



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:23 PM UTC

PDB ID : 5L0Y / pdb_00005l0y
Title : Crystal Structure of a Sec72-ssa1 c-terminal peptide fusion protein
Authors : Tripathi, A.; Rapoport, T.A.
Deposited on : 2016-07-28
Resolution : 2.87 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

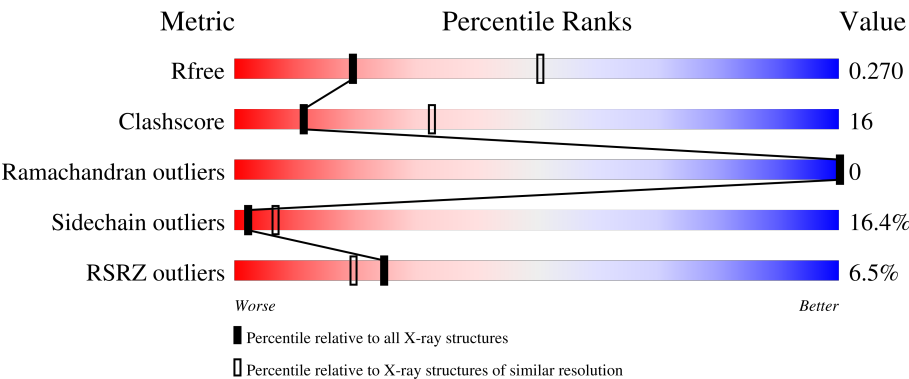
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.87 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	159	6% 62%30%5% . .
1	B	159	3% 58%32%. . 6%
1	C	159	8% 56%35%. 6%
1	D	159	6% 57%30%8% 6%
1	E	159	7% 57%32%6% 5%

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Mol	Chain	Length	Quality of chain
1	F	159	% 62% 22% 12%
1	G	159	6% 50% 36% 9%
1	H	159	12% 48% 28% 7% 16%
2	I	7	14% 57% 14% 14%
2	J	7	43% 43% 14%
2	K	7	29% 71% 14% 14%
2	L	7	29% 29% 29% 14%
2	M	7	14% 29% 29% 14% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9720 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 Sec72-ssa1 c-terminal peptide fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1248	772	233	237	6			
1	B	149	Total	C	N	O	S	0	0	0
			1201	743	227	225	6			
1	C	150	Total	C	N	O	S	0	0	0
			1209	747	229	227	6			
1	D	150	Total	C	N	O	S	0	0	0
			1212	749	224	233	6			
1	E	151	Total	C	N	O	S	0	0	0
			1220	756	228	230	6			
1	F	140	Total	C	N	O	S	0	0	0
			1132	702	211	213	6			
1	G	144	Total	C	N	O	S	0	0	0
			1162	722	222	212	6			
1	H	133	Total	C	N	O	S	0	0	0
			1089	677	205	201	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	215	HIS	-	linker	UNP G0SH41
A	216	ASP	-	linker	UNP G0SH41
A	217	ASN	-	linker	UNP G0SH41
A	218	ASP	-	linker	UNP G0SH41
B	215	HIS	-	linker	UNP G0SH41
B	216	ASP	-	linker	UNP G0SH41
B	217	ASN	-	linker	UNP G0SH41
B	218	ASP	-	linker	UNP G0SH41
C	215	HIS	-	linker	UNP G0SH41
C	216	ASP	-	linker	UNP G0SH41
C	217	ASN	-	linker	UNP G0SH41
C	218	ASP	-	linker	UNP G0SH41
D	215	HIS	-	linker	UNP G0SH41

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Chain	Residue	Modelled	Actual	Comment	Reference
D	216	ASP	-	linker	UNP G0SH41
D	217	ASN	-	linker	UNP G0SH41
D	218	ASP	-	linker	UNP G0SH41
E	215	HIS	-	linker	UNP G0SH41
E	216	ASP	-	linker	UNP G0SH41
E	217	ASN	-	linker	UNP G0SH41
E	218	ASP	-	linker	UNP G0SH41
F	215	HIS	-	linker	UNP G0SH41
F	216	ASP	-	linker	UNP G0SH41
F	217	ASN	-	linker	UNP G0SH41
F	218	ASP	-	linker	UNP G0SH41
G	215	HIS	-	linker	UNP G0SH41
G	216	ASP	-	linker	UNP G0SH41
G	217	ASN	-	linker	UNP G0SH41
G	218	ASP	-	linker	UNP G0SH41
H	215	HIS	-	linker	UNP G0SH41
H	216	ASP	-	linker	UNP G0SH41
H	217	ASN	-	linker	UNP G0SH41
H	218	ASP	-	linker	UNP G0SH41

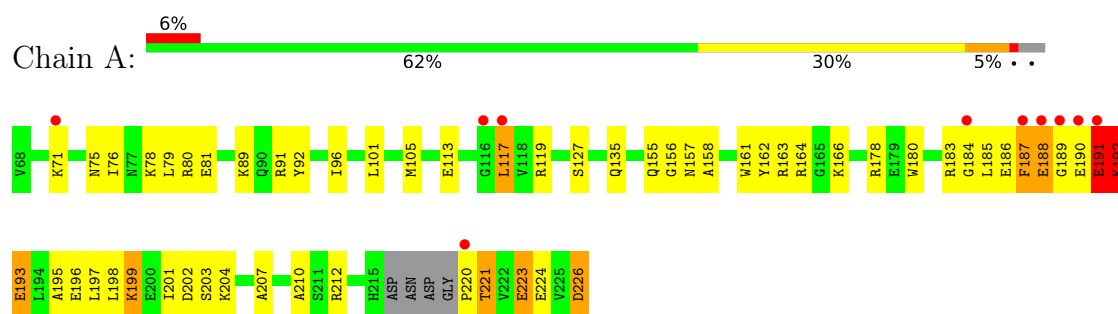
- Molecule 2 is a protein called PRO-THR-VAL-GLU-GLU-VAL-ASP.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	6	Total	C	N	O	0	0	0
			48	28	6	14			
2	J	7	Total	C	N	O	0	0	0
			55	33	7	15			
2	K	7	Total	C	N	O	0	0	0
			55	33	7	15			
2	L	6	Total	C	N	O	0	0	0
			48	28	6	14			
2	M	5	Total	C	N	O	0	0	0
			41	24	5	12			

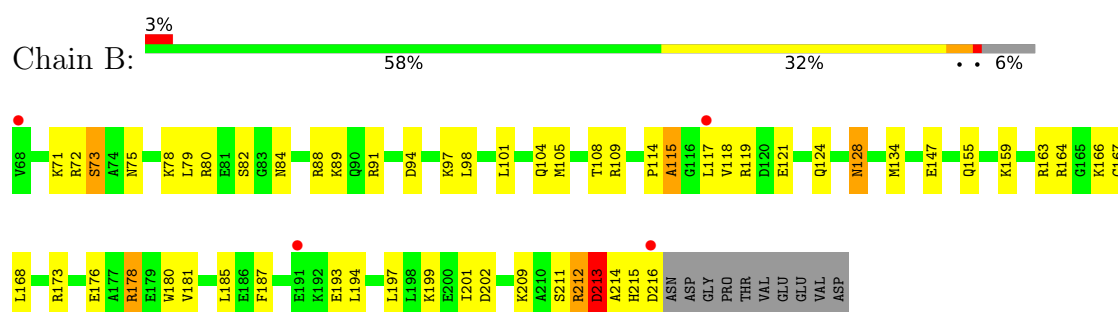
3 Residue-property plots

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.

