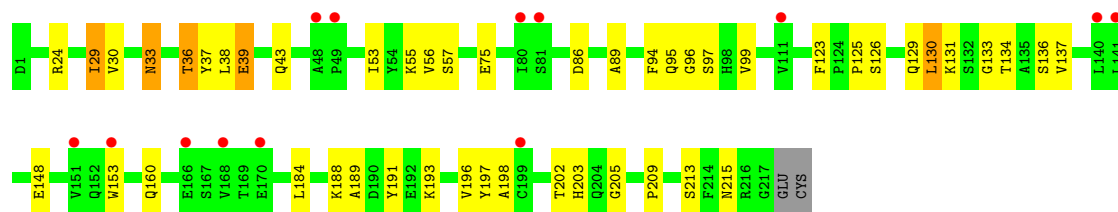
- Molecule 5: PA2.1 Fab Light Chain

Chain M:  82% 15% ..



- Molecule 5: PA2.1 Fab Light Chain

Chain O: 6% 77% 20% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.80Å 148.79Å 199.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.59 – 2.90 49.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.59-2.90) 84.6 (49.59-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.48 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.239 , 0.284 0.239 , 0.285	Depositor DCC
R_{free} test set	2101 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtrriage
Anisotropy	0.494	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19374	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/2311	0.69	0/3137
1	D	0.45	0/2302	0.65	0/3125
1	G	0.42	0/2311	0.62	0/3137
2	B	0.50	0/860	0.70	0/1162
2	E	0.38	0/859	0.59	0/1162
2	H	0.38	0/859	0.62	0/1162
3	C	0.42	0/76	0.67	0/103
3	F	0.55	0/76	0.77	0/103
3	I	0.65	0/76	0.79	0/103
4	J	0.47	0/1669	0.73	0/2276
4	K	0.37	0/1669	0.65	0/2276
4	N	0.41	0/1669	0.72	0/2276
5	L	0.55	1/1720 (0.1%)	0.78	2/2333 (0.1%)
5	M	0.41	0/1708	0.65	0/2317
5	O	0.35	0/1710	0.64	0/2319
All	All	0.44	1/19875 (0.0%)	0.68	2/26991 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	63	VAL	CA-C	5.78	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	81	SER	CA-C-N	-5.06	115.45	123.24
5	L	81	SER	C-N-CA	-5.06	115.45	123.24

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	2246	0	2096	50	0
1	D	2237	0	2090	49	0
1	G	2246	0	2096	39	0
2	B	837	0	803	8	0
2	E	836	0	803	12	0
2	H	836	0	803	8	0
3	C	75	0	83	4	0
3	F	75	0	83	7	0
3	I	75	0	83	7	0
4	J	1628	0	1585	39	0
4	K	1628	0	1585	32	0
4	N	1628	0	1585	46	0
5	L	1683	0	1637	25	0
5	M	1671	0	1622	16	0
5	O	1673	0	1627	27	0
All	All	19374	0	18581	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 9.

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)
1:G:70:HIS:HA	3:I:6:ILE:HD11	1.50	0.94
1:A:35:ARG:HD2	1:A:48:ARG:HE	1.35	0.91
1:G:154:GLU:HG3	1:G:157:ARG:HH22	1.36	0.90
1:A:108:ARG:NH1	4:K:99:GLU:OE2	2.11	0.84
4:K:100:GLU:O	4:K:102:THR:N	2.11	0.84
1:G:230:LEU:HD21	1:G:243:LYS:HE3	1.60	0.82
1:A:127:LYS:HD3	1:A:132:SER:HB2	1.61	0.80
4:J:74:GLU:OE1	4:J:74:GLU:N	2.15	0.78
5:L:130:LEU:HD12	5:L:188:LYS:HG3	1.67	0.77
4:J:55:ASN:O	4:J:57:ASN:N	2.17	0.77
1:A:162:GLY:HA2	4:K:101:ILE:HD13	1.67	0.77
5:L:18:ARG:HE	5:L:81:SER:HB2	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:100:GLU:HG2	4:J:101:ILE:HD13	1.71	0.73
5:O:125:PRO:HD3	5:O:137:VAL:HG22	1.70	0.73
5:L:18:ARG:HG3	5:L:81:SER:HA	1.71	0.72
4:N:91:THR:HG23	4:N:115:THR:HA	1.70	0.72
1:G:108:ARG:HH12	4:N:99:GLU:CD	1.96	0.72
1:A:169:ARG:HH12	4:K:101:ILE:HG22	1.55	0.69
1:A:87:GLN:OE1	1:A:93:HIS:NE2	2.26	0.69
4:N:29:PHE:HB2	4:N:77:ASN:HD22	1.58	0.69
4:K:124:PRO:HB3	4:K:150:TYR:HB3	1.74	0.69
4:N:55:ASN:C	4:N:57:ASN:H	2.01	0.68
