



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:21 PM UTC

PDB ID : 9DBT / pdb_00009dbt
Title : Crystal structure of human astrovirus 1 capsid spike bound to human neonatal Fc receptor
Authors : Lentz, A.; DuBois, R.M.
Deposited on : 2024-08-23
Resolution : 3.40 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

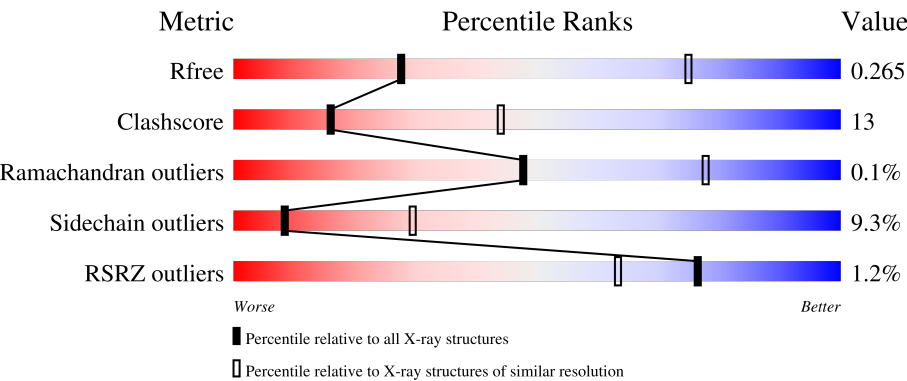
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	278	<div><div>4%</div><div>63%</div><div>29%</div><div>• 5%</div></div>
1	C	278	<div><div>2%</div><div>59%</div><div>32%</div><div>• 5%</div></div>
1	F	278	<div><div>2%</div><div>62%</div><div>29%</div><div>• •</div></div>
1	I	278	<div><div>%</div><div>48%</div><div>24%</div><div>5%</div><div>23%</div></div>
2	B	99	<div><div>%</div><div>63%</div><div>32%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	99	<div><div></div><div>62%</div><div>36%</div><div></div></div>
2	G	99	<div><div></div><div>60%</div><div>38%</div><div></div></div>
2	J	99	<div><div></div><div>57%</div><div>28%</div><div>12%</div><div></div></div>
3	E	228	<div><div></div><div>70%</div><div>23%</div><div>6%</div><div></div></div>
3	H	228	<div><div></div><div>70%</div><div>23%</div><div>6%</div><div></div></div>
3	K	228	<div><div></div><div>62%</div><div>32%</div><div>6%</div><div></div></div>
3	L	228	<div><div></div><div>71%</div><div>22%</div><div>6%</div><div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17924 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2079	1330	360	381	8			
1	F	266	Total	C	N	O	S	0	0	0
			2094	1338	362	386	8			
1	I	215	Total	C	N	O	S	0	0	0
			1709	1098	288	317	6			
1	C	263	Total	C	N	O	S	0	0	0
			2069	1324	357	380	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LEU	-	expression tag	UNP P55899
A	299	VAL	-	expression tag	UNP P55899
A	300	PRO	-	expression tag	UNP P55899
A	301	ARG	-	expression tag	UNP P55899
F	298	LEU	-	expression tag	UNP P55899
F	299	VAL	-	expression tag	UNP P55899
F	300	PRO	-	expression tag	UNP P55899
F	301	ARG	-	expression tag	UNP P55899
I	298	LEU	-	expression tag	UNP P55899
I	299	VAL	-	expression tag	UNP P55899
I	300	PRO	-	expression tag	UNP P55899
I	301	ARG	-	expression tag	UNP P55899
C	298	LEU	-	expression tag	UNP P55899
C	299	VAL	-	expression tag	UNP P55899
C	300	PRO	-	expression tag	UNP P55899
C	301	ARG	-	expression tag	UNP P55899

