



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:58 AM UTC

PDB ID : 8JDI / pdb_00008jdi
Title : Crystal structure of Cas7-AcrIF25 complex
Authors : Yang, J.; Wang, J.; Wang, Y.
Deposited on : 2023-05-14
Resolution : 3.37 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:

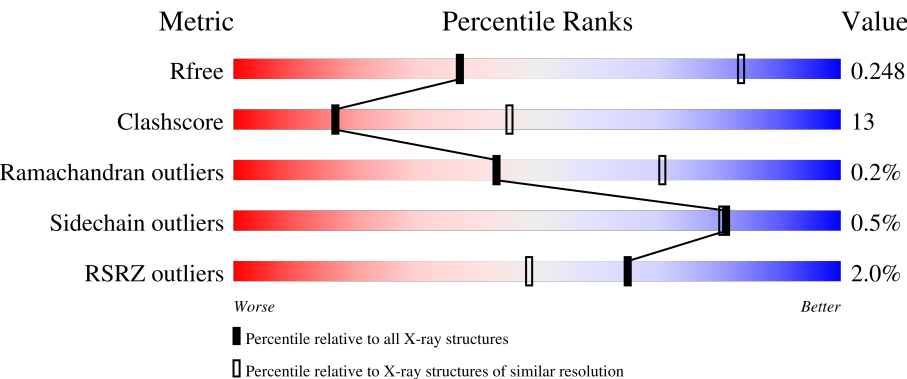
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.37 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	1047 (3.42-3.34)
Clashscore	190562	1067 (3.42-3.34)
Ramachandran outliers	187476	1056 (3.42-3.34)
Sidechain outliers	187428	1056 (3.42-3.34)
RSRZ outliers	180081	1047 (3.42-3.34)

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	342	% 67%21%11%
1	B	342	4% 64%19%16%
1	C	342	3% 61%28%10%
1	D	342	2% 66%21%12%
2	E	166	% 67%22%10%

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Mol	Chain	Length	Quality of chain
2	F	166	% 67%22%8%
2	G	166	% 77%14%8%
2	H	166	% 74%16%9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13487 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 CRISPR-associated protein Csy3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2303	1452	417	432	2			
1	C	309	Total	C	N	O	S	0	0	0
			2296	1452	409	433	2			
1	B	288	Total	C	N	O	S	0	0	0
			2089	1320	375	393	1			
1	D	302	Total	C	N	O	S	0	0	0
			2255	1425	410	419	1			

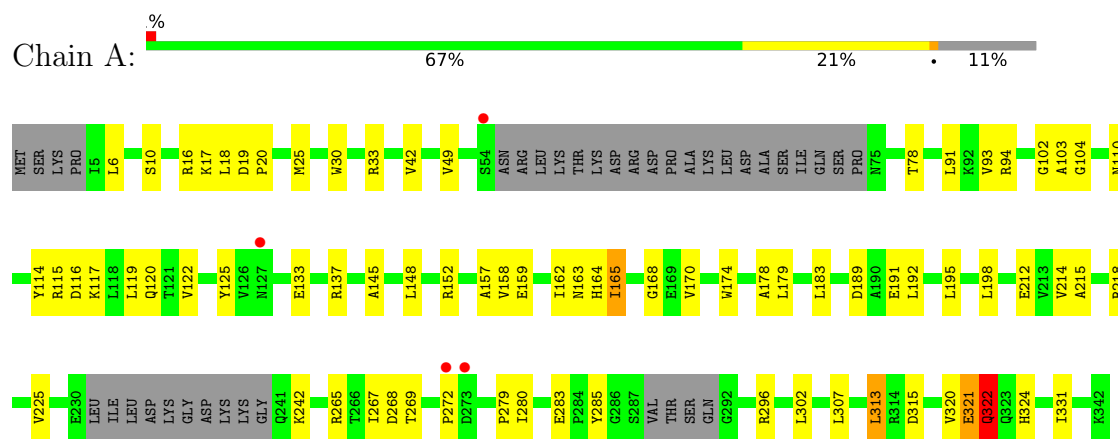
- Molecule 2 is a protein called AcrIF25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	150	Total	C	N	O	S	0	0	0
			1118	702	198	213	5			
2	G	152	Total	C	N	O	S	0	1	0
			1163	728	207	223	5			
2	F	152	Total	C	N	O	S	0	1	0
			1126	703	200	218	5			
2	H	151	Total	C	N	O	S	0	0	0
			1137	714	200	219	4			

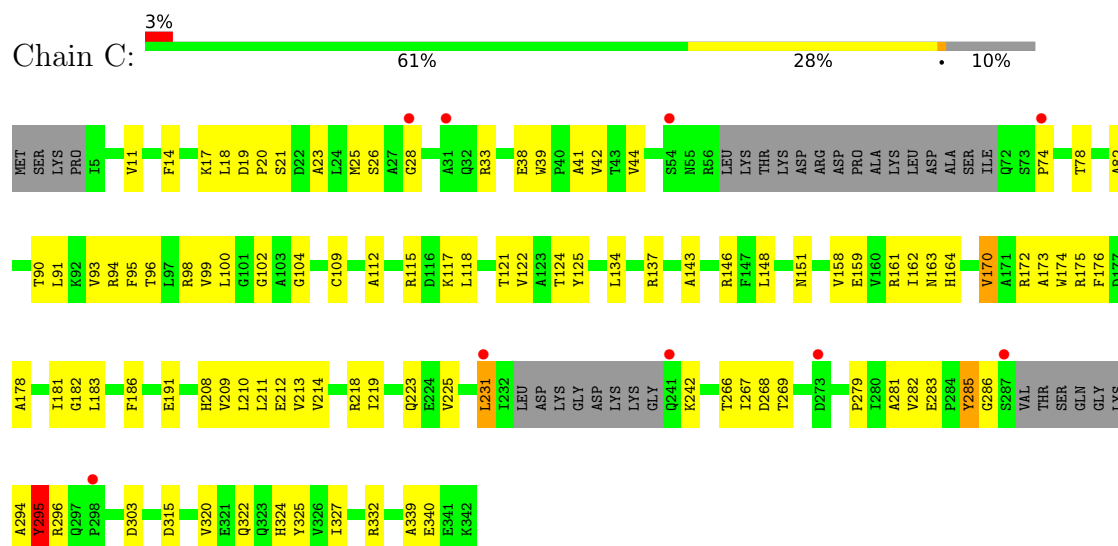
3 Residue-property plots [i](#)

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.