4:J:55:ASN:C	4:J:57:ASN:H	2.02	0.68
1:D:162:GLY:HA2	4:J:101:ILE:HG13	1.74	0.68
4:N:40:ALA:O	4:N:42:GLY:N	2.24	0.67
5:O:29:ILE:HG13	5:O:95:GLN:HB2	1.76	0.66
4:N:60:TYR:HE2	4:N:70:ILE:HG13	1.59	0.65
4:N:159:TRP:HB3	4:N:164:LEU:HD23	1.79	0.65
5:O:33:ASN:ND2	5:O:37:TYR:OH	2.29	0.65
1:A:230:LEU:HD11	1:A:243:LYS:HE3	1.80	0.63
5:O:30:VAL:HG22	5:O:36:THR:HB	1.79	0.63
2:H:7:ILE:HD12	2:H:82:VAL:HG21	1.80	0.63
4:J:36:TRP:CD2	4:J:81:MET:HG3	2.33	0.62
4:N:113:LEU:H	4:N:113:LEU:HD12	1.65	0.62
5:M:30:VAL:HG12	5:M:36:THR:HG23	1.80	0.62
1:G:230:LEU:CD2	1:G:243:LYS:HE3	2.29	0.61
5:M:24:ARG:HH11	5:M:24:ARG:HB3	1.66	0.60
1:A:189:MET:HE2	1:A:217:TRP:CH2	2.36	0.60
5:O:202:THR:HG22	5:O:209:PRO:HG3	1.83	0.60
5:L:198:ALA:HB2	5:L:213:SER:HB3	1.83	0.60
2:B:37:VAL:HG22	2:B:82:VAL:HG22	1.84	0.60
4:K:60:TYR:HE1	4:K:70:ILE:HG13	1.67	0.60
4:N:204:ASN:CG	4:N:211:LYS:HE2	2.26	0.60
1:D:108:ARG:NH1	4:J:99:GLU:OE1	2.32	0.59
1:A:13:SER:HA	1:A:20:PRO:HB3	1.83	0.59
1:G:143:THR:HG21	3:I:9:VAL:HG22	1.85	0.59
4:K:198:THR:HG23	4:K:215:LYS:HE3	1.84	0.58
1:D:107:TRP:O	1:D:169:ARG:NH2	2.36	0.58
5:L:145:TYR:CD1	5:L:146:PRO:HA	2.39	0.58
4:J:159:TRP:HB3	4:J:164:LEU:HD23	1.84	0.58
4:J:38:ARG:HB3	4:J:48:ILE:HD11	1.84	0.58
2:B:39:LEU:HD23	2:B:68:THR:HG22	1.86	0.58
1:A:176:LYS:NZ	4:K:54:GLY:O	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:37:VAL:HG22	4:N:47:TRP:HA	1.86	0.57
1:A:154:GLU:HG3	1:A:157:ARG:HH22	1.70	0.57
4:N:105:MET:HE2	5:O:94:PHE:CE2	2.40	0.57
1:D:13:SER:HA	1:D:20:PRO:HB3	1.86	0.57
4:N:51:ILE:HD11	4:N:56:VAL:HA	1.87	0.56
1:G:189:MET:HG2	1:G:274:TRP:CZ2	2.40	0.56
1:G:154:GLU:HG3	1:G:157:ARG:NH2	2.15	0.56
4:J:81:MET:HE1	4:J:94:TYR:CD2	2.41	0.56
4:N:100:GLU:OE1	4:N:101:ILE:HG12	2.05	0.56
4:N:67:LYS:O	4:N:83:LEU:HD12	2.05	0.56
5:O:33:ASN:OD1	5:O:33:ASN:N	2.26	0.56
1:A:22:PHE:HE1	1:A:74:HIS:HD1	1.54	0.56
5:L:113:ARG:HG3	5:L:145:TYR:CD2	2.41	0.55
1:A:154:GLU:HG3	1:A:157:ARG:NH2	2.21	0.55
1:A:143:THR:HG21	3:C:9:VAL:HG22	1.87	0.55
4:N:19:LYS:HA	4:N:81:MET:O	2.06	0.55
1:A:185:PRO:HD3	1:A:263:HIS:ND1	2.22	0.55
5:L:43:GLN:O	5:L:89:ALA:HB1	2.07	0.55
4:K:36:TRP:CE2	4:K:81:MET:HB2	2.42	0.55
5:O:198:ALA:HB2	5:O:213:SER:HB3	1.89	0.55
1:A:98:MET:HE1	1:A:113:TYR:CE1	2.43	0.54
1:A:274:TRP:HZ3	3:F:4:MET:HG2	1.72	0.54
5:L:188:LYS:O	5:L:192:GLU:HG2	2.07	0.54
5:L:29:ILE:HD11	5:L:76:PHE:CE2	2.43	0.54
1:D:169:ARG:HH12	4:J:101:ILE:HG22	1.73	0.53
4:J:54:GLY:O	4:J:55:ASN:HB2	2.08	0.53
1:G:108:ARG:NH1	4:N:99:GLU:OE2	2.33	0.53
1:D:219:ARG:O	1:D:222:GLU:HB3	2.09	0.53
2:H:75:LYS:HD3	2:H:75:LYS:H	1.74	0.53
4:N:74:GLU:HG3	4:N:75:SER:N	2.22	0.53
5:L:125:PRO:HD3	5:L:137:VAL:HG22	1.91	0.52
5:M:3:GLN:HB2	5:M:26:SER:HB3	1.90	0.52
1:D:22:PHE:HE1	1:D:74:HIS:HD1	1.57	0.52
5:L:166:GLU:HB2	5:L:180:LEU:HD21	1.92	0.52
5:M:29:ILE:O	5:M:36:THR:HG22	2.09	0.52
1:G:82:ARG:NE	1:G:89:GLU:HG2	2.24	0.52
1:G:219:ARG:HG3	1:G:257:TYR:CZ	2.45	0.52