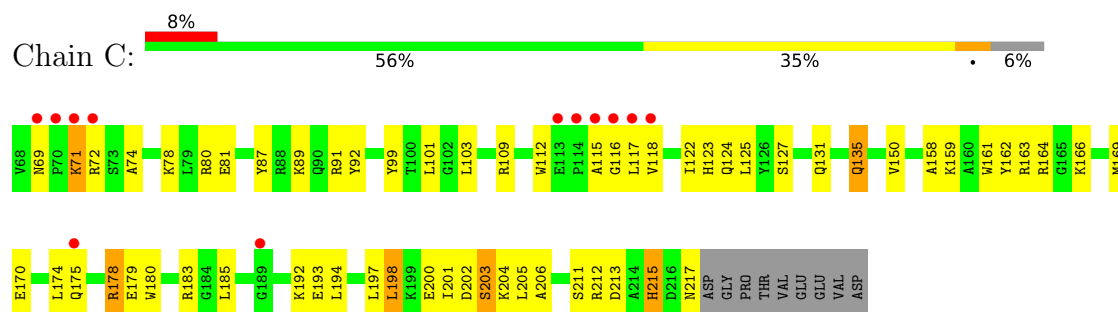
- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein



- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein

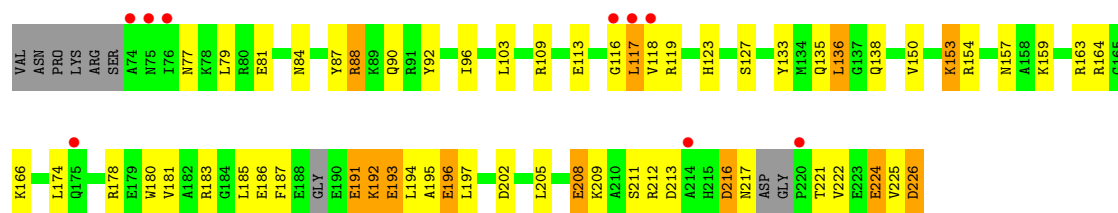


- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein

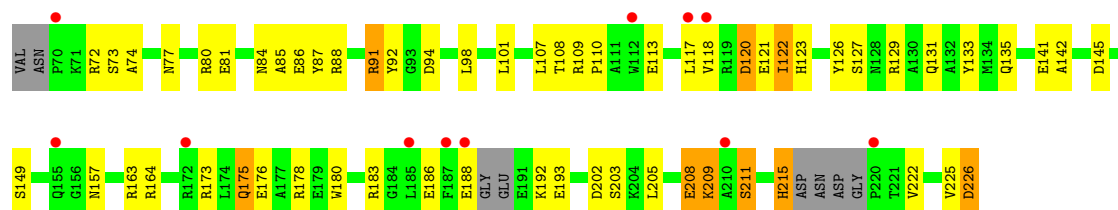


- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein

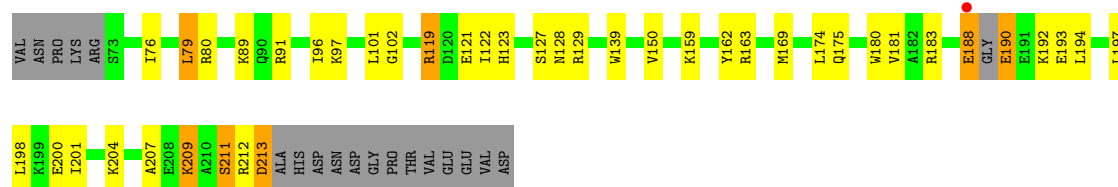




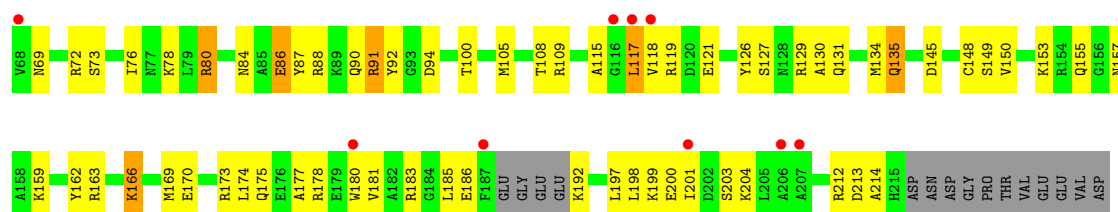
- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein



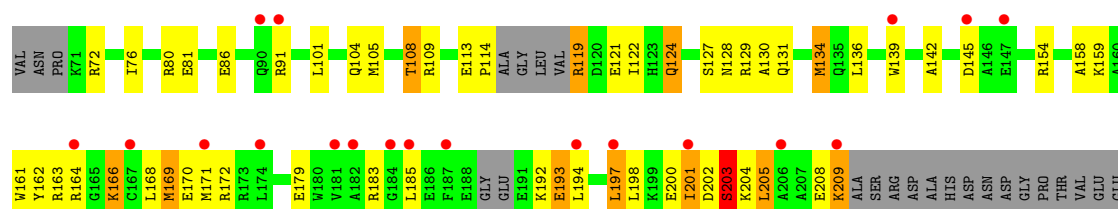
- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein



- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein

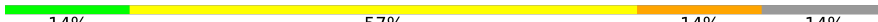


- Molecule 1: Sec72-ssa1 c-terminal peptide fusion protein



VAL
ASP

- Molecule 2: PRO-THR-VAL-GLU-GLU-VAL-ASP

Chain I:  14% 57% 14% 14%

PRO
T221
V222
E223
E224
V225
D226

- Molecule 2: PRO-THR-VAL-GLU-GLU-VAL-ASP

Chain J:  43% 43% 14%

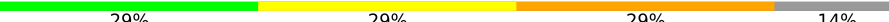
P220
T221
V222
V225
D226

- Molecule 2: PRO-THR-VAL-GLU-GLU-VAL-ASP

Chain K:  29% 71% 14% 14%

P220
T221
V222
D226

- Molecule 2: PRO-THR-VAL-GLU-GLU-VAL-ASP

Chain L:  29% 29% 29% 14%

PRO
T221
V222
E223
E224
V225
D226

- Molecule 2: PRO-THR-VAL-GLU-GLU-VAL-ASP

Chain M:  14% 29% 29% 14% 29%

PRO
THR
V222
E223
E224
V225
D226

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	76.50Å 118.53Å 164.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.08 – 2.87 96.08 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.3 (96.08-2.87) 99.3 (96.08-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.236 , 0.283 (Not available) , 0.270	Depositor DCC
R_{free} test set	1747 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9720	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.64	2/1268 (0.2%)	0.88	5/1700 (0.3%)
1	B	0.43	0/1221	0.83	2/1638 (0.1%)
1	C	0.48	0/1229	0.83	1/1649 (0.1%)
1	D	0.51	0/1230	0.85	1/1648 (0.1%)
1	E	0.45	0/1239	0.82	0/1658
1	F	0.49	1/1149 (0.1%)	0.81	0/1539
1	G	0.48	0/1181	0.87	1/1583 (0.1%)
1	H	0.50	0/1105	0.88	1/1476 (0.1%)
2	I	0.54	0/47	0.74	0/62
2	J	0.53	0/55	1.19	1/73 (1.4%)
2	K	0.46	0/55	0.98	0/73
2	L	0.29	0/47	0.79	0/62
2	M	0.15	0/40	0.62	0/52
All	All	0.50	3/9866 (0.0%)	0.85	12/13213 (0.1%)

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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	139	TRP	NE1-CE2	5.59	1.43	1.37
1	A	187	PHE	N-CA	-5.16	1.40	1.46
1	A	187	PHE	CA-C	-5.07	1.46	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	ALA	N-CA-C	8.22	122.10	110.50
1	A	192	LYS	N-CA-C	6.94	122.76	111.37
1	A	221	THR	N-CA-C	6.92	118.82	111.28
2	J	221	THR	N-CA-C	6.50	118.37	111.28
1	H	203	SER	N-CA-C	-6.46	104.16	111.14
1	A	191	GLU	N-CA-C	6.01	118.94	110.23
1	D	192	LYS	N-CA-C	6.00	117.49	111.07
1	A	190	GLU	N-CA-C	-5.96	104.67	113.61
1	C	116	GLY	N-CA-C	-5.67	99.75	113.18
1	B	213	ASP	N-CA-C	-5.58	105.09	111.07
1	G	69	ASN	N-CA-C	-5.41	103.26	110.07
1	A	187	PHE	N-CA-C	5.10	117.50	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	114	PRO	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1248	0	1230	42	0
1	B	1201	0	1186	44	1
1	C	1209	0	1192	46	0
1	D	1212	0	1183	42	0
1	E	1220	0	1206	35	0
1	F	1132	0	1118	27	1
1	G	1162	0	1160	40	0
1	H	1089	0	1082	46	0
2	I	48	0	40	7	0
2	J	55	0	48	4	0
2	K	55	0	48	3	0
2	L	48	0	40	4	0
2	M	41	0	33	3	0
All	All	9720	0	9566	311	1

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 16.