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	J	87	Total	C	N	O	S	0	0	0
			738	474	125	136	3			
2	D	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 3 is a protein called Structural protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	215	Total	C	N	O	S	0	0	0
			1687	1085	274	320	8			
3	K	215	Total	C	N	O	S	0	0	0
			1687	1085	274	320	8			
3	L	215	Total	C	N	O	S	0	0	0
			1687	1085	274	320	8			
3	E	215	Total	C	N	O	S	0	0	0
			1687	1085	274	320	8			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	428	MET	-	initiating methionine	UNP Q82452
H	646	ALA	-	expression tag	UNP Q82452
H	647	ALA	-	expression tag	UNP Q82452
H	648	ALA	-	expression tag	UNP Q82452
H	649	GLU	-	expression tag	UNP Q82452
H	650	LEU	-	expression tag	UNP Q82452
H	651	ALA	-	expression tag	UNP Q82452
H	652	LEU	-	expression tag	UNP Q82452
H	653	VAL	-	expression tag	UNP Q82452
H	654	PRO	-	expression tag	UNP Q82452
H	655	ARG	-	expression tag	UNP Q82452
K	428	MET	-	initiating methionine	UNP Q82452
K	646	ALA	-	expression tag	UNP Q82452
K	647	ALA	-	expression tag	UNP Q82452
K	648	ALA	-	expression tag	UNP Q82452
K	649	GLU	-	expression tag	UNP Q82452
K	650	LEU	-	expression tag	UNP Q82452
K	651	ALA	-	expression tag	UNP Q82452
K	652	LEU	-	expression tag	UNP Q82452

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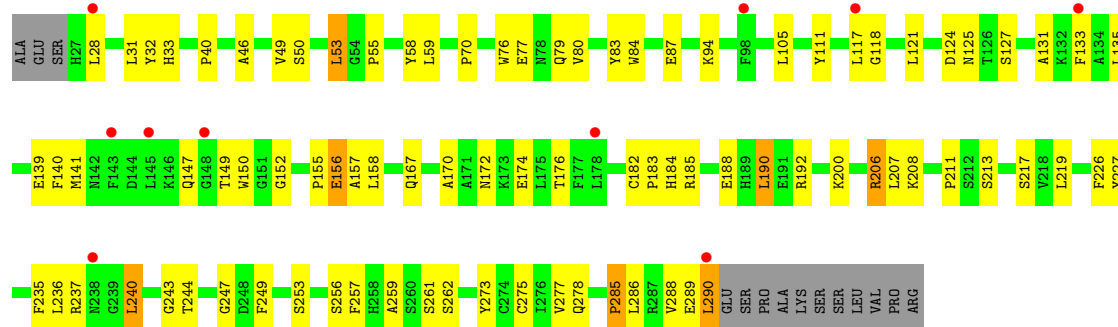
Chain	Residue	Modelled	Actual	Comment	Reference
K	653	VAL	-	expression tag	UNP Q82452
K	654	PRO	-	expression tag	UNP Q82452
K	655	ARG	-	expression tag	UNP Q82452
L	428	MET	-	initiating methionine	UNP Q82452
L	646	ALA	-	expression tag	UNP Q82452
L	647	ALA	-	expression tag	UNP Q82452
L	648	ALA	-	expression tag	UNP Q82452
L	649	GLU	-	expression tag	UNP Q82452
L	650	LEU	-	expression tag	UNP Q82452
L	651	ALA	-	expression tag	UNP Q82452
L	652	LEU	-	expression tag	UNP Q82452
L	653	VAL	-	expression tag	UNP Q82452
L	654	PRO	-	expression tag	UNP Q82452
L	655	ARG	-	expression tag	UNP Q82452
E	428	MET	-	initiating methionine	UNP Q82452
E	646	ALA	-	expression tag	UNP Q82452
E	647	ALA	-	expression tag	UNP Q82452
E	648	ALA	-	expression tag	UNP Q82452
E	649	GLU	-	expression tag	UNP Q82452
E	650	LEU	-	expression tag	UNP Q82452
E	651	ALA	-	expression tag	UNP Q82452
E	652	LEU	-	expression tag	UNP Q82452
E	653	VAL	-	expression tag	UNP Q82452
E	654	PRO	-	expression tag	UNP Q82452
E	655	ARG	-	expression tag	UNP Q82452

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.