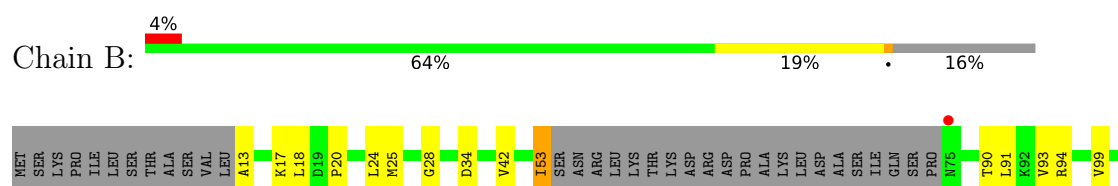
• Molecule 1: CRISPR-associated protein Csy3

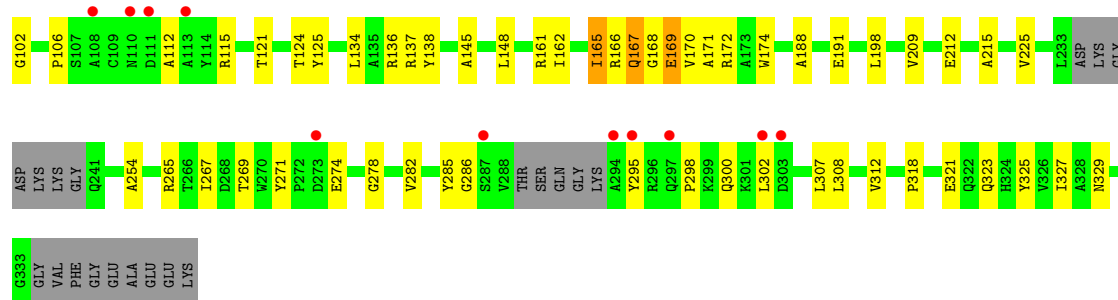


• Molecule 1: CRISPR-associated protein Csy3

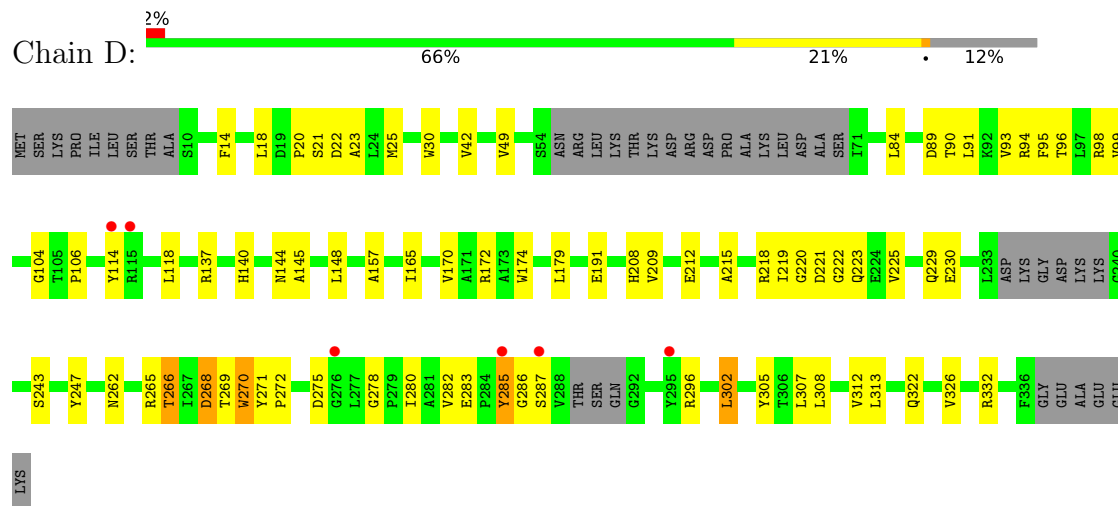


• Molecule 1: CRISPR-associated protein Csy3

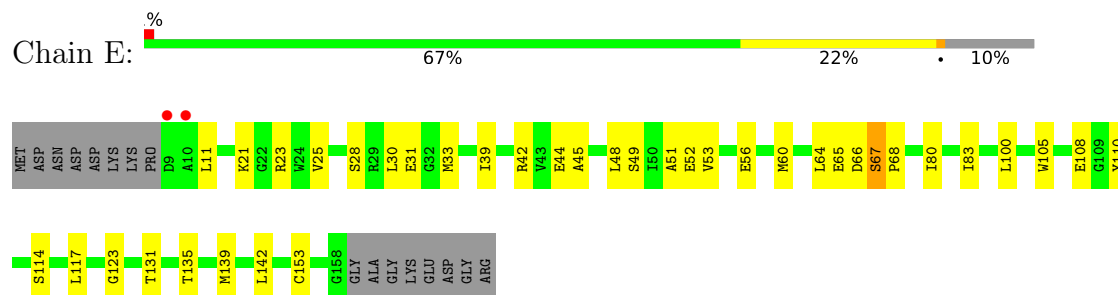




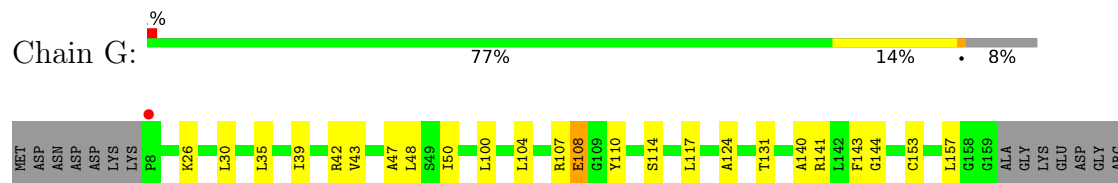
• Molecule 1: CRISPR-associated protein Csy3