All (311) 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:155:GLN:HA	1:A:188:GLU:HB2	1.34	1.09
1:H:109:ARG:HD2	1:H:119:ARG:HE	1.30	0.96
1:A:156:GLY:N	1:A:188:GLU:OE1	1.99	0.94
1:A:158:ALA:N	1:A:188:GLU:OE2	2.03	0.92
1:A:157:ASN:N	1:A:188:GLU:OE1	2.04	0.91
1:A:191:GLU:OE1	1:A:193:GLU:N	2.04	0.88
1:A:157:ASN:C	1:A:188:GLU:OE2	2.19	0.85
1:F:209:LYS:HE2	1:F:212:ARG:HE	1.41	0.85
1:A:80:ARG:NH1	1:D:226:ASP:O	2.10	0.85
1:A:157:ASN:H	1:A:188:GLU:CD	1.85	0.83
1:A:76:ILE:HG13	1:A:105:MET:HE2	1.60	0.83
1:B:212:ARG:HG3	1:B:212:ARG:HH11	1.42	0.83
1:G:131:GLN:OE1	1:G:163:ARG:NH1	2.11	0.82
1:C:80:ARG:NH1	2:I:226:ASP:O	2.15	0.79
1:B:211:SER:O	1:B:214:ALA:HB2	1.81	0.79
1:G:129:ARG:NH2	1:G:145:ASP:OD1	2.14	0.79
1:B:134:MET:HE1	1:B:163:ARG:HB3	1.64	0.79
1:B:97:LYS:HB3	1:C:71:LYS:HD2	1.63	0.78
1:B:212:ARG:HG3	1:B:212:ARG:NH1	1.99	0.77
1:E:226:ASP:O	1:H:80:ARG:NH1	2.17	0.77
1:D:117:LEU:HD13	1:D:118:VAL:HG23	1.65	0.76
1:C:161:TRP:O	1:C:180:TRP:HZ3	1.70	0.75
1:D:193:GLU:HG2	2:L:222:VAL:HG13	1.69	0.75
1:G:80:ARG:HD3	1:G:121:GLU:OE1	1.87	0.74
1:D:221:THR:HA	1:D:224:GLU:HG3	1.71	0.73
1:D:77:ASN:ND2	1:D:81:GLU:OE2	2.21	0.73
1:A:220:PRO:HG2	1:A:223:GLU:HG3	1.72	0.71
1:C:159:LYS:HD2	2:I:222:VAL:HA	1.70	0.71
1:H:127:SER:OG	1:H:163:ARG:NH1	2.23	0.71
1:A:155:GLN:HA	1:A:188:GLU:CB	2.17	0.71
1:B:212:ARG:HD2	1:B:212:ARG:O	1.91	0.70
1:B:213:ASP:O	1:B:215:HIS:CD2	2.44	0.70
1:G:86:GLU:OE1	1:G:91:ARG:NH1	2.23	0.70
1:F:212:ARG:NH2	1:F:213:ASP:OD2	2.25	0.69
1:B:109:ARG:HD3	1:B:118:VAL:HG21	1.74	0.69
1:F:169:MET:HE2	1:F:204:LYS:HE3	1.74	0.69
1:D:193:GLU:HG2	2:L:222:VAL:CG1	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LYS:HG3	1:D:193:GLU:N	2.09	0.68
1:A:117:LEU:H	1:A:117:LEU:HD23	1.59	0.67
1:H:109:ARG:HD2	1:H:119:ARG:NE	2.06	0.67
1:A:75:ASN:HB2	1:A:105:MET:HE1	1.77	0.67
1:E:120:ASP:OD2	1:E:120:ASP:N	2.24	0.67
1:E:178:ARG:NH1	1:E:202:ASP:OD1	2.27	0.67
1:C:115:ALA:HB1	1:C:118:VAL:H	1.60	0.66
1:F:80:ARG:NE	1:F:121:GLU:OE2	2.24	0.66
1:F:193:GLU:OE1	2:J:221:THR:OG1	2.13	0.66
1:F:162:TYR:CD2	2:J:222:VAL:HG11	2.31	0.66
1:C:169:MET:HE2	1:C:201:ILE:HG13	1.76	0.65
1:F:127:SER:OG	1:F:163:ARG:NH1	2.29	0.65
1:G:87:TYR:OH	1:G:135:GLN:OE1	2.07	0.65
1:G:166:LYS:NZ	1:G:170:GLU:OE2	2.29	0.65
1:C:166:LYS:NZ	1:C:170:GLU:OE2	2.29	0.64
1:C:162:TYR:CD2	2:I:222:VAL:HG11	2.32	0.64
1:H:158:ALA:HA	1:H:161:TRP:HD1	1.61	0.64
1:F:174:LEU:HD21	1:F:204:LYS:HB3	1.78	0.64
1:A:158:ALA:CA	1:A:188:GLU:OE2	2.46	0.64
1:D:127:SER:OG	1:D:163:ARG:NH1	2.31	0.64
1:F:159:LYS:NZ	2:J:226:ASP:OD2	2.24	0.63
1:C:174:LEU:HD21	1:C:204:LYS:HB2	1.80	0.63
1:F:169:MET:HE3	1:F:201:ILE:HG12	1.79	0.63
1:F:169:MET:HE1	1:F:200:GLU:HG2	1.80	0.63
1:H:124:GLN:O	1:H:128:ASN:ND2	2.31	0.63
1:C:127:SER:OG	1:C:163:ARG:NH1	2.32	0.62
1:E:85:ALA:HA	1:E:88:ARG:HD2	1.81	0.62
1:C:164:ARG:HB3	1:C:180:TRP:CH2	2.35	0.62
1:D:116:GLY:O	1:D:119:ARG:HB2	2.00	0.62
1:H:202:ASP:HA	1:H:205:LEU:HB3	1.81	0.61
1:F:207:ALA:O	1:F:211:SER:OG	2.19	0.61
1:D:192:LYS:O	1:D:196:GLU:HG2	2.00	0.61
1:G:72:ARG:NH1	1:G:105:MET:O	2.33	0.60
1:B:181:VAL:HG13	1:B:194:LEU:HD22	1.82	0.60
2:I:224:GLU:HG2	2:I:225:VAL:H	1.64	0.60
1:G:150:VAL:HG21	1:G:180:TRP:HZ2	1.67	0.59
1:D:178:ARG:NH1	1:D:202:ASP:OD2	2.35	0.59
1:A:187:PHE:HD1	1:A:187:PHE:O	1.85	0.59
1:G:86:GLU:HG2	1:G:94:ASP:HB2	1.85	0.59
1:B:82:SER:HB3	1:B:98:LEU:HD13	1.85	0.59
1:A:221:THR:OG1	1:E:193:GLU:OE1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:LYS:O	1:G:163:ARG:HG2	2.04	0.58
1:A:158:ALA:HA	1:A:188:GLU:OE2	2.04	0.57
1:A:162:TYR:CE2	1:D:222:VAL:HG11	2.39	0.57
1:A:185:LEU:O	1:A:189:GLY:O	2.22	0.57
1:H:127:SER:O	1:H:130:ALA:HB3	2.04	0.57
1:C:159:LYS:HG3	2:I:222:VAL:HG13	1.86	0.57
1:G:183:ARG:HA	1:G:186:GLU:HG3	1.87	0.57
1:C:164:ARG:HB3	1:C:180:TRP:CZ3	2.40	0.57
1:B:159:LYS:NZ	2:M:224:GLU:O	2.34	0.56
1:D:92:TYR:HB2	1:D:136:LEU:HD23	1.87	0.56
1:H:197:LEU:O	1:H:201:ILE:HG23	2.04	0.56
1:C:202:ASP:HA	1:C:205:LEU:HD12	1.88	0.56
1:C:161:TRP:HA	1:C:180:TRP:CH2	2.40	0.56
1:C:193:GLU:OE2	2:I:222:VAL:HG23	2.05	0.56
1:C:158:ALA:HA	1:C:161:TRP:HD1	1.71	0.56
1:E:86:GLU:O	1:E:91:ARG:HB3	2.06	0.56
1:B:173:ARG:NH2	1:B:176:GLU:OE2	2.35	0.55
1:D:159:LYS:O	1:D:163:ARG:HG3	2.06	0.55
1:E:127:SER:OG	1:E:163:ARG:NH1	2.38	0.55
1:D:191:GLU:O	1:D:195:ALA:CB	2.54	0.55
1:B:73:SER:HB2	1:B:117:LEU:HD23	1.89	0.55
1:F:197:LEU:O	1:F:201:ILE:HG13	2.07	0.55
1:H:193:GLU:OE2	1:H:193:GLU:N	2.40	0.55
1:H:202:ASP:OD1	1:H:203:SER:N	2.39	0.55
1:G:197:LEU:O	1:G:201:ILE:HG22	2.07	0.55
1:H:80:ARG:NE	1:H:121:GLU:OE1	2.40	0.55
1:H:159:LYS:O	1:H:163:ARG:HD2	2.07	0.55
1:B:147:GLU:HB2	1:B:164:ARG:HD2	1.89	0.54
1:C:197:LEU:O	1:C:201:ILE:HD12	2.06	0.54
1:H:129:ARG:NH2	1:H:145:ASP:OD1	2.41	0.54
1:H:169:MET:HE3	1:H:201:ILE:HG22	1.87	0.54
1:A:202:ASP:HB3	1:D:178:ARG:HH21	1.73	0.54
1:B:212:ARG:HH11	1:B:212:ARG:CG	2.14	0.54
1:G:177:ALA:O	1:G:181:VAL:HG23	2.08	0.53
1:G:84:ASN:ND2	2:K:226:ASP:OXT	2.41	0.53
1:G:174:LEU:HB3	1:G:201:ILE:CD1	2.39	0.53
1:H:179:GLU:O	1:H:183:ARG:HG3	2.09	0.53
1:D:226:ASP:OD1	1:D:226:ASP:N	2.41	0.53
1:B:124:GLN:O	1:B:128:ASN:ND2	2.42	0.53
1:H:134:MET:HE2	1:H:142:ALA:HB1	1.91	0.53
1:D:88:ARG:O	1:D:90:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:201:ILE:O	1:H:201:ILE:HG12	2.09	0.52
1:A:226:ASP:N	1:A:226:ASP:OD1	2.42	0.52
1:H:205:LEU:O	1:H:209:LYS:HG2	2.09	0.52
1:C:212:ARG:HA	1:C:215:HIS:HB2	1.90	0.52
1:H:119:ARG:HB3	1:H:122:ILE:HD11	1.91	0.52
1:B:164:ARG:HD3	1:B:180:TRP:CZ2	2.45	0.52
1:G:90:GLN:HB2	1:G:92:TYR:CZ	2.45	0.52
1:E:222:VAL:HG21	1:H:162:TYR:CD2	2.45	0.52
1:C:123:HIS:CE1	1:C:124:GLN:HG2	2.45	0.52
1:D:109:ARG:HH21	1:D:113:GLU:HB3	1.75	0.52
1:E:84:ASN:HB3	1:E:88:ARG:HH21	1.75	0.52
1:G:109:ARG:NH2	1:G:118:VAL:HG11	2.25	0.52
1:E:131:GLN:OE1	1:E:163:ARG:NE	2.38	0.52
1:H:154:ARG:O	1:H:161:TRP:HZ2	1.92	0.51
1:D:191:GLU:O	1:D:195:ALA:HB3	2.10	0.51
1:D:192:LYS:CG	1:D:193:GLU:N	2.73	0.51
1:E:91:ARG:HD2	1:E:94:ASP:CG	2.34	0.51
1:E:173:ARG:HH21	1:E:176:GLU:CD	2.19	0.51
1:A:92:TYR:CE2	1:A:135:GLN:HB3	2.45	0.51
1:A:127:SER:OG	1:A:163:ARG:NH1	2.44	0.51
1:F:76:ILE:HG22	1:F:121:GLU:HG2	1.93	0.51
1:F:79:LEU:HD23	1:F:102:GLY:HA2	1.93	0.51
1:F:209:LYS:HE2	1:F:212:ARG:NE	2.17	0.51
1:A:161:TRP:CE3	1:A:184:GLY:HA3	2.46	0.51
1:B:164:ARG:HD3	1:B:180:TRP:CH2	2.45	0.51
1:G:163:ARG:NH1	2:K:222:VAL:O	2.44	0.51
1:H:201:ILE:HA	1:H:204:LYS:HB3	1.93	0.51
1:B:109:ARG:CD	1:B:118:VAL:HG21	2.40	0.51
1:F:181:VAL:HG13	1:F:194:LEU:HD22	1.92	0.50
1:H:139:TRP:CD2	1:H:170:GLU:HG3	2.45	0.50
1:E:107:LEU:HD11	1:E:126:TYR:OH	2.12	0.50
1:C:175:GLN:O	1:C:178:ARG:HB3	2.12	0.50
1:G:92:TYR:CZ	1:G:135:GLN:HG2	2.46	0.50
1:G:213:ASP:OD2	1:G:214:ALA:N	2.45	0.50
1:H:72:ARG:HD2	1:H:109:ARG:HE	1.77	0.49
1:H:162:TYR:CD2	1:H:162:TYR:C	2.90	0.49
1:G:127:SER:O	1:G:130:ALA:HB3	2.11	0.49