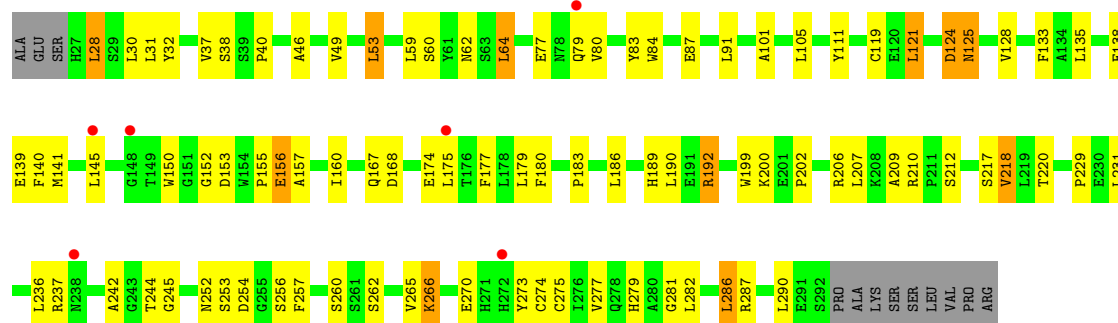
• Molecule 1: IgG receptor FcRn large subunit p51

Chain A: 



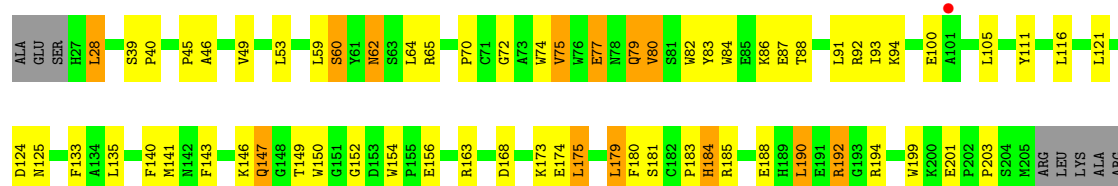
• Molecule 1: IgG receptor FcRn large subunit p51

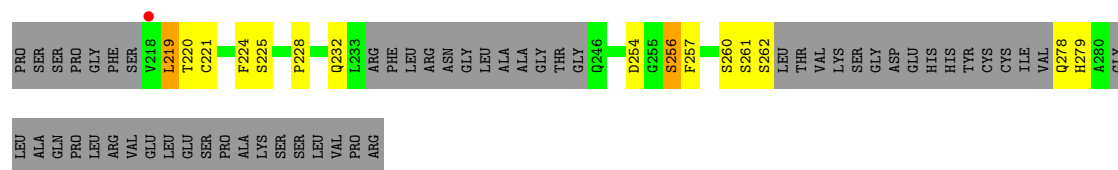
Chain F: 



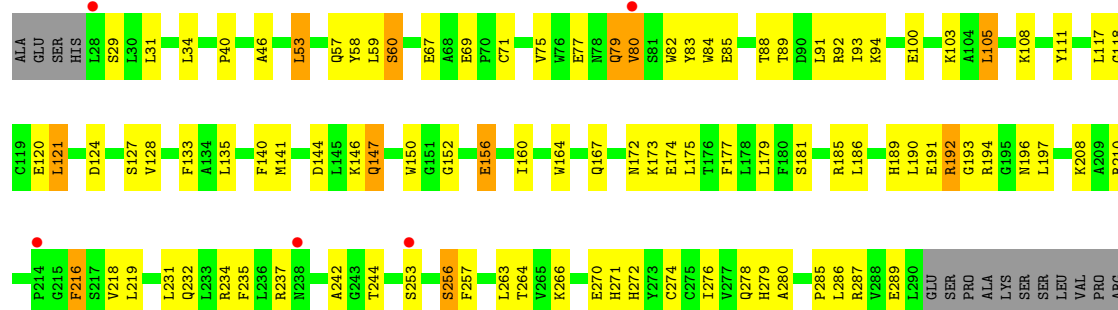
• Molecule 1: IgG receptor FcRn large subunit p51

Chain I: 





• Molecule 1: IgG receptor FcRn large subunit p51



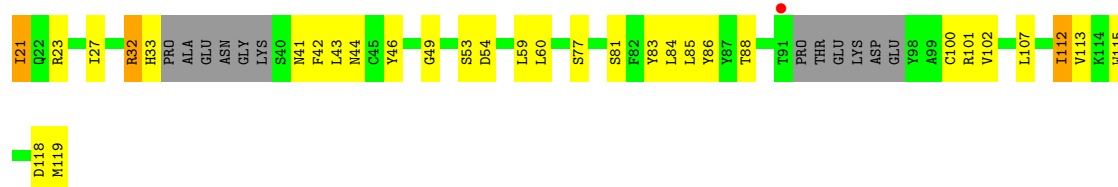
• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