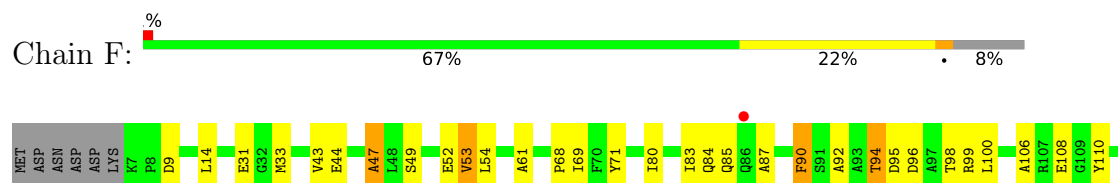
• Molecule 2: AcrIF25



• Molecule 2: AcrIF25

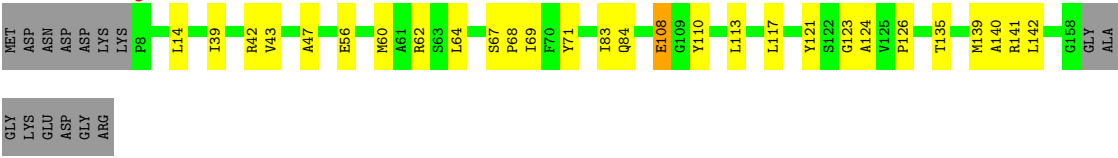


• Molecule 2: AcrIF25





● Molecule 2: AcrIF25



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	108.67Å 119.01Å 215.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 3.37 49.43 – 3.37	Depositor EDS
% Data completeness (in resolution range)	89.3 (49.43-3.37) 89.2 (49.43-3.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.218 , 0.247 0.219 , 0.248	Depositor DCC
R_{free} test set	1753 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	13487	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% 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	0.51	4/2345 (0.2%)	0.55	1/3187 (0.0%)
1	B	0.48	3/2128 (0.1%)	0.58	1/2910 (0.0%)
1	C	0.37	0/2338	0.67	6/3188 (0.2%)
1	D	0.44	0/2298	0.71	9/3131 (0.3%)
2	E	0.59	2/1138 (0.2%)	0.68	3/1548 (0.2%)
2	F	0.60	0/1150	0.78	6/1566 (0.4%)
2	G	0.20	0/1187	0.50	1/1608 (0.1%)
2	H	0.39	0/1158	0.57	2/1573 (0.1%)
All	All	0.46	9/13742 (0.1%)	0.63	29/18711 (0.2%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	321	GLU	C-O	-8.07	1.14	1.24
1	B	169	GLU	C-O	-7.17	1.14	1.23
1	A	320	VAL	C-O	-6.74	1.15	1.24
2	E	51	ALA	C-O	-6.36	1.16	1.24
1	B	165	ILE	C-O	-6.31	1.16	1.24
1	A	320	VAL	CA-C	-6.30	1.44	1.52
1	A	322	GLN	C-O	-5.66	1.17	1.24
1	B	167	GLN	C-O	-5.54	1.18	1.24
2	E	64	LEU	C-O	-5.33	1.17	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	92	ALA	N-CA-C	-10.11	94.79	109.96
2	E	67	SER	CA-C-N	9.23	130.18	119.47
2	E	67	SER	C-N-CA	9.23	130.18	119.47
1	C	295	TYR	N-CA-C	8.36	120.47	111.36
2	G	108	GLU	N-CA-C	-8.17	102.45	111.36
2	F	108	GLU	N-CA-C	-7.83	102.75	111.28
1	C	170	VAL	N-CA-C	7.60	119.46	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	14	LEU	N-CA-C	7.22	120.78	107.99
2	H	108	GLU	N-CA-C	-6.74	103.93	111.28
1	C	74	PRO	N-CA-CB	6.68	110.27	103.25
1	B	165	ILE	N-CA-C	6.30	117.37	108.36
1	A	313	LEU	N-CA-C	6.13	118.04	111.36
1	D	302	LEU	N-CA-C	6.04	120.51	113.20
2	F	90	PHE	N-CA-C	6.01	117.83	111.28
1	D	266	THR	N-CA-C	-5.94	102.42	110.68
1	D	243	SER	N-CA-C	5.93	120.24	112.89
1	D	230	GLU	N-CA-CB	5.88	118.42	110.59
1	D	285	TYR	N-CA-C	-5.83	103.19	111.24
2	F	53	VAL	CB-CA-C	-5.75	104.50	112.04
1	D	270	TRP	N-CA-C	5.74	119.26	112.72
1	D	229	GLN	N-CA-C	5.64	119.43	109.96
1	D	287	SER	N-CA-C	5.61	117.77	110.53
1	C	339	ALA	CA-C-N	5.60	132.24	121.54
1	C	339	ALA	C-N-CA	5.60	132.24	121.54
1	D	268	ASP	N-CA-C	5.56	117.28	108.67
2	E	44	GLU	N-CA-C	-5.30	105.27	112.26
1	C	285	TYR	N-CA-C	-5.23	99.88	108.41
2	F	108	GLU	N-CA-CB	5.16	117.70	110.12
2	F	92	ALA	N-CA-CB	5.05	117.38	109.85

There are no chirality outliers.

There are no planarity outliers.

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	2303	0	2231	51	0
1	B	2089	0	1930	54	0
1	C	2296	0	2178	80	0
1	D	2255	0	2146	56	0
2	E	1118	0	1075	32	0
2	F	1126	0	1058	37	0
2	G	1163	0	1143	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1137	0	1102	24	0
All	All	13487	0	12863	336	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 13.