1:G:66:LYS:HD3	3:I:4:MET:HA	1.91	0.52
1:G:189:MET:HE2	1:G:217:TRP:CH2	2.45	0.52
4:K:11:VAL:HG21	4:K:152:PRO:HG3	1.91	0.52
1:G:81:LEU:HD21	3:I:9:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:PHE:CD2	1:D:34:VAL:HG13	2.44	0.52
4:J:12:LYS:HE3	4:J:18:VAL:HG23	1.91	0.52
1:D:219:ARG:HG3	1:D:257:TYR:CZ	2.44	0.51
4:J:198:THR:HG23	4:J:215:LYS:HE3	1.93	0.51
1:A:6:ARG:HG2	1:A:98:MET:HE2	1.91	0.51
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.45	0.51
4:J:31:SER:HA	4:J:52:TYR:OH	2.10	0.51
5:L:192:GLU:O	5:L:216:ARG:NH2	2.43	0.51
4:K:55:ASN:OD1	4:K:57:ASN:HB2	2.11	0.51
5:L:202:THR:HG22	5:L:209:PRO:HG3	1.92	0.51
4:N:141:ALA:HB3	4:N:189:VAL:O	2.11	0.51
1:A:274:TRP:CZ3	3:F:4:MET:HG2	2.46	0.50
1:G:62:GLY:O	1:G:66:LYS:HG3	2.10	0.50
4:K:67:LYS:O	4:K:83:LEU:HD12	2.11	0.50
1:D:195:SER:HB3	1:D:198:GLU:HB2	1.92	0.50
4:J:6:GLN:O	4:J:110:GLN:NE2	2.44	0.50
4:K:60:TYR:CE1	4:K:70:ILE:HG13	2.46	0.50
4:N:142:ALA:HB1	5:O:123:PHE:HZ	1.76	0.50
1:A:106:ASP:CG	1:A:108:ARG:HG3	2.37	0.50
3:C:8:GLN:CD	3:C:8:GLN:H	2.18	0.50
4:J:24:ALA:HB1	4:J:27:TYR:CE1	2.46	0.50
1:D:82:ARG:CZ	1:D:89:GLU:HG2	2.42	0.50
4:J:36:TRP:CG	4:J:81:MET:HG3	2.47	0.50
4:N:55:ASN:C	4:N:57:ASN:N	2.69	0.50
1:A:27:TYR:CE2	1:A:32:GLN:HB2	2.47	0.50
3:F:4:MET:HB3	3:F:5:TRP:HE3	1.77	0.49
1:D:50:PRO:O	1:D:53:GLU:HB2	2.12	0.49
2:H:55:SER:HB3	2:H:63:TYR:CZ	2.47	0.49
5:M:42:GLN:HG3	5:M:91:TYR:CE1	2.47	0.49
4:N:55:ASN:O	4:N:57:ASN:N	2.46	0.49
4:N:142:ALA:CB	5:O:123:PHE:HZ	2.25	0.49
1:A:189:MET:HE2	1:A:217:TRP:HH2	1.77	0.49
3:I:6:ILE:H	3:I:6:ILE:HD12	1.76	0.49
1:D:234:ARG:HD2	2:E:10:TYR:CE1	2.48	0.49
4:J:158:SER:OG	4:J:202:ASN:HB2	2.13	0.49
4:K:159:TRP:CH2	4:K:201:CYS:HB3	2.48	0.49
2:B:0:MET:HG2	2:B:1:ILE:H	1.78	0.49
1:A:195:SER:O	1:D:76:VAL:HG11	2.12	0.48
4:K:159:TRP:CZ3	4:K:201:CYS:HB3	2.47	0.48
1:G:74:HIS:CD2	1:G:97:ARG:HH21	2.31	0.48
5:L:180:LEU:HD23	5:L:181:SER:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:60:TYR:HE1	4:J:70:ILE:HG13	1.79	0.48
5:M:202:THR:HG22	5:M:209:PRO:HG3	1.95	0.48
1:D:82:ARG:HD2	1:D:89:GLU:HA	1.95	0.48
5:L:166:GLU:HA	5:L:181:SER:O	2.14	0.48
5:L:31:HIS:HB3	5:L:33:ASN:OD1	2.14	0.48
4:N:124:PRO:HB3	4:N:150:TYR:HB3	1.95	0.47
1:D:169:ARG:NH1	4:J:101:ILE:HG22	2.30	0.47
1:G:227:ASP:O	1:G:247:VAL:HG23	2.15	0.47
2:E:27:VAL:HG23	2:E:30:PHE:HE2	1.79	0.47
4:J:175:LEU:HD13	4:J:181:TYR:CE1	2.49	0.47
5:L:125:PRO:HG3	5:L:135:ALA:HB1	1.96	0.47
4:K:24:ALA:HB1	4:K:27:TYR:HE1	1.79	0.47
4:N:16:SER:O	4:N:86:LEU:HG	2.15	0.47
4:N:37:VAL:HG13	4:N:46:GLU:O	2.15	0.47
1:A:194:VAL:HG13	1:A:195:SER:H	1.78	0.47
1:A:35:ARG:HG2	1:A:48:ARG:CG	2.45	0.47
4:N:12:LYS:HE2	4:N:12:LYS:HA	1.95	0.47
5:O:43:GLN:O	5:O:89:ALA:HB1	2.14	0.47
5:L:69:GLY:HA2	5:L:77:THR:O	2.15	0.46
1:A:116:TYR:HD2	1:A:123:TYR:HD2	1.64	0.46
4:N:174:VAL:O	4:N:181:TYR:HA	2.15	0.46
1:G:35:ARG:HG2	1:G:48:ARG:HE	1.80	0.46
1:G:234:ARG:HD2	2:H:10:TYR:CE1	2.51	0.46