• Molecule 2: Beta-2-microglobulin



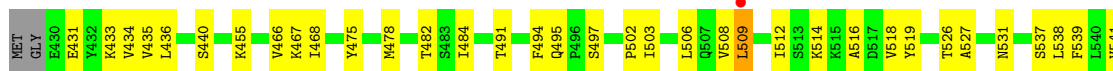
• Molecule 2: Beta-2-microglobulin





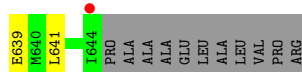
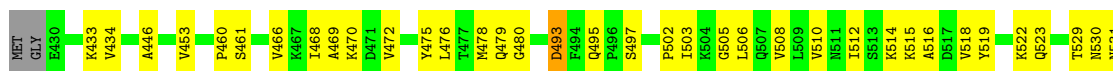
- Molecule 3: Structural protein

Chain H: 70% 23% 6%



- Molecule 3: Structural protein

Chain K: 62% 32% 6%



- Molecule 3: Structural protein

Chain L: 71% 22% 6%



- Molecule 3: Structural protein

Chain E: 70% 23% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	87.00Å 153.00Å 255.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.03 – 3.40 98.03 – 3.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (98.03-3.40) 97.7 (98.03-3.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.85 (at 3.41Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.209 , 0.263 0.210 , 0.265	Depositor DCC
R_{free} test set	1634 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	97.6	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17924	wwPDB-VP
Average B, all atoms (Å ²)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.54	0/2145	0.76	1/2915 (0.0%)
1	C	0.64	1/2134 (0.0%)	0.82	3/2900 (0.1%)
1	F	0.62	0/2160	0.78	0/2935
1	I	0.50	0/1764	0.70	0/2396
2	B	0.54	0/852	0.74	0/1152
2	D	0.55	0/852	0.78	0/1152
2	G	0.49	0/852	0.74	0/1152
2	J	0.48	0/757	0.71	0/1020
3	E	0.60	0/1732	0.80	0/2367
3	H	0.57	0/1732	0.80	0/2367
3	K	0.55	0/1732	0.82	0/2367
3	L	0.54	0/1732	0.78	0/2367
All	All	0.56	1/18444 (0.0%)	0.78	4/25090 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	192	ARG	CA-C	7.35	1.62	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	GLU	N-CA-C	-6.31	104.33	111.14
1	C	192	ARG	N-CA-C	5.79	119.60	112.54
1	A	243	GLY	CA-C-O	-5.77	118.25	122.23
1	C	192	ARG	CA-C-O	5.41	126.03	119.38