1:B:185:LEU:HD21	1:B:194:LEU:HB3	1.93	0.49
1:E:164:ARG:HD3	1:E:180:TRP:CZ2	2.47	0.49
1:C:74:ALA:O	1:C:78:LYS:HG3	2.13	0.49
1:C:179:GLU:OE1	1:C:183:ARG:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:126:TYR:CE2	1:G:148:CYS:HB3	2.48	0.49
1:A:161:TRP:CE3	1:A:184:GLY:CA	2.95	0.49
1:B:213:ASP:O	1:B:215:HIS:NE2	2.46	0.49
1:C:161:TRP:HA	1:C:180:TRP:CZ3	2.48	0.49
1:D:181:VAL:HG13	1:D:194:LEU:HD22	1.93	0.49
1:F:150:VAL:HG21	1:F:180:TRP:CZ2	2.48	0.49
1:G:87:TYR:C	1:G:87:TYR:CD2	2.91	0.49
1:A:196:GLU:HG2	1:D:209:LYS:HE3	1.94	0.49
1:E:92:TYR:OH	1:E:135:GLN:NE2	2.37	0.49
1:F:89:LYS:HD2	1:F:91:ARG:NH2	2.28	0.48
1:B:212:ARG:HD2	1:B:212:ARG:C	2.35	0.48
1:H:131:GLN:HG2	1:H:163:ARG:NE	2.29	0.48
1:B:117:LEU:O	1:B:121:GLU:HG2	2.13	0.48
1:A:178:ARG:NH1	1:A:202:ASP:OD2	2.46	0.48
1:B:84:ASN:O	1:B:88:ARG:HG3	2.14	0.48
1:B:89:LYS:HD3	1:B:89:LYS:N	2.28	0.48
1:F:212:ARG:HG2	1:F:212:ARG:HH21	1.79	0.48
1:A:156:GLY:CA	1:A:188:GLU:OE1	2.60	0.48
1:D:174:LEU:H	1:D:174:LEU:HD12	1.79	0.48
1:E:205:LEU:C	1:E:209:LYS:HE2	2.38	0.47
1:G:130:ALA:O	1:G:134:MET:HG3	2.14	0.47
1:G:174:LEU:HB3	1:G:201:ILE:HD11	1.95	0.47
1:B:128:ASN:OD1	2:M:225:VAL:HB	2.15	0.47
1:C:69:ASN:HB3	1:C:71:LYS:HE2	1.95	0.47
1:H:121:GLU:O	1:H:124:GLN:N	2.46	0.47
1:A:192:LYS:O	1:A:195:ALA:N	2.47	0.47
1:C:162:TYR:CG	2:I:222:VAL:HG11	2.50	0.47
1:C:192:LYS:HG3	1:C:193:GLU:N	2.30	0.47
1:E:91:ARG:HG2	1:E:94:ASP:HB2	1.96	0.47
1:E:129:ARG:NE	1:E:145:ASP:OD2	2.28	0.47
1:E:208:GLU:O	1:E:211:SER:HB3	2.14	0.47
1:G:153:LYS:HB3	1:G:157:ASN:ND2	2.29	0.47
1:B:94:ASP:HA	1:B:97:LYS:HD2	1.96	0.47
1:C:92:TYR:CZ	1:C:135:GLN:HG2	2.49	0.47
1:D:153:LYS:HG2	1:D:157:ASN:HB2	1.96	0.47
1:C:158:ALA:HB1	1:C:194:LEU:HD11	1.97	0.46
1:G:76:ILE:HD12	1:G:117:LEU:HD23	1.96	0.46
1:C:178:ARG:HE	1:C:198:LEU:HD21	1.79	0.46
1:H:166:LYS:N	1:H:197:LEU:HD21	2.30	0.46
1:H:204:LYS:HG3	1:H:208:GLU:OE1	2.15	0.46
1:E:74:ALA:O	1:E:77:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:O	1:B:215:HIS:CG	2.68	0.46
1:H:158:ALA:HA	1:H:161:TRP:CD1	2.48	0.46
1:C:158:ALA:O	1:C:161:TRP:HB2	2.16	0.46
1:H:127:SER:HG	1:H:163:ARG:HH11	1.61	0.46
1:B:71:LYS:NZ	1:D:138:GLN:OE1	2.36	0.46
1:C:89:LYS:HD3	1:C:91:ARG:HH11	1.81	0.46
1:G:72:ARG:O	1:G:76:ILE:HG13	2.16	0.45
1:E:175:GLN:O	1:E:178:ARG:HB3	2.17	0.45
1:C:71:LYS:HE3	1:C:71:LYS:HB2	1.66	0.45
1:C:159:LYS:HG2	1:C:163:ARG:NH1	2.32	0.45
1:E:173:ARG:NH2	1:E:176:GLU:OE2	2.34	0.45
1:A:164:ARG:HD3	1:A:180:TRP:CZ2	2.52	0.45
1:C:164:ARG:HD3	1:C:180:TRP:CE2	2.52	0.45
1:B:104:GLN:HE22	1:C:72:ARG:HH12	1.63	0.45
1:C:72:ARG:NE	1:C:109:ARG:HH11	2.15	0.45
1:F:128:ASN:CG	2:J:225:VAL:HG13	2.42	0.45
1:F:150:VAL:HG21	1:F:180:TRP:HZ2	1.82	0.45
1:G:169:MET:SD	1:G:201:ILE:HB	2.57	0.45
1:E:215:HIS:ND1	1:E:215:HIS:C	2.74	0.45
1:A:183:ARG:O	1:A:187:PHE:HB2	2.17	0.45
1:B:128:ASN:N	1:B:128:ASN:HD22	2.15	0.44
1:C:118:VAL:O	1:C:122:ILE:HG23	2.17	0.44
1:D:154:ARG:HD3	1:D:187:PHE:CZ	2.53	0.44
1:E:149:SER:OG	1:E:157:ASN:ND2	2.46	0.44
1:G:115:ALA:O	1:G:118:VAL:HG12	2.17	0.44
1:D:164:ARG:HD3	1:D:180:TRP:CZ2	2.52	0.44
1:E:91:ARG:CD	1:E:94:ASP:H	2.31	0.44
1:F:204:LYS:HB2	1:F:204:LYS:HE2	1.79	0.44
1:D:208:GLU:O	1:D:212:ARG:HG3	2.18	0.44
1:B:75:ASN:HB2	1:B:105:MET:HE1	1.99	0.44
1:C:72:ARG:CD	1:C:109:ARG:HD2	2.48	0.44
1:F:209:LYS:HE3	1:F:209:LYS:HA	2.00	0.44
1:H:104:GLN:O	1:H:108:THR:OG1	2.26	0.44
1:A:197:LEU:O	1:A:201:ILE:HG13	2.18	0.44
1:D:92:TYR:O	1:D:96:ILE:HG12	2.17	0.44
1:H:134:MET:HE3	1:H:134:MET:HB2	1.87	0.44
1:B:155:GLN:HG3	1:B:187:PHE:HD1	1.83	0.44
1:G:118:VAL:HG13	1:G:119:ARG:N	2.32	0.44
1:D:87:TYR:HE1	1:D:135:GLN:HG3	1.82	0.44
1:D:88:ARG:HH11	1:D:88:ARG:HG3	1.82	0.44
1:D:192:LYS:HG3	1:D:193:GLU:H	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HE2	1:A:91:ARG:HE	1.83	0.43
1:B:75:ASN:CB	1:B:105:MET:HE1	2.48	0.43
1:B:213:ASP:O	1:B:215:HIS:CE1	2.71	0.43
1:B:159:LYS:HB3	1:B:163:ARG:NH1	2.34	0.43
1:D:185:LEU:HD23	1:D:185:LEU:HA	1.84	0.43
1:F:188:GLU:H	1:F:188:GLU:HG2	1.39	0.43
1:G:149:SER:OG	1:G:157:ASN:ND2	2.52	0.43
1:H:134:MET:HE1	1:H:163:ARG:HG2	1.99	0.43
1:A:92:TYR:O	1:A:96:ILE:HG13	2.19	0.43
1:E:80:ARG:NE	1:E:121:GLU:OE2	2.50	0.43
1:B:178:ARG:NH1	1:B:202:ASP:OD1	2.45	0.43
1:G:175:GLN:O	1:G:178:ARG:HB3	2.18	0.43
1:B:134:MET:HE1	1:B:163:ARG:CB	2.44	0.43
1:C:162:TYR:CE1	1:C:197:LEU:HD13	2.53	0.43
1:E:98:LEU:HD23	1:E:98:LEU:HA	1.77	0.42
1:B:197:LEU:O	1:B:201:ILE:HG13	2.19	0.42
1:C:158:ALA:HA	1:C:161:TRP:CD1	2.53	0.42
1:E:133:TYR:HB3	1:E:142:ALA:HB2	2.02	0.42
1:E:183:ARG:O	1:E:186:GLU:HB2	2.19	0.42
1:H:86:GLU:HG3	1:H:91:ARG:HB3	2.00	0.42
1:H:113:GLU:HB2	1:H:114:PRO:HD2	2.01	0.42
1:H:119:ARG:CB	1:H:122:ILE:HD11	2.49	0.42
1:H:185:LEU:HD23	1:H:185:LEU:HA	1.92	0.42
1:C:87:TYR:OH	1:C:131:GLN:HG3	2.19	0.42
1:G:185:LEU:HD23	1:G:185:LEU:HA	1.83	0.42
1:H:72:ARG:O	1:H:76:ILE:HG13	2.18	0.42
1:H:109:ARG:HD3	1:H:113:GLU:HG3	2.01	0.42
1:A:187:PHE:O	1:A:187:PHE:CD1	2.70	0.42
1:E:109:ARG:HG3	1:E:110:PRO:HD2	2.00	0.42
1:A:76:ILE:HG12	1:A:105:MET:HB3	2.01	0.42
1:B:124:GLN:HE22	2:M:226:ASP:HB3	1.84	0.42
1:C:203:SER:O	1:C:206:ALA:HB3	2.20	0.42
1:E:205:LEU:O	1:E:209:LYS:HE2	2.19	0.42
1:H:72:ARG:HD2	1:H:109:ARG:HH21	1.84	0.42
1:D:84:ASN:ND2	2:L:226:ASP:O	2.53	0.42
1:E:164:ARG:HD3	1:E:180:TRP:CE2	2.54	0.42
1:D:103:LEU:HD23	1:D:103:LEU:HA	1.88	0.42
1:A:178:ARG:NH1	1:A:198:LEU:HD11	2.35	0.42
1:D:205:LEU:HD23	1:D:205:LEU:HA	1.82	0.42
1:C:99:TYR:O	1:C:125:LEU:HD12	2.20	0.41
1:D:209:LYS:HD3	1:D:209:LYS:HA	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:LEU:HD23	1:E:205:LEU:HA	1.81	0.41
1:G:150:VAL:HG21	1:G:180:TRP:CZ2	2.52	0.41
1:H:113:GLU:O	1:H:119:ARG:NH2	2.52	0.41
1:H:122:ILE:HD12	1:H:122:ILE:H	1.84	0.41
1:H:136:LEU:HD23	1:H:136:LEU:HA	1.86	0.41
1:A:207:ALA:O	1:A:210:ALA:HB3	2.20	0.41
1:B:134:MET:HE2	1:B:167:CYS:SG	2.61	0.41
1:H:164:ARG:O	1:H:168:LEU:HG	2.20	0.41
1:B:159:LYS:O	1:B:163:ARG:HG3	2.20	0.41
1:E:122:ILE:HG23	1:E:126:TYR:CE2	2.55	0.41
1:B:168:LEU:HD13	1:B:176:GLU:HB3	2.02	0.41
1:A:199:LYS:HD2	1:D:205:LEU:HD13	2.03	0.41
1:F:119:ARG:O	1:F:122:ILE:HG12	2.21	0.41
1:A:199:LYS:HD2	1:D:205:LEU:CD1	2.51	0.41
1:A:204:LYS:HE2	1:A:204:LYS:HB2	1.92	0.41
1:G:118:VAL:HG13	1:G:119:ARG:HD2	2.03	0.41
1:G:162:TYR:CE2	2:K:222:VAL:HG11	2.56	0.41
1:G:198:LEU:O	1:G:201:ILE:HG23	2.21	0.41
1:C:164:ARG:HD3	1:C:180:TRP:CZ2	2.55	0.41
1:C:185:LEU:HD23	1:C:185:LEU:HA	1.94	0.40
1:D:216:ASP:O	1:D:217:ASN:CB	2.69	0.40
1:G:117:LEU:HD22	1:G:118:VAL:N	2.36	0.40
1:A:223:GLU:O	1:E:87:TYR:OH	2.13	0.40
1:D:150:VAL:HG21	1:D:180:TRP:HZ2	1.87	0.40
1:F:96:ILE:HG23	1:F:129:ARG:HD2	2.03	0.40
1:G:88:ARG:C	1:G:90:GLN:H	2.29	0.40
2:L:221:THR:HG23	2:L:222:VAL:H	1.86	0.40
1:B:115:ALA:HB3	1:B:118:VAL:HG22	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ASP:OD1	1:F:190:GLU:OE1[2_655]	1.42	0.78