4:J:204:ASN:HD22	4:J:211:LYS:HG2	1.79	0.46
4:K:47:TRP:CE3	4:K:61:ASN:HB2	2.51	0.46
1:D:49:ALA:O	1:D:52:ILE:HG22	2.16	0.46
2:B:38:ASP:HB2	2:B:81:ARG:HB3	1.98	0.46
4:N:35:HIS:O	4:N:96:CYS:HA	2.15	0.46
4:J:155:VAL:HG22	4:J:183:LEU:HD21	1.97	0.46
4:J:83:LEU:HA	4:J:83:LEU:HD12	1.68	0.46
4:J:124:PRO:HD2	4:J:210:THR:HG21	1.98	0.46
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.51	0.46
1:G:107:TRP:CE3	4:N:52:TYR:CE2	3.03	0.46
1:A:35:ARG:HG2	1:A:48:ARG:HG3	1.98	0.46
1:G:27:TYR:CE2	1:G:32:GLN:HB2	2.51	0.46
1:G:66:LYS:NZ	3:I:4:MET:HE2	2.31	0.46
1:G:106:ASP:CG	1:G:108:ARG:HG3	2.41	0.45
5:L:4:MET:HE3	5:L:23:CYS:SG	2.55	0.45
5:O:196:VAL:HG22	5:O:215:ASN:OD1	2.16	0.45
5:O:203:HIS:CE1	5:O:205:GLY:H	2.35	0.45
1:A:52:ILE:HG13	1:A:52:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:212:GLU:O	1:G:263:HIS:HD2	1.99	0.45
5:M:24:ARG:HB3	5:M:24:ARG:NH1	2.31	0.45
1:A:219:ARG:HD3	1:A:256:ARG:CZ	2.47	0.45
1:D:8:PHE:O	1:D:24:ALA:HA	2.16	0.45
2:B:6:LYS:O	2:B:27:VAL:HA	2.17	0.45
1:A:201:LEU:HD12	1:A:249:VAL:HG11	1.99	0.45
5:M:147:ARG:HB2	5:M:178:TYR:CE2	2.51	0.45
5:O:191:TYR:HA	5:O:197:TYR:OH	2.16	0.45
5:M:94:PHE:CZ	5:M:101:ARG:HB2	2.52	0.45
5:M:198:ALA:HB2	5:M:213:SER:HB3	1.99	0.45
4:N:11:VAL:HG21	4:N:151:PHE:CZ	2.52	0.45
1:D:5:MET:HE2	1:D:164:CYS:SG	2.56	0.45
1:G:219:ARG:HB2	1:G:224:GLN:HG3	1.99	0.45
5:O:153:TRP:HB2	5:O:160:GLN:HB2	1.98	0.45
1:D:189:MET:HE1	1:D:272:LEU:O	2.17	0.45
4:N:210:THR:HG22	4:N:212:VAL:HG23	1.99	0.45
1:A:255:GLN:CD	1:A:255:GLN:H	2.25	0.44
4:J:204:ASN:ND2	4:J:211:LYS:HG2	2.32	0.44
4:K:24:ALA:HB1	4:K:27:TYR:CE1	2.52	0.44
4:N:69:THR:N	4:N:82:GLU:O	2.42	0.44
1:A:107:TRP:CE3	4:K:52:TYR:CZ	3.05	0.44
1:D:266:LEU:HD13	1:D:270:LEU:HG	1.99	0.44
2:E:29:GLY:HA2	2:E:61:SER:CB	2.47	0.44
1:D:196:ASP:OD1	1:D:196:ASP:N	2.45	0.44
1:G:52:ILE:HG13	1:G:52:ILE:O	2.17	0.44
4:N:98:ARG:HG2	4:N:99:GLU:N	2.32	0.44
5:O:129:GLN:HG2	5:O:134:THR:O	2.17	0.44
1:G:137:ASP:O	1:G:141:GLN:HG2	2.17	0.44
4:J:170:THR:HG23	4:J:185:SER:HB2	2.00	0.44
5:L:40:TRP:CE2	5:L:78:LEU:HB2	2.52	0.44
4:K:37:VAL:HG13	4:K:46:GLU:O	2.17	0.44
5:M:18:ARG:HG3	5:M:81:SER:HA	1.99	0.44
4:N:209:ASN:OD1	4:N:211:LYS:HE3	2.17	0.44
4:J:55:ASN:C	4:J:57:ASN:N	2.66	0.44
1:D:99:TYR:CE2	3:F:3:LEU:HD12	2.52	0.44
5:L:124:PRO:HB3	5:L:214:PHE:CE1	2.53	0.44
5:M:40:TRP:CZ3	5:M:93:CYS:HB3	2.53	0.44
1:D:99:TYR:CZ	3:F:3:LEU:HD12	2.53	0.44
1:G:73:THR:HB	3:I:6:ILE:HD13	2.00	0.44
1:G:185:PRO:HA	1:G:208:PHE:HB3	1.99	0.44
1:G:203:CYS:HB2	1:G:217:TRP:CZ2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HA	1:D:108:ARG:O	2.18	0.43
1:D:106:ASP:CG	1:D:108:ARG:HG3	2.42	0.43
2:H:95:TRP:CH2	2:H:97:ARG:HG2	2.52	0.43
4:K:38:ARG:HB2	4:K:94:TYR:CE1	2.53	0.43
4:K:81:MET:HE3	4:K:81:MET:HB3	1.80	0.43
4:K:117:SER:HB3	4:K:151:PHE:CZ	2.52	0.43
2:B:84:HIS:CE1	2:B:86:THR:HG23	2.53	0.43
2:E:5:PRO:HB3	2:E:30:PHE:HB3	1.99	0.43
2:H:73:THR:O	2:H:97:ARG:NH2	2.52	0.43