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	2079	0	1990	54	0
1	C	2069	0	1983	72	0
1	F	2094	0	2001	71	0
1	I	1709	0	1609	64	0
2	B	829	0	791	21	0
2	D	829	0	791	24	0
2	G	829	0	791	24	0
2	J	738	0	706	23	0
3	E	1687	0	1653	32	0
3	H	1687	0	1653	42	0
3	K	1687	0	1653	48	0
3	L	1687	0	1653	38	0
All	All	17924	0	17274	466	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 (466) 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)
2:J:60:LEU:HD11	2:J:101:ARG:HG3	1.37	1.03
3:H:527:ALA:HB3	3:K:530:ASN:ND2	1.82	0.94
3:H:527:ALA:CB	3:K:530:ASN:ND2	2.35	0.90
1:C:208:LYS:HD2	2:D:118:ASP:HA	1.54	0.88
3:L:528:GLN:OE1	3:L:532:LYS:HE2	1.74	0.88
1:F:220:THR:HG21	2:G:118:ASP:HB3	1.56	0.87
1:F:79:GLN:NE2	1:F:192:ARG:HG3	1.90	0.87
2:J:60:LEU:CD1	2:J:101:ARG:HG3	2.05	0.86
1:C:194:ARG:NH2	1:C:197:LEU:HD12	1.91	0.85
1:I:152:GLY:HA2	3:L:512:ILE:HG22	1.59	0.85
1:F:79:GLN:HE21	1:F:192:ARG:HG3	1.45	0.82
1:C:194:ARG:NH2	1:C:197:LEU:CD1	2.42	0.82
1:C:152:GLY:HA2	3:E:512:ILE:HG22	1.61	0.82
1:F:237:ARG:HG3	1:F:242:ALA:HB2	1.60	0.82
3:K:609:VAL:HG11	3:K:612:LYS:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:PRO:HG3	1:C:46:ALA:HB2	1.63	0.80
3:L:433:LYS:HG2	3:L:639:GLU:HG3	1.64	0.77
2:B:27:ILE:HG12	2:B:102:VAL:HG21	1.66	0.77
1:I:150:TRP:CZ2	1:I:174:GLU:HG3	2.20	0.77
1:F:152:GLY:HA2	3:H:512:ILE:CG2	2.16	0.77
2:J:60:LEU:HD11	2:J:101:ARG:CG	2.13	0.76
1:F:152:GLY:HA2	3:H:512:ILE:HG22	1.68	0.75
2:B:44:ASN:HB3	2:B:85:LEU:HD11	1.68	0.75
1:I:82:TRP:CZ3	1:I:86:LYS:HD2	2.22	0.74
1:C:79:GLN:HA	1:C:192:ARG:HH11	1.52	0.74
1:F:145:LEU:HD13	1:F:179:LEU:HD21	1.69	0.72
1:I:254:ASP:HB3	2:J:32:ARG:HH21	1.53	0.72
1:A:275:CYS:HB3	1:A:288:VAL:HB	1.72	0.71
1:A:152:GLY:HA2	3:K:512:ILE:HG22	1.71	0.71
1:A:211:PRO:HA	1:A:217:SER:HA	1.71	0.71
1:A:70:PRO:HG3	1:A:84:TRP:CE2	2.26	0.70
3:H:527:ALA:CB	3:K:530:ASN:HD22	2.05	0.69
1:F:139:GLU:HG2	3:H:512:ILE:HD11	1.74	0.69
1:I:150:TRP:HZ2	1:I:174:GLU:HG3	1.55	0.69
1:F:124:ASP:OD1	1:F:124:ASP:N	2.21	0.68
1:A:249:PHE:HD1	1:A:259:ALA:HB2	1.59	0.68
3:L:435:VAL:HG22	3:L:637:CYS:HB3	1.76	0.67
3:H:512:ILE:HG22	3:H:512:ILE:O	1.94	0.67
1:I:180:PHE:HD1	1:C:172:ASN:HD22	1.43	0.67
3:L:446:ALA:HB3	3:L:449:LYS:HG3	1.75	0.67
2:G:32:ARG:HB2	2:G:42:PHE:HB2	1.77	0.67
1:C:79:GLN:HA	1:C:192:ARG:NH1	2.10	0.67
1:C:219:LEU:HD21	1:C:270:GLU:HB3	1.77	0.66