All (336) 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:C:231:LEU:HD12	1:C:231:LEU:H	1.24	1.00
1:C:268:ASP:OD2	1:C:296:ARG:NH1	1.95	1.00
2:E:67:SER:HB2	2:E:68:PRO:CD	1.97	0.94
2:G:104:LEU:O	2:G:108:GLU:HG3	1.66	0.94
1:D:137:ARG:NH1	1:D:270:TRP:CZ2	2.40	0.88
2:G:107:ARG:HH11	2:G:143:PHE:HB3	1.41	0.86
1:D:302:LEU:HD22	1:D:322:GLN:NE2	1.95	0.82
1:C:162:ILE:HG12	1:C:213:VAL:HG12	1.62	0.81
2:F:95:ASP:OD2	2:F:98:THR:OG1	1.98	0.81
2:G:107:ARG:HH11	2:G:143:PHE:CB	1.94	0.79
2:E:67:SER:HB2	2:E:68:PRO:HD3	1.64	0.79
2:E:48:LEU:HD22	2:E:53:VAL:HG22	1.67	0.77
1:C:176:PHE:HB3	1:C:181:ILE:HD11	1.65	0.77
2:E:48:LEU:HD22	2:E:53:VAL:CG2	2.17	0.75
2:G:107:ARG:NH1	2:G:143:PHE:CB	2.49	0.75
1:B:286:GLY:O	1:B:295:TYR:HA	1.87	0.74
1:D:165:ILE:HG22	1:D:170:VAL:HG12	1.70	0.74
2:E:67:SER:HB2	2:E:68:PRO:HD2	1.66	0.74
2:F:99:ARG:HB2	2:F:157:LEU:HD13	1.68	0.74
1:B:278:GLY:HA3	2:F:124:ALA:HB2	1.69	0.74
1:B:166:ARG:HG2	1:B:166:ARG:HH11	1.53	0.73
1:B:318:PRO:HG2	1:B:323:GLN:NE2	2.04	0.72
1:C:285:TYR:HE1	1:C:303:ASP:OD2	1.72	0.72
1:B:318:PRO:HG2	1:B:323:GLN:HE21	1.55	0.72
1:A:33:ARG:NH1	1:A:159:GLU:OE1	2.24	0.71
1:D:84:LEU:HD11	1:D:219:ILE:HD11	1.71	0.71
1:A:114:TYR:HE1	1:A:313:LEU:HD11	1.55	0.70
2:G:107:ARG:NH1	2:G:143:PHE:HB2	2.06	0.70
1:A:313:LEU:N	1:A:313:LEU:HD12	2.06	0.70
1:B:125:TYR:CE1	1:B:327:ILE:HD13	2.27	0.70
2:H:60:MET:HE2	2:H:135:THR:HG23	1.72	0.70
1:C:269:THR:HG22	1:C:279:PRO:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:107:ARG:NH1	2:G:143:PHE:HB3	2.08	0.69
2:G:43:VAL:HA	2:H:42:ARG:HG2	1.76	0.68
1:B:321:GLU:OE1	1:B:321:GLU:N	2.27	0.67
1:D:285:TYR:CZ	1:D:305:TYR:HD2	2.12	0.67
1:C:231:LEU:HD12	1:C:231:LEU:N	2.04	0.67
2:E:67:SER:CB	2:E:68:PRO:CD	2.64	0.67
1:B:325:TYR:CE1	1:B:329:ASN:ND2	2.62	0.66
2:F:80:ILE:O	2:F:84:GLN:HG3	1.95	0.66
2:H:135:THR:HG22	2:H:139:MET:HE2	1.76	0.66
1:B:265:ARG:HB3	1:B:282:VAL:HG22	1.77	0.66
1:A:307:LEU:HD21	1:A:322:GLN:HG3	1.78	0.66
1:D:283:GLU:OE1	1:D:332:ARG:NE	2.30	0.65
2:E:31:GLU:HB3	2:E:33:MET:HE3	1.77	0.65
1:C:33:ARG:NH1	1:C:159:GLU:OE1	2.29	0.65
2:G:42:ARG:HH12	2:H:47:ALA:HA	1.62	0.64
1:A:268:ASP:OD2	1:A:296:ARG:NH1	2.31	0.64
2:E:42:ARG:O	2:E:45:ALA:HB2	1.99	0.63
2:F:49:SER:HB3	2:F:52:GLU:CG	2.28	0.63
1:C:78:THR:HG23	1:C:242:LYS:H	1.63	0.63
1:C:137:ARG:HB3	1:C:267:ILE:HG12	1.81	0.63
1:D:42:VAL:HG11	1:D:225:VAL:HG21	1.80	0.63
1:C:282:VAL:HG23	1:C:282:VAL:O	1.99	0.62
1:D:285:TYR:OH	1:D:305:TYR:HD2	1.82	0.62
1:C:125:TYR:CE1	1:C:327:ILE:HD13	2.34	0.62
2:F:94:THR:HG23	2:F:94:THR:O	2.00	0.62
1:C:219:ILE:O	2:G:141:ARG:NH1	2.32	0.62
1:D:104:GLY:O	1:D:106:PRO:HD3	1.99	0.62
2:E:67:SER:CB	2:E:68:PRO:HD3	2.25	0.62
1:B:285:TYR:HE1	1:B:298:PRO:HB3	1.64	0.62
1:A:49:VAL:HG13	2:E:108:GLU:HB3	1.82	0.61
1:C:25:MET:HG2	1:C:93:VAL:HG22	1.82	0.61
2:F:43:VAL:O	2:F:47:ALA:HB2	1.99	0.61
1:C:170:VAL:HG23	1:C:170:VAL:O	2.01	0.61
1:D:14:PHE:HZ	1:D:118:LEU:HD21	1.65	0.61
1:D:285:TYR:CZ	1:D:305:TYR:CD2	2.89	0.61
1:D:296:ARG:NH2	1:D:322:GLN:OE1	2.33	0.61
1:C:23:ALA:HA	1:C:95:PHE:HB3	1.82	0.60
1:D:282:VAL:HG23	1:D:282:VAL:O	2.00	0.60
1:D:308:LEU:O	1:D:312:VAL:HG22	2.02	0.60
1:C:320:VAL:HG12	1:C:324:HIS:HE1	1.66	0.60
2:F:114:SER:HA	2:F:117:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:135:THR:HG22	2:E:139:MET:HE2	1.83	0.60
1:C:99:VAL:HB	1:C:209:VAL:HG22	1.83	0.60
2:H:56:GLU:O	2:H:60:MET:HG3	2.02	0.60
1:A:313:LEU:N	1:A:313:LEU:CD1	2.65	0.60
1:C:295:TYR:HD1	1:C:295:TYR:H	1.50	0.59
1:C:296:ARG:HH21	1:C:322:GLN:HE22	1.50	0.59
1:C:285:TYR:CD1	1:C:303:ASP:OD1	2.56	0.59
1:D:137:ARG:CZ	1:D:270:TRP:CZ2	2.85	0.59
2:F:49:SER:HB3	2:F:52:GLU:HB2	1.83	0.58
1:A:313:LEU:CD1	1:A:313:LEU:H	2.16	0.58
2:H:62:ARG:HG3	2:H:84:GLN:OE1	2.02	0.58
2:E:11:LEU:HA	2:F:14:LEU:O	2.04	0.58
1:C:279:PRO:HD2	2:G:124:ALA:HB2	1.83	0.58