1:D:73:THR:HG23	3:F:8:GLN:HG3	2.00	0.43
1:G:68:LYS:O	1:G:71:SER:HB3	2.18	0.43
4:J:99:GLU:HA	4:J:104:ALA:O	2.18	0.43
5:O:39:GLU:HG3	5:O:94:PHE:HB3	2.00	0.43
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.98	0.43
5:M:12:SER:HB3	5:M:110:GLU:OE2	2.19	0.43
2:E:39:LEU:HD23	2:E:68:THR:HG22	2.01	0.43
5:O:126:SER:O	5:O:130:LEU:HD22	2.19	0.43
4:J:47:TRP:CZ2	4:J:49:GLY:HA2	2.54	0.43
4:J:103:TYR:CD1	4:J:103:TYR:N	2.85	0.43
1:D:87:GLN:HE21	1:D:87:GLN:HB2	1.67	0.43
4:J:30:THR:HA	4:J:53:PRO:HB2	2.01	0.43
1:A:118:TYR:O	1:A:121:LYS:HG2	2.19	0.43
1:D:13:SER:HB3	1:D:78:LEU:HD13	2.01	0.43
5:L:129:GLN:O	5:L:132:SER:OG	2.26	0.43
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.54	0.42
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.87	0.42
1:D:8:PHE:HB2	1:D:25:VAL:HG23	2.01	0.42
1:D:126:LEU:HD13	1:D:133:TRP:CH2	2.54	0.42
1:D:195:SER:OG	1:D:196:ASP:OD1	2.37	0.42
4:N:205:HIS:CD2	4:N:207:PRO:HD2	2.54	0.42
1:D:218:GLN:OE1	1:D:260:HIS:NE2	2.52	0.42
2:E:46:ILE:HG22	2:E:48:LYS:H	1.84	0.42
4:K:214:LYS:HB2	4:K:214:LYS:NZ	2.33	0.42
1:A:169:ARG:NH1	4:K:101:ILE:HG22	2.28	0.42
2:E:29:GLY:HA2	2:E:61:SER:HB2	2.00	0.42
2:E:59:ASP:OD1	2:E:59:ASP:N	2.53	0.42
4:J:36:TRP:CE2	4:J:81:MET:HG3	2.54	0.42
5:L:151:VAL:HG22	5:L:201:VAL:HG22	2.01	0.42
4:K:27:TYR:CE2	4:K:98:ARG:HD2	2.55	0.42
1:G:108:ARG:NH1	4:N:99:GLU:OE1	2.53	0.42
5:L:11:LEU:HD11	5:L:19:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:100:GLU:C	4:K:102:THR:N	2.76	0.42
4:N:105:MET:HE2	5:O:94:PHE:CZ	2.54	0.42
5:O:133:GLY:HA2	5:O:188:LYS:HB2	2.02	0.42
1:D:52:ILE:O	1:D:52:ILE:HG13	2.20	0.42
1:D:194:VAL:HG13	1:D:195:SER:H	1.85	0.42
1:D:253:GLN:HB3	1:D:256:ARG:HD3	2.02	0.42
2:H:80:CYS:O	2:H:92:ILE:HA	2.19	0.42
1:A:49:ALA:O	1:A:52:ILE:HG22	2.20	0.42
2:E:39:LEU:HB2	2:E:49:VAL:HG21	2.02	0.42
5:M:18:ARG:HE	5:M:81:SER:HB3	1.84	0.42
4:N:124:PRO:HD2	4:N:210:THR:HB	2.00	0.42
1:D:44:ARG:O	1:D:46:GLU:HG3	2.19	0.42
1:D:73:THR:HB	3:F:6:ILE:HD11	2.02	0.42
5:O:136:SER:HA	5:O:184:LEU:O	2.20	0.42
4:J:98:ARG:HG2	4:J:99:GLU:N	2.35	0.42
4:J:124:PRO:HB3	4:J:150:TYR:HB3	2.02	0.42
4:N:94:TYR:O	4:N:111:GLY:HA2	2.20	0.42
4:N:123:GLY:HA3	4:N:210:THR:OG1	2.20	0.42
4:N:153:GLU:OE2	4:N:173:ALA:HB3	2.19	0.42
5:O:55:LYS:O	5:O:57:SER:N	2.42	0.42
5:O:55:LYS:C	5:O:56:VAL:HG12	2.45	0.42
1:G:51:TRP:CZ2	1:G:179:LEU:HD11	2.55	0.42
1:A:190:THR:HG22	1:D:65:ARG:HD2	2.01	0.41
4:K:98:ARG:HG2	4:K:99:GLU:N	2.35	0.41
5:M:155:VAL:HG22	5:M:197:TYR:CD1	2.54	0.41
1:A:77:ASP:CG	3:C:9:VAL:HB	2.45	0.41
1:D:190:THR:OG1	1:D:202:ARG:HB3	2.20	0.41
2:E:29:GLY:HA2	2:E:61:SER:OG	2.21	0.41
4:K:45:LEU:HD12	5:M:92:TYR:CD2	2.55	0.41
1:A:215:LEU:HD23	1:A:215:LEU:HA	1.85	0.41
1:G:184:ALA:HB1	1:G:266:LEU:HD23	2.03	0.41
4:K:18:VAL:O	4:K:82:GLU:HA	2.21	0.41
4:N:198:THR:HG23	4:N:215:LYS:HE3	2.02	0.41
4:J:167:GLY:O	4:J:187:VAL:HA	2.20	0.41
5:L:4:MET:HB2	5:L:104:GLY:HA2	2.03	0.41