2:G:84:LEU:HD13	2:G:86:TYR:HE1	1.60	0.66
2:D:44:ASN:HB3	2:D:85:LEU:HD11	1.78	0.66
1:F:40:PRO:HG3	1:F:46:ALA:HB2	1.78	0.65
1:I:201:GLU:OE2	1:I:225:SER:HB3	1.95	0.65
3:H:531:ASN:HD21	3:K:600:MET:H	1.42	0.65
2:D:93:THR:HG23	2:D:96:ASP:OD2	1.96	0.65
2:J:32:ARG:HD3	2:J:42:PHE:HB2	1.78	0.65
3:H:630:LEU:HD13	3:H:634:THR:HG21	1.76	0.65
1:C:140:PHE:CE2	1:C:141:MET:HE3	2.32	0.65
1:I:141:MET:HE2	1:I:150:TRP:HB3	1.78	0.65
3:K:433:LYS:HE2	3:K:639:GLU:OE2	1.95	0.65
1:C:105:LEU:HD23	1:C:111:TYR:CD2	2.32	0.64
1:I:133:PHE:HB2	1:I:141:MET:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:468:ILE:HG21	3:H:539:PHE:CD2	2.33	0.64
3:L:433:LYS:HE2	3:L:639:GLU:OE2	1.97	0.64
1:F:135:LEU:HD23	1:F:156:GLU:HG3	1.80	0.63
1:I:179:LEU:HD11	1:C:175:LEU:HD22	1.79	0.63
3:K:534:GLN:NE2	3:K:618:HIS:O	2.31	0.63
1:I:175:LEU:O	1:I:179:LEU:HB2	1.99	0.63
3:K:510:VAL:HG23	3:K:515:LYS:HG3	1.81	0.63
1:C:278:GLN:HG2	1:C:285:PRO:HB3	1.81	0.62
3:E:630:LEU:HD13	3:E:634:THR:HG21	1.82	0.62
1:C:31:LEU:HD23	1:C:118:GLY:HA3	1.82	0.61
2:D:59:LEU:HD13	2:D:88:THR:HG22	1.81	0.61
1:I:62:ASN:HD21	1:I:65:ARG:HB2	1.65	0.61
2:G:44:ASN:HB3	2:G:85:LEU:HD11	1.81	0.61
1:I:49:VAL:HG21	1:I:91:LEU:HD22	1.82	0.61
3:H:573:GLY:HA2	3:H:613:THR:HG21	1.82	0.61
1:I:82:TRP:HZ3	1:I:86:LYS:HD2	1.64	0.61
3:L:528:GLN:NE2	3:L:595:ILE:CD1	2.64	0.61
1:A:31:LEU:HD23	1:A:118:GLY:HA3	1.84	0.60
2:G:84:LEU:HD13	2:G:86:TYR:CE1	2.36	0.60
2:B:60:LEU:HD12	2:B:112:ILE:HD11	1.84	0.60
3:K:624:VAL:HB	3:L:624:VAL:HB	1.82	0.59
3:E:503:ILE:HD12	3:E:518:VAL:HG12	1.85	0.59
1:A:278:GLN:HG2	1:A:285:PRO:HB3	1.83	0.59
1:F:83:TYR:OH	1:F:189:HIS:NE2	2.27	0.59
2:D:61:LYS:HD3	2:D:98:TYR:CE1	2.37	0.59
1:F:254:ASP:OD1	2:G:32:ARG:NH1	2.36	0.59
1:F:254:ASP:CG	2:G:32:ARG:HH12	2.10	0.59
3:H:431:GLU:HG3	3:H:641:LEU:HD23	1.84	0.59
1:C:232:GLN:NE2	1:C:278:GLN:OE1	2.36	0.59
1:F:133:PHE:HB2	1:F:141:MET:HB3	1.84	0.58
1:I:179:LEU:CD1	1:C:175:LEU:HD22	2.33	0.58
1:I:93:ILE:HG21	1:I:173:LYS:HD3	1.85	0.58
1:I:203:PRO:HD3	1:I:279:HIS:CD2	2.38	0.58
1:A:167:GLN:HB2	1:A:170:ALA:HB2	1.84	0.58
3:K:503:ILE:HD12	3:K:518:VAL:HG12	1.83	0.58
2:B:59:LEU:HD13	2:B:88:THR:HG22	1.85	0.58
2:G:49:GLY:HA2	2:G:81:SER:OG	2.03	0.58
1:C:80:VAL:H	1:C:192:ARG:HH12	1.52	0.58
1:I:135:LEU:HB2	1:I:140:PHE:CE1	2.39	0.58
3:L:493:ASP:OD1	3:L:493:ASP:N	2.36	0.58