1:A:42:VAL:HG11	1:A:225:VAL:HG21	1.86	0.58
1:B:94:ARG:NH1	1:B:212:GLU:OE1	2.36	0.58
1:A:117:LYS:NZ	1:A:315:ASP:OD2	2.36	0.57
1:C:94:ARG:NH1	1:C:212:GLU:OE1	2.38	0.57
2:E:49:SER:OG	2:E:52:GLU:CB	2.52	0.57
1:C:295:TYR:CD1	1:C:295:TYR:N	2.73	0.57
2:G:30:LEU:HD21	2:H:142:LEU:HD23	1.85	0.57
2:F:90:PHE:CD1	2:F:90:PHE:C	2.83	0.57
1:D:220:GLY:O	1:D:223:GLN:HG2	2.04	0.57
1:B:325:TYR:HE1	1:B:329:ASN:HD21	1.50	0.57
1:C:320:VAL:HG12	1:C:324:HIS:CE1	2.40	0.57
1:B:138:TYR:CE1	1:B:267:ILE:HD11	2.40	0.57
1:C:137:ARG:HD3	1:C:267:ILE:HG23	1.87	0.56
1:C:285:TYR:CE1	1:C:303:ASP:OD2	2.55	0.56
1:C:28:GLY:HA3	1:C:39:TRP:CE2	2.40	0.56
1:B:166:ARG:HD3	1:B:171:ALA:HB2	1.87	0.56
1:D:266:THR:HG22	1:D:266:THR:O	2.04	0.56
2:F:96:ASP:HA	2:F:99:ARG:HG3	1.88	0.56
1:B:99:VAL:HB	1:B:209:VAL:HG22	1.88	0.56
2:F:83:ILE:HD11	2:F:110:TYR:HA	1.88	0.56
2:F:68:PRO:HA	2:F:71:TYR:CZ	2.42	0.55
1:A:94:ARG:HG3	1:A:214:VAL:HG22	1.89	0.55
1:A:78:THR:HG23	1:A:242:LYS:HB2	1.88	0.55
1:A:163:ASN:HB3	1:A:170:VAL:HG13	1.87	0.55
2:G:26:LYS:HD3	2:H:141:ARG:O	2.05	0.55
1:B:166:ARG:HG2	1:B:166:ARG:NH1	2.15	0.55
1:A:116:ASP:O	1:A:120:GLN:HG3	2.07	0.55
1:D:84:LEU:HB2	1:D:222:GLY:HA2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LYS:HE3	1:A:102:GLY:O	2.07	0.55
1:A:269:THR:HG22	1:A:279:PRO:HB3	1.89	0.54
2:H:68:PRO:HA	2:H:71:TYR:CZ	2.43	0.54
1:A:94:ARG:NH1	1:A:212:GLU:OE1	2.41	0.54
1:B:137:ARG:HH12	1:B:269:THR:HG23	1.73	0.54
1:C:121:THR:O	1:C:124:THR:HG22	2.08	0.53
1:D:145:ALA:HB1	1:D:148:LEU:HD12	1.89	0.53
2:F:49:SER:HB3	2:F:52:GLU:CB	2.38	0.53
1:A:174:TRP:CD1	1:A:191:GLU:HG3	2.44	0.53
1:C:94:ARG:HG3	1:C:214:VAL:HG22	1.91	0.53
1:B:42:VAL:HG11	1:B:225:VAL:HG21	1.90	0.53
1:B:174:TRP:HD1	1:B:191:GLU:HG3	1.74	0.52
1:C:109:CYS:SG	1:C:115:ARG:HB3	2.48	0.52
1:B:325:TYR:CD1	1:B:325:TYR:C	2.88	0.52
2:G:104:LEU:O	2:G:108:GLU:CG	2.48	0.52
2:F:54:LEU:CD2	2:F:54:LEU:N	2.72	0.52
1:D:174:TRP:HD1	1:D:191:GLU:HG3	1.74	0.52
2:G:43:VAL:HG21	2:H:39:ILE:HG23	1.92	0.52
1:C:223:GLN:HE22	2:G:144:GLY:HA2	1.75	0.52
1:D:94:ARG:NH1	1:D:212:GLU:OE1	2.42	0.52
1:C:11:VAL:HG11	2:F:138:GLN:HG3	1.92	0.52
1:C:146:ARG:O	1:C:146:ARG:HG2	2.10	0.52
1:D:137:ARG:HH12	1:D:269:THR:HG22	1.75	0.52
1:A:17:LYS:HB2	1:A:331:ILE:HG23	1.92	0.52
1:C:38:GLU:O	1:C:39:TRP:HB2	2.10	0.52
1:C:285:TYR:HD1	1:C:303:ASP:OD1	1.92	0.51
1:B:174:TRP:CD1	1:B:191:GLU:HG3	2.46	0.51
2:E:105:TRP:O	2:E:105:TRP:HD1	1.94	0.51
2:G:30:LEU:HD13	2:H:141:ARG:HB2	1.91	0.51
1:C:231:LEU:H	1:C:231:LEU:CD1	2.04	0.51
1:B:112:ALA:O	1:B:115:ARG:HG2	2.11	0.51
1:B:169:GLU:OE2	1:B:169:GLU:HA	2.11	0.51
1:B:166:ARG:HD3	1:B:171:ALA:CB	2.40	0.50
1:C:296:ARG:NH2	1:C:322:GLN:OE1	2.44	0.50
2:G:43:VAL:HG22	2:H:42:ARG:HB3	1.92	0.50
1:D:172:ARG:HG2	1:D:174:TRP:CH2	2.46	0.50
2:H:121:TYR:CE2	2:H:126:PRO:HG3	2.46	0.50
1:C:268:ASP:CG	1:C:296:ARG:HH12	2.19	0.50
1:B:172:ARG:HG2	1:B:172:ARG:HH11	1.77	0.50
1:D:137:ARG:NH1	1:D:270:TRP:CH2	2.78	0.50
1:C:286:GLY:H	1:C:296:ARG:HB2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ARG:HH22	1:B:188:ALA:HA	1.77	0.50
1:D:157:ALA:HA	1:D:179:LEU:HD11	1.93	0.50
2:F:61:ALA:HB1	2:F:80:ILE:HG23	1.93	0.50
1:C:172:ARG:HG2	1:C:173:ALA:N	2.26	0.50
2:E:114:SER:HA	2:E:117:LEU:HD12	1.94	0.50
1:A:16:ARG:NH2	1:A:19:ASP:OD1	2.45	0.50
1:D:25:MET:HG2	1:D:93:VAL:HG22	1.93	0.50
1:C:18:LEU:O	1:C:20:PRO:HD3	2.12	0.49
1:A:18:LEU:O	1:A:20:PRO:HD3	2.12	0.49
1:D:174:TRP:CD1	1:D:191:GLU:HG3	2.46	0.49
1:A:30:TRP:CE3	1:A:218:ARG:HB2	2.47	0.49
2:E:42:ARG:HB2	2:F:43:VAL:HG22	1.94	0.49
2:E:100:LEU:HD12	2:E:153:CYS:HB3	1.94	0.49
2:G:114:SER:HA	2:G:117:LEU:HD12	1.94	0.49
1:B:18:LEU:O	1:B:20:PRO:HD3	2.12	0.49
1:C:91:LEU:HD13	1:C:225:VAL:HG11	1.93	0.49
2:F:54:LEU:N	2:F:54:LEU:HD22	2.27	0.49
1:D:18:LEU:O	1:D:20:PRO:HD3	2.13	0.49
1:C:283:GLU:OE2	1:C:332:ARG:NH1	2.46	0.49