5:O:39:GLU:HA	5:O:53:ILE:O	2.21	0.41
1:A:19:GLU:HG2	1:A:75:ARG:NH2	2.36	0.41
1:D:127:LYS:HD3	1:D:132:SER:OG	2.21	0.41
1:D:185:PRO:HD3	1:D:263:HIS:ND1	2.35	0.41
5:O:39:GLU:HG3	5:O:94:PHE:HD2	1.86	0.41
1:A:266:LEU:HD13	1:A:270:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:86:LEU:HB3	4:N:116:VAL:HG11	2.02	0.41
1:A:99:TYR:CE2	3:C:3:LEU:HD12	2.56	0.41
1:A:116:TYR:HD2	1:A:123:TYR:CD2	2.39	0.41
1:D:107:TRP:CD1	1:D:107:TRP:N	2.86	0.41
1:D:220:ASP:OD1	1:D:256:ARG:HB3	2.21	0.41
1:G:185:PRO:HD3	1:G:263:HIS:ND1	2.36	0.41
1:A:273:ARG:HE	1:A:273:ARG:HB3	1.51	0.41
1:G:12:VAL:HG22	1:G:94:THR:HG23	2.02	0.41
1:G:44:ARG:HD2	1:G:64:THR:HG21	2.02	0.41
2:H:70:PHE:HD2	2:H:78:TYR:CZ	2.39	0.41
5:O:189:ALA:O	5:O:193:LYS:HG3	2.21	0.41
4:N:10:GLU:HB2	4:N:11:VAL:H	1.56	0.40
1:A:62:GLY:O	1:A:66:LYS:HG3	2.20	0.40
1:D:51:TRP:CZ2	1:D:179:LEU:HD11	2.55	0.40
1:D:154:GLU:HG3	1:D:157:ARG:NH2	2.36	0.40
1:A:218:GLN:O	1:A:257:TYR:HA	2.21	0.40
1:D:81:LEU:HD23	1:D:81:LEU:HA	1.82	0.40
1:D:154:GLU:HG3	1:D:157:ARG:HH22	1.85	0.40
2:E:29:GLY:C	2:E:61:SER:HB2	2.47	0.40
4:K:93:VAL:HG22	4:K:113:LEU:HG	2.03	0.40
4:J:103:TYR:N	4:J:103:TYR:HD1	2.20	0.40
4:K:47:TRP:CZ2	4:K:49:GLY:HA2	2.57	0.40
4:N:98:ARG:O	4:N:105:MET:HA	2.21	0.40
5:O:148:GLU:O	5:O:203:HIS:HD2	2.04	0.40
1:A:212:GLU:O	1:A:263:HIS:HD2	2.03	0.40
1:G:64:THR:O	1:G:67:VAL:HG12	2.22	0.40
1:G:138:MET:O	1:G:141:GLN:HB2	2.21	0.40
4:J:24:ALA:HB1	4:J:27:TYR:HE1	1.86	0.40
4:N:27:TYR:CE2	4:N:98:ARG:HD2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	273/275 (99%)	264 (97%)	9 (3%)	0	100	100
1	D	272/275 (99%)	261 (96%)	11 (4%)	0	100	100
1	G	273/275 (99%)	260 (95%)	13 (5%)	0	100	100
2	B	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
2	E	98/100 (98%)	90 (92%)	8 (8%)	0	100	100
2	H	98/100 (98%)	93 (95%)	5 (5%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	F	7/9 (78%)	7 (100%)	0	0	100	100
3	I	7/9 (78%)	7 (100%)	0	0	100	100
4	J	211/221 (96%)	197 (93%)	12 (6%)	2 (1%)	14	41
4	K	211/221 (96%)	193 (92%)	14 (7%)	4 (2%)	6	23
4	N	211/221 (96%)	192 (91%)	11 (5%)	8 (4%)	2	10
5	L	216/219 (99%)	208 (96%)	8 (4%)	0	100	100
5	M	215/219 (98%)	204 (95%)	11 (5%)	0	100	100
5	O	215/219 (98%)	204 (95%)	10 (5%)	1 (0%)	24	54
All	All	2412/2472 (98%)	2284 (95%)	113 (5%)	15 (1%)	21	51

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	55	ASN
4	J	56	VAL
4	K	101	ILE
4	N	56	VAL
4	N	103	TYR
4	K	42	GLY
4	N	141	ALA
4	K	132	SER
4	N	9	ALA
4	N	139	GLY
4	N	31	SER
4	N	41	PRO
4	N	42	GLY
5	O	96	GLY
4	K	56	VAL

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	231/231 (100%)	226 (98%)	5 (2%)	45 77
1	D	230/231 (100%)	228 (99%)	2 (1%)	70 90
1	G	231/231 (100%)	223 (96%)	8 (4%)	32 66
2	B	95/95 (100%)	92 (97%)	3 (3%)	34 68
2	E	95/95 (100%)	94 (99%)	1 (1%)	65 88
2	H	95/95 (100%)	90 (95%)	5 (5%)	20 52
3	C	9/9 (100%)	7 (78%)	2 (22%)	1 3
3	F	9/9 (100%)	7 (78%)	2 (22%)	1 3