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	115/159 (72%)	111 (96%)	4 (4%)	0	100	100
1	B	147/159 (92%)	142 (97%)	5 (3%)	0	100	100
1	C	78/159 (49%)	72 (92%)	6 (8%)	0	100	100
1	D	72/159 (45%)	71 (99%)	1 (1%)	0	100	100
1	E	145/159 (91%)	137 (94%)	8 (6%)	0	100	100
1	F	136/159 (86%)	133 (98%)	3 (2%)	0	100	100
1	G	140/159 (88%)	131 (94%)	9 (6%)	0	100	100
1	H	127/159 (80%)	124 (98%)	3 (2%)	0	100	100
2	I	4/7 (57%)	4 (100%)	0	0	100	100
2	J	5/7 (71%)	5 (100%)	0	0	100	100
2	K	5/7 (71%)	5 (100%)	0	0	100	100
2	L	4/7 (57%)	4 (100%)	0	0	100	100
2	M	3/7 (43%)	3 (100%)	0	0	100	100
All	All	981/1307 (75%)	942 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	124/127 (98%)	104 (84%)	20 (16%)	2	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	118/127 (93%)	100 (85%)	18 (15%)	3	8
1	C	119/127 (94%)	103 (87%)	16 (13%)	4	11
1	D	120/127 (94%)	99 (82%)	21 (18%)	2	5
1	E	121/127 (95%)	98 (81%)	23 (19%)	1	4
1	F	111/127 (87%)	97 (87%)	14 (13%)	4	12
1	G	114/127 (90%)	96 (84%)	18 (16%)	2	7
1	H	107/127 (84%)	86 (80%)	21 (20%)	1	4
2	I	6/7 (86%)	4 (67%)	2 (33%)	0	0
2	J	7/7 (100%)	7 (100%)	0	100	100
2	K	7/7 (100%)	6 (86%)	1 (14%)	3	9
2	L	6/7 (86%)	3 (50%)	3 (50%)	0	0
2	M	5/7 (71%)	4 (80%)	1 (20%)	1	4
All	All	965/1051 (92%)	807 (84%)	158 (16%)	2	7