1:D:148:LEU:HD11	1:D:215:ALA:HB1	1.95	0.49
2:G:35:LEU:O	2:G:39:ILE:HG13	2.12	0.48
1:B:121:THR:O	1:B:124:THR:HG22	2.13	0.48
2:E:30:LEU:HG	2:F:141:ARG:HB3	1.96	0.48
2:E:48:LEU:HD22	2:E:53:VAL:HG23	1.94	0.48
1:C:296:ARG:HH21	1:C:322:GLN:NE2	2.11	0.48
1:D:285:TYR:OH	1:D:305:TYR:CD2	2.58	0.48
1:D:322:GLN:O	1:D:326:VAL:HG23	2.12	0.48
1:C:143:ALA:HB1	1:C:181:ILE:HD13	1.95	0.48
1:A:17:LYS:HE3	1:A:103:ALA:HA	1.96	0.48
2:G:107:ARG:HH12	2:G:143:PHE:HB2	1.78	0.48
1:B:162:ILE:O	1:B:174:TRP:HE3	1.97	0.48
1:D:30:TRP:HE3	1:D:90:THR:HG21	1.78	0.48
1:A:313:LEU:HD12	1:A:313:LEU:H	1.77	0.47
2:E:60:MET:HE3	2:E:142:LEU:HD11	1.96	0.47
1:C:90:THR:HG22	1:C:218:ARG:HA	1.96	0.47
1:C:266:THR:HA	1:C:281:ALA:HA	1.94	0.47
1:C:17:LYS:HE2	1:C:102:GLY:O	2.14	0.47
1:C:182:GLY:O	1:C:183:LEU:HB2	2.13	0.47
1:B:13:ALA:HA	1:B:106:PRO:HA	1.96	0.47
1:D:283:GLU:OE1	1:D:332:ARG:CZ	2.62	0.47
1:A:125:TYR:OH	1:A:324:HIS:ND1	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LEU:N	1:C:231:LEU:CD1	2.72	0.47
2:F:54:LEU:CD1	2:F:106:ALA:CB	2.92	0.47
1:A:25:MET:HG2	1:A:93:VAL:HG22	1.97	0.47
1:C:148:LEU:O	1:C:151:ASN:ND2	2.47	0.47
1:D:302:LEU:HA	1:D:307:LEU:HD21	1.97	0.47
1:B:25:MET:HG2	1:B:93:VAL:HG22	1.96	0.47
1:D:280:ILE:HG22	2:H:123:GLY:HA2	1.96	0.47
1:A:148:LEU:HD11	1:A:215:ALA:HB1	1.96	0.47
1:D:262:ASN:OD1	1:D:265:ARG:NH2	2.47	0.47
1:C:21:SER:HB3	1:C:96:THR:H	1.80	0.46
1:C:44:VAL:HG22	1:C:82:ALA:HB2	1.97	0.46
1:D:99:VAL:HB	1:D:209:VAL:HG23	1.97	0.46
1:D:268:ASP:HB2	1:D:282:VAL:HG12	1.96	0.46
2:H:67:SER:HB3	2:H:69:ILE:HG22	1.95	0.46
1:A:165:ILE:O	1:A:165:ILE:HG13	2.15	0.46
1:A:307:LEU:HD21	1:A:322:GLN:CG	2.44	0.46
1:B:172:ARG:HD3	1:B:174:TRP:CZ2	2.50	0.46
2:F:49:SER:HB3	2:F:52:GLU:HG3	1.98	0.46
1:A:91:LEU:HD13	1:A:225:VAL:HG11	1.98	0.46
1:C:320:VAL:O	1:C:324:HIS:ND1	2.47	0.46
1:B:167:GLN:HB3	1:B:168:GLY:H	1.54	0.46
2:E:23:ARG:NH1	2:F:44:GLU:OE1	2.49	0.46
1:C:161:ARG:HG2	1:C:175:ARG:HG2	1.96	0.46
2:G:39:ILE:HG23	2:H:43:VAL:HG21	1.97	0.46
1:D:22:ASP:OD2	1:D:247:TYR:OH	2.25	0.46
1:D:25:MET:HB3	1:D:91:LEU:HD11	1.98	0.46
2:F:100:LEU:HD12	2:F:153:CYS:HB3	1.98	0.46
1:D:49:VAL:HG13	2:H:108:GLU:HB3	1.98	0.46
2:E:65:GLU:HB2	2:E:80:ILE:HG21	1.98	0.45
1:D:90:THR:HG22	1:D:218:ARG:HA	1.98	0.45
2:E:28:SER:OG	2:E:33:MET:O	2.33	0.45
1:C:19:ASP:HB3	1:C:98:ARG:HG3	1.98	0.45
1:C:42:VAL:HG11	1:C:225:VAL:HG21	1.98	0.45
1:C:137:ARG:HG2	1:C:186:PHE:CD2	2.51	0.45
1:D:278:GLY:HA3	2:H:124:ALA:HB2	1.99	0.45
1:A:322:GLN:OE1	1:A:322:GLN:N	2.50	0.45
2:G:117:LEU:HD22	2:G:131:THR:O	2.16	0.45
1:A:265:ARG:NH2	1:A:283:GLU:OE2	2.50	0.45
2:G:110:TYR:OH	2:G:140:ALA:HB2	2.17	0.45
1:B:24:LEU:HD23	1:B:254:ALA:HB2	1.99	0.45
1:D:271:TYR:HB2	1:D:272:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:LEU:HD22	2:E:131:THR:O	2.17	0.45
1:B:148:LEU:HD11	1:B:215:ALA:HB1	1.98	0.45
1:B:265:ARG:HB3	1:B:282:VAL:CG2	2.44	0.45
1:C:78:THR:CG2	1:C:242:LYS:H	2.28	0.45
1:C:283:GLU:O	1:C:325:TYR:OH	2.23	0.45
1:B:53:ILE:HB	2:F:85:GLN:OE1	2.17	0.45
1:B:17:LYS:HE2	1:B:102:GLY:O	2.17	0.45
1:B:34:ASP:HA	1:B:161:ARG:HH12	1.82	0.44
1:A:272:PRO:HD3	1:A:296:ARG:HD2	1.99	0.44
1:B:172:ARG:HG2	1:B:172:ARG:NH1	2.31	0.44
1:B:307:LEU:HD12	1:B:307:LEU:HA	1.65	0.44
1:A:162:ILE:HG21	1:A:195:LEU:HD11	1.98	0.44
1:A:10:SER:HB3	1:A:110:ASN:HD21	1.82	0.44
1:B:91:LEU:HD13	1:B:225:VAL:HG11	2.00	0.44
1:A:104:GLY:HA3	1:A:122:VAL:HG11	1.99	0.44
1:A:133:GLU:OE1	1:A:137:ARG:NE	2.41	0.44
2:E:42:ARG:HB3	2:F:43:VAL:HA	2.00	0.44
1:C:14:PHE:HZ	1:C:118:LEU:HD11	1.82	0.44
1:C:174:TRP:CD1	1:C:191:GLU:HG3	2.52	0.44
1:D:98:ARG:HB2	1:D:208:HIS:NE2	2.32	0.44
1:A:17:LYS:CE	1:A:102:GLY:O	2.66	0.44
2:H:64:LEU:HD22	2:H:69:ILE:HG21	2.00	0.44
1:C:28:GLY:HA3	1:C:39:TRP:CD2	2.53	0.43
1:B:134:LEU:HD11	1:B:327:ILE:HG13	1.98	0.43
1:C:26:SER:HA	1:C:41:ALA:HA	2.00	0.43