3	I	9/9 (100%)	7 (78%)	2 (22%)	1 3
4	J	182/188 (97%)	166 (91%)	16 (9%)	9 29
4	K	182/188 (97%)	173 (95%)	9 (5%)	22 54
4	N	182/188 (97%)	159 (87%)	23 (13%)	4 14
5	L	193/194 (100%)	182 (94%)	11 (6%)	18 49
5	M	191/194 (98%)	173 (91%)	18 (9%)	8 26
5	O	192/194 (99%)	180 (94%)	12 (6%)	16 45
All	All	2126/2151 (99%)	2007 (94%)	119 (6%)	19 50

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	88	SER
1	A	132	SER
1	A	178	THR
1	A	275	GLU
2	B	39	LEU
2	B	57	SER
2	B	99	MET
3	C	4	MET
3	C	9	VAL

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Mol	Chain	Res	Type
1	D	173	GLU
1	D	194	VAL
2	E	99	MET
3	F	8	GLN
3	F	9	VAL
1	G	35	ARG
1	G	124	ILE
1	G	194	VAL
1	G	216	THR
1	G	230	LEU
1	G	268	LYS
1	G	273	ARG
1	G	275	GLU
2	H	1	ILE
2	H	39	LEU
2	H	75	LYS
2	H	85	VAL
2	H	99	MET
3	I	6	ILE
3	I	9	VAL
4	J	1	GLN
4	J	6	GLN
4	J	67	LYS
4	J	81	MET
4	J	83	LEU
4	J	101	ILE
4	J	102	THR
4	J	103	TYR
4	J	105	MET
4	J	132	SER
4	J	143	LEU
4	J	174	VAL
4	J	177	SER
4	J	183	LEU
4	J	214	LYS
4	J	219	LYS
5	L	2	ILE
5	L	3	GLN
5	L	12	SER
5	L	30	VAL
5	L	38	LEU
5	L	39	GLU

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Mol	Chain	Res	Type
5	L	97	SER
5	L	130	LEU
5	L	131	LYS
5	L	185	THR
5	L	218	GLU
4	K	56	VAL
4	K	67	LYS
4	K	101	ILE
4	K	113	LEU
4	K	140	THR
4	K	143	LEU
4	K	214	LYS
4	K	217	GLU
4	K	219	LYS
5	M	4	MET
5	M	10	THR
5	M	24	ARG
5	M	29	ILE
5	M	32	SER
5	M	36	THR
5	M	39	GLU
5	M	50	LYS
5	M	55	LYS
5	M	59	ARG
5	M	75	GLU
5	M	81	SER
5	M	86	ASP
5	M	99	VAL
5	M	101	ARG
5	M	130	LEU
5	M	131	LYS
5	M	181	SER
4	N	5	VAL
4	N	7	SER
4	N	10	GLU
4	N	11	VAL
4	N	12	LYS
4	N	38	ARG
4	N	43	GLN
4	N	51	ILE
4	N	56	VAL
4	N	63	LYS

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Mol	Chain	Res	Type
4	N	67	LYS
4	N	74	GLU
4	N	87	ARG
4	N	101	ILE
4	N	105	MET
4	N	110	GLN
4	N	113	LEU
4	N	114	VAL
4	N	117	SER
4	N	140	THR
4	N	143	LEU
4	N	214	LYS
4	N	219	LYS
5	O	24	ARG
5	O	29	ILE
5	O	33	ASN
5	O	36	THR
5	O	38	LEU
5	O	39	GLU
5	O	75	GLU
5	O	86	ASP
5	O	97	SER
5	O	99	VAL
5	O	130	LEU
5	O	131	LYS

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

Mol	Chain	Res	Type
1	A	54	GLN
1	A	96	GLN
1	A	180	GLN
1	A	253	GLN
1	D	87	GLN
1	D	145	HIS
1	D	180	GLN
2	E	2	GLN
2	H	2	GLN
2	H	13	HIS
4	J	204	ASN
5	L	35	ASN
5	L	58	ASN

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Mol	Chain	Res	Type
5	L	165	GLN
5	M	58	ASN
4	N	110	GLN
4	N	197	GLN
4	N	204	ASN
5	O	58	ASN
5	O	98	HIS
5	O	142	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	275/275 (100%)	0.18	1 (0%) 88 85	46, 64, 87, 123	0
1	D	274/275 (99%)	0.37	8 (2%) 53 45	45, 66, 163, 202	0
1	G	275/275 (100%)	0.39	4 (1%) 72 64	50, 83, 116, 169	0
2	B	100/100 (100%)	0.13	2 (2%) 65 56	42, 58, 92, 125	0
2	E	100/100 (100%)	0.53	5 (5%) 34 27	54, 93, 139, 158	0
2	H	100/100 (100%)	0.48	5 (5%) 34 27	61, 82, 120, 132	0
3	C	9/9 (100%)	0.69	1 (11%) 10 9	57, 61, 72, 75	0
3	F	9/9 (100%)	0.10	0 100 100	46, 51, 58, 60	0