1:C:210:ARG:HB3	1:C:218:VAL:HG13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:57:VAL:HG22	2:G:102:VAL:HG22	1.86	0.57
1:C:231:LEU:HD12	1:C:279:HIS:HB2	1.86	0.57
1:F:245:GLY:HA3	1:F:262:SER:O	2.05	0.57
2:G:33:HIS:O	2:G:41:ASN:ND2	2.30	0.57
2:D:84:LEU:HD13	2:D:86:TYR:HE1	1.67	0.57
1:A:156:GLU:CD	1:A:156:GLU:H	2.12	0.57
3:L:534:GLN:NE2	3:L:618:HIS:O	2.31	0.57
3:H:502:PRO:HG3	3:H:519:TYR:CZ	2.40	0.56
1:C:83:TYR:HE1	1:C:185:ARG:HG3	1.70	0.56
1:I:175:LEU:HD11	1:C:179:LEU:HD13	1.86	0.56
1:I:220:THR:HA	1:I:261:SER:O	2.04	0.56
1:A:133:PHE:CD2	1:A:141:MET:HE3	2.41	0.56
1:A:155:PRO:HA	1:A:158:LEU:HD12	1.88	0.56
3:K:508:VAL:HB	3:K:516:ALA:HB3	1.86	0.56
1:C:141:MET:HE1	1:C:160:ILE:HB	1.88	0.56
2:D:61:LYS:HD3	2:D:98:TYR:HE1	1.71	0.56
2:J:32:ARG:HB2	2:J:42:PHE:HB2	1.88	0.56
1:A:83:TYR:HE1	1:A:185:ARG:HG3	1.72	0.55
1:A:40:PRO:HG3	1:A:46:ALA:HB2	1.87	0.55
1:F:167:GLN:HG3	1:F:168:ASP:H	1.69	0.55
3:E:434:VAL:O	3:E:637:CYS:HA	2.06	0.55
1:A:208:LYS:HD2	2:B:118:ASP:HA	1.87	0.55
3:H:518:VAL:HG22	3:H:541:VAL:HG12	1.89	0.55
2:J:44:ASN:HB3	2:J:85:LEU:HD11	1.88	0.55
3:H:467:LYS:HB3	3:H:475:TYR:HD2	1.71	0.55
2:B:27:ILE:HG13	2:B:47:VAL:HG13	1.87	0.55
3:K:609:VAL:CG1	3:K:612:LYS:HE3	2.33	0.55
1:F:237:ARG:HG2	1:F:273:TYR:CZ	2.42	0.55
3:L:528:GLN:HE22	3:L:595:ILE:CD1	2.19	0.54
2:B:75:SER:HB2	2:B:83:TYR:CZ	2.41	0.54
1:A:155:PRO:HD2	1:A:156:GLU:OE2	2.07	0.54
1:I:179:LEU:HD13	1:C:175:LEU:HD13	1.88	0.54
2:J:27:ILE:HG12	2:J:102:VAL:HG21	1.89	0.54
1:A:32:TYR:HE1	1:A:59:LEU:HD13	1.71	0.54
3:L:532:LYS:HG2	3:L:597:ASP:OD1	2.08	0.54
2:D:41:ASN:HB3	2:D:90:PHE:CE1	2.43	0.54
1:F:32:TYR:OH	1:F:87:GLU:OE2	2.26	0.54
1:A:105:LEU:HD21	1:A:135:LEU:HD21	1.90	0.54
1:A:184:HIS:NE2	1:A:188:GLU:OE2	2.41	0.54
3:H:433:LYS:HE2	3:H:639:GLU:OE2	2.08	0.54
1:C:189:HIS:O	1:C:193:GLY:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:479:GLN:NE2	3:K:611:LEU:HG	2.23	0.54
3:H:434:VAL:O	3:H:637:CYS:HA	2.08	0.53
3:H:494:PHE:HB3	3:E:494:PHE:HB3	1.90	0.53
3:K:434:VAL:O	3:K:637:CYS:HA	2.08	0.53
1:I:40:PRO:HG3	1:I:46:ALA:HB2	1.88	0.53
1:C:59:LEU:HD21	1:C:91:LEU:HD11	1.88	0.53
1:C:235:PHE:CG	1:C:263:LEU:HD22	2.43	0.53
1:A:140:PHE:CD2	1:A:157:ALA:HB2	2.43	0.53
1:C:144:ASP:OD2	1:C:147:GLN:HB2	2.08	0.53
3:E:433:LYS:HE3	3:E:492:ILE:CD1	2.38	0.53