2:H:83:ILE:HD11	2:H:110:TYR:HA	2.00	0.43
1:A:137:ARG:HD3	1:A:267:ILE:HG13	2.00	0.43
2:F:9:ASP:OD1	2:F:9:ASP:N	2.43	0.43
1:B:136:ARG:NH2	1:B:188:ALA:HA	2.33	0.43
2:H:113:LEU:O	2:H:117:LEU:HD13	2.18	0.43
1:C:104:GLY:HA3	1:C:122:VAL:HG21	2.00	0.43
1:A:17:LYS:NZ	1:A:102:GLY:O	2.51	0.43
1:B:308:LEU:O	1:B:312:VAL:HG23	2.19	0.43
1:A:6:LEU:HD12	1:A:313:LEU:HG	1.99	0.43
1:C:146:ARG:CZ	1:C:183:LEU:CD2	2.95	0.43
1:C:286:GLY:O	1:C:294:ALA:HA	2.18	0.43
1:D:269:THR:OG1	1:D:275:ASP:OD2	2.37	0.43
1:A:302:LEU:HD12	1:A:302:LEU:HA	1.85	0.43
2:E:66:ASP:CG	2:E:66:ASP:O	2.59	0.43
2:H:60:MET:HE2	2:H:60:MET:HB3	1.70	0.43
1:C:95:PHE:CZ	1:C:213:VAL:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLU:HB3	1:C:39:TRP:H	1.71	0.42
1:B:285:TYR:CE1	1:B:298:PRO:HB3	2.50	0.42
2:H:110:TYR:OH	2:H:140:ALA:HB2	2.19	0.42
1:A:145:ALA:HB1	1:A:148:LEU:HD12	2.02	0.42
1:C:112:ALA:O	1:C:115:ARG:HG2	2.18	0.42
2:G:100:LEU:HD12	2:G:153:CYS:HB3	2.01	0.42
2:E:21:LYS:O	2:E:25:VAL:HG23	2.20	0.42
1:B:174:TRP:HH2	1:B:198:LEU:HD22	1.83	0.42
1:A:152:ARG:CZ	1:A:183:LEU:HD13	2.50	0.42
1:C:98:ARG:HB3	1:C:210:LEU:HD13	2.01	0.42
1:B:145:ALA:HB1	1:B:148:LEU:HD12	2.01	0.42
1:C:117:LYS:NZ	1:C:315:ASP:OD1	2.47	0.42
1:B:137:ARG:NH1	1:B:267:ILE:O	2.51	0.42
2:F:68:PRO:HA	2:F:71:TYR:CE2	2.55	0.42
1:D:89:ASP:CB	1:D:221:ASP:H	2.33	0.42
1:A:115:ARG:O	1:A:119:LEU:HD23	2.20	0.42
2:E:56:GLU:O	2:E:60:MET:HG3	2.19	0.42
2:F:117:LEU:HD22	2:F:131:THR:O	2.19	0.42
2:E:83:ILE:HD11	2:E:110:TYR:HA	2.01	0.42
1:B:300:GLN:C	1:B:302:LEU:H	2.28	0.42
1:D:302:LEU:HA	1:D:307:LEU:CD2	2.50	0.42
1:A:164:HIS:CE1	1:A:198:LEU:HD11	2.55	0.41
1:D:23:ALA:HA	1:D:95:PHE:HB3	2.02	0.41
1:D:21:SER:HB3	1:D:96:THR:H	1.85	0.41
1:D:285:TYR:HA	1:D:296:ARG:O	2.20	0.41
1:B:28:GLY:O	1:B:90:THR:HG22	2.21	0.41
1:D:137:ARG:CZ	1:D:270:TRP:HZ2	2.31	0.41
1:B:325:TYR:HE1	1:B:329:ASN:ND2	2.10	0.41
1:C:163:ASN:HB2	1:C:212:GLU:HG2	2.02	0.41
2:F:31:GLU:HG3	2:F:33:MET:HE2	2.03	0.41
1:C:223:GLN:NE2	2:G:144:GLY:HA2	2.35	0.41
1:B:165:ILE:HG12	1:B:170:VAL:HG12	2.02	0.41
1:A:189:ASP:HB3	1:A:192:LEU:HB3	2.02	0.41
1:A:280:ILE:HG22	2:E:123:GLY:HA2	2.03	0.41
1:A:285:TYR:C	1:A:296:ARG:HB2	2.46	0.41
1:C:100:LEU:HD23	1:C:208:HIS:HB2	2.03	0.41
1:C:158:VAL:HB	1:C:178:ALA:HB3	2.03	0.41
2:F:137:SER:O	2:F:141:ARG:HG2	2.21	0.41
1:A:157:ALA:HA	1:A:179:LEU:HD11	2.03	0.41
1:A:158:VAL:HB	1:A:178:ALA:HB3	2.01	0.41
2:E:105:TRP:CD1	2:E:105:TRP:C	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:LEU:CD1	1:C:327:ILE:HD11	2.51	0.41
2:G:107:ARG:NH2	2:G:144:GLY:O	2.54	0.41
1:D:114:TYR:CE2	1:D:313:LEU:HD21	2.55	0.41
2:E:39:ILE:HD11	2:F:14:LEU:HG	2.03	0.40
2:G:47:ALA:O	2:G:48:LEU:HG	2.20	0.40
1:D:140:HIS:O	1:D:144:ASN:N	2.51	0.40
1:C:137:ARG:HH12	1:C:269:THR:HG23	1.86	0.40
1:D:91:LEU:HD13	1:D:225:VAL:HG11	2.03	0.40
1:C:164:HIS:HA	1:C:211:LEU:HD23	2.03	0.40
2:F:31:GLU:CG	2:F:33:MET:HE2	2.51	0.40
2:F:69:ILE:HD11	2:F:117:LEU:HD23	2.04	0.40
2:F:83:ILE:O	2:F:87:ALA:HB2	2.22	0.40
2:H:60:MET:CE	2:H:135:THR:HG23	2.45	0.40
2:G:50:ILE:HD13	2:G:157:LEU:HD11	2.04	0.40
1:B:271:TYR:HE1	1:B:274:GLU:CB	2.34	0.40
2:F:49:SER:O	2:F:53:VAL:HG23	2.22	0.40
1:D:23:ALA:HB1	1:D:93:VAL:HG13	2.04	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	296/342 (86%)	278 (94%)	17 (6%)	1 (0%)	36	64
1	B	280/342 (82%)	267 (95%)	13 (5%)	0	100	100
1	C	301/342 (88%)	279 (93%)	21 (7%)	1 (0%)	36	64
1	D	294/342 (86%)	276 (94%)	17 (6%)	1 (0%)	36	64
2	E	148/166 (89%)	145 (98%)	3 (2%)	0	100	100
2	F	151/166 (91%)	146 (97%)	4 (3%)	1 (1%)	18	46
2	G	151/166 (91%)	141 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	149/166 (90%)	143 (96%)	6 (4%)	0	100	100
All	All	1770/2032 (87%)	1675 (95%)	91 (5%)	4 (0%)	43	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	340	GLU
1	D	286	GLY
1	A	168	GLY
2	F	47	ALA