3	I	9/9 (100%)	0.62	0 100 100	73, 88, 97, 100	0
4	J	215/221 (97%)	0.13	3 (1%) 73 65	46, 68, 106, 127	0
4	K	215/221 (97%)	0.64	8 (3%) 45 37	62, 107, 153, 183	0
4	N	215/221 (97%)	1.81	84 (39%) 1 0	80, 167, 239, 299	0
5	L	218/219 (99%)	-0.04	0 100 100	42, 55, 82, 110	0
5	M	217/219 (99%)	0.34	0 100 100	61, 80, 130, 147	0
5	O	217/219 (99%)	0.84	13 (5%) 27 21	74, 130, 192, 239	0
All	All	2448/2472 (99%)	0.49	134 (5%) 30 24	42, 79, 176, 299	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	N	198	THR	5.0
4	N	203	VAL	4.9
4	N	152	PRO	4.8
2	B	98	ASP	4.7
4	N	155	VAL	4.7
4	N	212	VAL	4.5
4	N	143	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
4	N	18	VAL	4.4
2	H	99	MET	4.4
4	N	216	VAL	4.1
4	J	56	VAL	4.0
2	E	1	ILE	4.0
4	N	147	VAL	4.0
4	N	191	SER	3.9
4	N	214	LYS	3.8
4	N	124	PRO	3.7
4	K	113	LEU	3.7
4	N	190	PRO	3.5
5	O	81	SER	3.5
4	N	159	TRP	3.5
4	N	199	TYR	3.5
4	N	204	ASN	3.5
1	D	264	GLU	3.4
4	N	194	LEU	3.4
4	N	215	LYS	3.4
4	N	217	GLU	3.4
4	N	163	ALA	3.4
4	N	187	VAL	3.4
4	N	201	CYS	3.3
2	H	98	ASP	3.3
4	N	209	ASN	3.3
4	N	192	SER	3.3
4	N	183	LEU	3.2
4	N	112	THR	3.2
4	N	188	THR	3.2
4	N	122	LYS	3.1
4	N	157	VAL	3.1
4	N	146	LEU	3.1
4	N	213	ASP	3.1
4	K	40	ALA	3.0
4	N	142	ALA	3.0
4	N	164	LEU	3.0
4	N	5	VAL	3.0
1	D	212	GLU	2.9
2	E	98	ASP	2.9
4	N	154	PRO	2.9
4	N	218	PRO	2.9
4	N	156	THR	2.9
5	O	166	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
4	N	113	LEU	2.9
1	G	177	GLU	2.9
4	N	174	VAL	2.9
4	N	40	ALA	2.9
4	N	189	VAL	2.8
4	N	206	LYS	2.8
4	N	9	ALA	2.8
4	N	130	ALA	2.8
1	D	35	ARG	2.7
1	D	274	TRP	2.7
4	N	145	CYS	2.7
4	N	115	THR	2.7
4	K	101	ILE	2.7
4	K	138	GLY	2.7
2	E	18	GLY	2.7
4	N	173	ALA	2.6
4	N	4	LEU	2.6
4	N	211	LYS	2.5
4	N	14	PRO	2.5
5	O	140	LEU	2.5
2	H	96	ASP	2.5
1	G	1	GLY	2.5
4	N	123	GLY	2.5
4	N	193	SER	2.5
4	N	81	MET	2.5
4	N	196	THR	2.5
4	N	133	SER	2.5
4	N	138	GLY	2.5
4	N	12	LYS	2.5
4	N	22	CYS	2.5
2	B	0	MET	2.4
4	J	138	GLY	2.4
4	N	150	TYR	2.4
4	N	41	PRO	2.4
4	N	44	GLY	2.4
1	D	230	LEU	2.4
4	N	200	ILE	2.4
4	N	162	GLY	2.4
4	N	108	TRP	2.4
4	N	94	TYR	2.4
5	O	153	TRP	2.3
5	O	141	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
5	O	170	GLU	2.3
4	N	153	GLU	2.3
4	N	181	TYR	2.3
4	N	208	SER	2.3
3	C	9	VAL	2.3
4	N	11	VAL	2.3
4	N	92	ALA	2.2
4	K	194	LEU	2.2
4	N	16	SER	2.2
5	O	151	VAL	2.2
2	H	94	LYS	2.2
4	N	205	HIS	2.2
4	N	207	PRO	2.2
5	O	168	VAL	2.2
5	O	199	CYS	2.2
4	N	127	PHE	2.2
4	N	160	ASN	2.2
1	D	249	VAL	2.2
4	N	20	VAL	2.2
4	N	165	THR	2.2
4	K	195	GLY	2.1
4	J	133	SER	2.1
2	E	16	GLU	2.1
5	O	49	PRO	2.1
4	N	167	GLY	2.1
1	G	229	GLU	2.1
4	N	184	SER	2.1
5	O	111	VAL	2.1
1	D	265	GLY	2.1
1	G	91	GLY	2.1
1	D	211	ALA	2.1
2	H	1	ILE	2.1
4	N	118	SER	2.1
1	A	53	GLU	2.1
4	K	203	VAL	2.0
4	N	126	VAL	2.0
5	O	48	ALA	2.0
4	N	166	SER	2.0
4	N	169	HIS	2.0
2	E	14	PRO	2.0
4	K	83	LEU	2.0
5	O	80	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
4	N	219	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.