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	LYS
1	A	78	LYS
1	A	79	LEU
1	A	81	GLU
1	A	101	LEU
1	A	113	GLU
1	A	117	LEU
1	A	119	ARG
1	A	166	LYS
1	A	186	GLU
1	A	188	GLU
1	A	191	GLU
1	A	192	LYS
1	A	193	GLU
1	A	199	LYS
1	A	203	SER
1	A	212	ARG
1	A	223	GLU
1	A	224	GLU
1	A	226	ASP
1	B	72	ARG

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Mol	Chain	Res	Type
1	B	73	SER
1	B	78	LYS
1	B	79	LEU
1	B	80	ARG
1	B	91	ARG
1	B	101	LEU
1	B	108	THR
1	B	119	ARG
1	B	128	ASN
1	B	166	LYS
1	B	178	ARG
1	B	193	GLU
1	B	199	LYS
1	B	209	LYS
1	B	212	ARG
1	B	213	ASP
1	B	216	ASP
1	C	71	LYS
1	C	81	GLU
1	C	101	LEU
1	C	103	LEU
1	C	112	TRP
1	C	117	LEU
1	C	135	GLN
1	C	150	VAL
1	C	178	ARG
1	C	198	LEU
1	C	200	GLU
1	C	203	SER
1	C	211	SER
1	C	213	ASP
1	C	215	HIS
1	C	217	ASN
1	D	79	LEU
1	D	88	ARG
1	D	117	LEU
1	D	123	HIS
1	D	133	TYR
1	D	136	LEU
1	D	153	LYS
1	D	166	LYS
1	D	183	ARG