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	224/273 (82%)	221 (99%)	3 (1%)	61	71
1	B	187/273 (68%)	186 (100%)	1 (0%)	81	80
1	C	217/273 (80%)	215 (99%)	2 (1%)	70	76
1	D	212/273 (78%)	212 (100%)	0	100	100
2	E	107/128 (84%)	107 (100%)	0	100	100
2	F	106/128 (83%)	105 (99%)	1 (1%)	70	76
2	G	116/128 (91%)	116 (100%)	0	100	100
2	H	111/128 (87%)	111 (100%)	0	100	100
All	All	1280/1604 (80%)	1273 (100%)	7 (0%)	81	80

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	ILE
1	A	321	GLU
1	A	322	GLN
1	C	231	LEU

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Mol	Chain	Res	Type
1	C	295	TYR
1	B	53	ILE
2	F	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	164	HIS
1	C	258	GLN
1	C	322	GLN
2	G	111	GLN
1	B	322	GLN
1	B	323	GLN
2	F	84	GLN
1	D	75	ASN
1	D	229	GLN

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 ⓘ

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	304/342 (88%)	-0.08	4 (1%) 75 60	17, 39, 68, 79	0
1	B	288/342 (84%)	0.20	12 (4%) 40 29	28, 58, 100, 112	0
1	C	309/342 (90%)	0.24	9 (2%) 53 39	32, 57, 88, 103	0
1	D	302/342 (88%)	0.17	6 (1%) 65 49	18, 49, 93, 107	0
2	E	150/166 (90%)	-0.06	2 (1%) 75 60	27, 50, 79, 95	0
2	F	152/166 (91%)	0.23	1 (0%) 84 72	39, 70, 105, 118	1 (0%)
2	G	152/166 (91%)	-0.13	1 (0%) 84 72	26, 47, 76, 91	1 (0%)
2	H	151/166 (90%)	-0.16	1 (0%) 84 72	20, 42, 87, 96	0
All	All	1808/2032 (88%)	0.08	36 (1%) 65 49	17, 52, 91, 118	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	287	SER	3.6
1	B	108	ALA	3.3
1	B	110	ASN	3.1
1	B	111	ASP	3.0
2	E	9	ASP	2.9
1	C	273	ASP	2.7
1	C	298	PRO	2.7
1	B	287	SER	2.6
1	C	31	ALA	2.6
1	D	114	TYR	2.5
1	B	294	ALA	2.5
1	B	75	ASN	2.4
2	G	8	PRO	2.4
1	A	127	ASN	2.4
1	A	54	SER	2.4
1	C	241	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	8	PRO	2.3
1	A	273	ASP	2.3
1	B	297	GLN	2.3
1	D	287	SER	2.3
1	D	285	TYR	2.2
1	D	295	TYR	2.2
1	C	28	GLY	2.2
2	E	10	ALA	2.2
1	A	272	PRO	2.2
1	B	113	ALA	2.2
1	C	54	SER	2.2
2	F	86	GLN	2.2
1	B	302	LEU	2.2
1	B	295	TYR	2.1
1	B	303	ASP	2.1
1	D	115	ARG	2.1
1	B	273	ASP	2.1
1	C	74	PRO	2.1
1	D	276	GLY	2.0
1	C	231	LEU	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.