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Mol	Chain	Res	Type
1	D	186	GLU
1	D	191	GLU
1	D	193	GLU
1	D	196	GLU
1	D	197	LEU
1	D	208	GLU
1	D	211	SER
1	D	213	ASP
1	D	216	ASP
1	D	224	GLU
1	D	225	VAL
1	D	226	ASP
1	E	72	ARG
1	E	73	SER
1	E	81	GLU
1	E	91	ARG
1	E	101	LEU
1	E	108	THR
1	E	113	GLU
1	E	117	LEU
1	E	118	VAL
1	E	120	ASP
1	E	122	ILE
1	E	123	HIS
1	E	141	GLU
1	E	175	GLN
1	E	188	GLU
1	E	192	LYS
1	E	203	SER
1	E	208	GLU
1	E	209	LYS
1	E	211	SER
1	E	215	HIS
1	E	225	VAL
1	E	226	ASP
1	F	79	LEU
1	F	97	LYS
1	F	101	LEU
1	F	119	ARG
1	F	123	HIS
1	F	175	GLN
1	F	183	ARG

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Mol	Chain	Res	Type
1	F	188	GLU
1	F	190	GLU
1	F	192	LYS
1	F	198	LEU
1	F	209	LYS
1	F	211	SER
1	F	213	ASP
1	G	73	SER
1	G	78	LYS
1	G	80	ARG
1	G	86	GLU
1	G	91	ARG
1	G	100	THR
1	G	108	THR
1	G	117	LEU
1	G	135	GLN
1	G	155	GLN
1	G	166	LYS
1	G	173	ARG
1	G	192	LYS
1	G	199	LYS
1	G	200	GLU
1	G	203	SER
1	G	204	LYS
1	G	212	ARG
1	H	81	GLU
1	H	101	LEU
1	H	105	MET
1	H	108	THR
1	H	119	ARG
1	H	124	GLN
1	H	134	MET
1	H	166	LYS
1	H	169	MET
1	H	171	MET
1	H	172	ARG
1	H	192	LYS
1	H	193	GLU
1	H	194	LEU
1	H	197	LEU
1	H	198	LEU
1	H	200	GLU

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Mol	Chain	Res	Type
1	H	201	ILE
1	H	203	SER
1	H	205	LEU
1	H	209	LYS
2	I	221	THR
2	I	226	ASP
2	K	226	ASP
2	L	221	THR
2	L	222	VAL
2	L	224	GLU
2	M	226	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	135	GLN
1	B	128	ASN
1	B	215	HIS
1	C	124	GLN
1	C	138	GLN
1	D	90	GLN
1	E	104	GLN
1	E	135	GLN
1	E	138	GLN
1	G	75	ASN
1	G	84	ASN

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, 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	155/159 (97%)	0.20	10 (6%) 25 20	24, 58, 105, 152	0
1	B	149/159 (93%)	0.25	4 (2%) 56 47	34, 67, 110, 158	0
1	C	150/159 (94%)	0.46	12 (8%) 18 15	38, 77, 148, 256	0
1	D	150/159 (94%)	0.41	9 (6%) 27 21	35, 73, 132, 294	0
1	E	151/159 (94%)	0.70	11 (7%) 21 17	46, 84, 123, 142	0
1	F	140/159 (88%)	-0.19	1 (0%) 84 80	32, 54, 102, 133	0
1	G	144/159 (90%)	0.56	9 (6%) 26 20	46, 87, 131, 170	0
1	H	133/159 (83%)	0.92	19 (14%) 6 5	36, 86, 168, 233	0
2	I	6/7 (85%)	0.36	0 100 100	73, 86, 99, 99	0
2	J	7/7 (100%)	0.37	0 100 100	40, 59, 71, 72	0
2	K	7/7 (100%)	1.16	2 (28%) 1 1	95, 110, 114, 116	0
2	L	6/7 (85%)	0.77	0 100 100	82, 101, 110, 116	0
2	M	5/7 (71%)	0.58	1 (20%) 3 2	72, 82, 94, 98	0
All	All	1203/1307 (92%)	0.42	78 (6%) 25 20	24, 73, 133, 294	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	118	VAL	6.2
1	D	74	ALA	6.0
1	A	188	GLU	5.3
1	A	190	GLU	4.5
1	D	76	ILE	4.3
1	D	75	ASN	4.0
1	C	114	PRO	3.8
1	H	194	LEU	3.7
1	A	189	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	115	ALA	3.5
1	A	184	GLY	3.5
1	C	118	VAL	3.5
1	D	220	PRO	3.4
1	G	117	LEU	3.4
1	E	118	VAL	3.2
1	G	118	VAL	3.2
1	A	220	PRO	3.2
1	H	185	LEU	3.2
1	H	164	ARG	3.2
1	C	70	PRO	3.2
1	H	167	CYS	3.1
1	A	117	LEU	3.1
1	A	116	GLY	3.1
1	H	197	LEU	2.9
1	E	70	PRO	2.9
1	A	71	LYS	2.9
1	E	220	PRO	2.8
1	H	90	GLN	2.8
1	C	113	GLU	2.8
1	H	91	ARG	2.8
1	G	201	ILE	2.8
1	C	71	LYS	2.8
1	C	117	LEU	2.7
1	G	207	ALA	2.7
1	A	191	GLU	2.7
1	C	72	ARG	2.7
1	D	117	LEU	2.7
1	C	116	GLY	2.6
1	H	174	LEU	2.6
1	G	180	TRP	2.6
1	H	184	GLY	2.6
1	E	155	GLN	2.6
2	M	222	VAL	2.6
1	E	117	LEU	2.5
1	B	191	GLU	2.5
1	H	147	GLU	2.5
1	H	181	VAL	2.5
1	G	68	VAL	2.4
1	C	189	GLY	2.4
1	H	145	ASP	2.4
1	H	171	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	201	ILE	2.4
2	K	220	PRO	2.3
1	B	117	LEU	2.3
1	G	187	PHE	2.3
1	H	182	ALA	2.2
1	D	175	GLN	2.2
1	B	216	ASP	2.2
1	C	69	ASN	2.2
1	A	187	PHE	2.2
1	G	116	GLY	2.2
1	C	175	GLN	2.2
1	E	112	TRP	2.2
1	G	206	ALA	2.2
2	K	222	VAL	2.1
1	H	209	LYS	2.1
1	E	187	PHE	2.1
1	B	68	VAL	2.1
1	D	116	GLY	2.1
1	H	187	PHE	2.1
1	E	172	ARG	2.1
1	F	188	GLU	2.1
1	E	185	LEU	2.0
1	D	214	ALA	2.0
1	H	206	ALA	2.0
1	E	188	GLU	2.0
1	E	210	ALA	2.0
1	H	139	TRP	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.