1:F:38:SER:HB3	1:F:111:TYR:HB2	1.89	0.53
1:C:67:GLU:HA	1:C:88:THR:CG2	2.39	0.53
3:E:433:LYS:HE3	3:E:492:ILE:HD12	1.90	0.53
2:B:49:GLY:HA2	2:B:81:SER:OG	2.08	0.53
1:I:70:PRO:HB3	1:I:84:TRP:CZ2	2.44	0.53
3:H:512:ILE:CG2	3:H:512:ILE:O	2.56	0.53
1:F:237:ARG:HG2	1:F:273:TYR:CE2	2.44	0.53
1:I:28:LEU:HG	1:I:190:LEU:HD11	1.90	0.53
3:K:510:VAL:CG2	3:K:515:LYS:HG3	2.39	0.53
2:D:49:GLY:HA2	2:D:81:SER:OG	2.09	0.53
3:L:468:ILE:HG21	3:L:539:PHE:CD2	2.43	0.52
1:I:83:TYR:HD2	1:I:84:TRP:CD1	2.28	0.52
1:F:212:SER:H	1:F:217:SER:HA	1.73	0.52
1:A:156:GLU:OE1	3:K:472:VAL:HG22	2.10	0.52
2:D:77:SER:HB3	2:D:78:LYS:HE2	1.91	0.52
2:B:43:LEU:O	2:B:87:TYR:HA	2.10	0.52
1:F:286:LEU:HD22	1:F:287:ARG:H	1.74	0.52
1:F:138:GLU:OE2	3:H:475:TYR:CZ	2.63	0.52
1:C:194:ARG:NH2	1:C:197:LEU:HD13	2.23	0.52
1:F:202:PRO:HB3	1:F:281:GLY:HA3	1.91	0.52
1:I:62:ASN:N	1:I:62:ASN:HD22	2.07	0.52
3:K:446:ALA:O	3:K:629:PRO:HG2	2.10	0.52
3:L:508:VAL:HB	3:L:516:ALA:HB3	1.91	0.52
2:D:90:PHE:CD2	2:D:98:TYR:CE2	2.98	0.52
1:F:135:LEU:HB2	1:F:140:PHE:CE1	2.45	0.51
2:J:112:ILE:HG12	2:J:113:VAL:N	2.25	0.51
3:H:564:ASP:OD1	3:H:564:ASP:N	2.35	0.51
3:K:545:THR:HA	3:K:584:GLN:HE21	1.75	0.51
3:K:601:PRO:HG2	3:K:605:VAL:HG22	1.93	0.51
3:L:493:ASP:OD2	3:L:495:GLN:HG2	2.10	0.51
1:I:146:LYS:HE3	1:C:146:LYS:HE3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:479:GLN:CD	3:K:611:LEU:HG	2.36	0.51
1:A:219:LEU:O	1:A:262:SER:HA	2.11	0.51
2:J:60:LEU:HD11	2:J:101:ARG:CD	2.39	0.51
2:B:61:LYS:HD3	2:B:98:TYR:CE2	2.46	0.51
1:I:232:GLN:HB2	1:I:278:GLN:HB2	1.93	0.51
1:C:216:PHE:HD2	1:C:264:THR:HG22	1.75	0.51
1:A:87:GLU:OE2	1:A:185:ARG:HD3	2.11	0.51
3:H:436:LEU:HD22	3:H:484:ILE:HG21	1.93	0.51
1:C:80:VAL:H	1:C:192:ARG:NH1	2.09	0.51
1:A:150:TRP:CZ2	1:A:174:GLU:HG3	2.46	0.50
3:K:433:LYS:HG2	3:K:639:GLU:HG3	1.93	0.50
1:I:87:GLU:OE2	1:I:185:ARG:HD3	2.12	0.50
1:C:67:GLU:HA	1:C:88:THR:HG23	1.93	0.50
3:E:433:LYS:HE2	3:E:639:GLU:OE2	2.12	0.50
1:F:80:VAL:HG23	1:F:83:TYR:H	1.76	0.50
1:C:133:PHE:HB2	1:C:141:MET:HB3	1.93	0.50
1:C:135:LEU:HD23	1:C:156:GLU:HG3	1.93	0.50
3:E:518:VAL:HG22	3:E:541:VAL:HG12	1.94	0.50
2:B:74:LEU:HD23	2:B:84:LEU:HG	1.93	0.50
1:F:138:GLU:OE2	3:H:467:LYS:NZ	2.44	0.50
1:I:59:LEU:HD23	1:I:60:SER:N	2.27	0.50
1:C:194:ARG:HH22	1:C:197:LEU:HD13	1.75	0.50
1:I:180:PHE:C	1:I:183:PRO:HD2	2.37	0.50
1:F:180:PHE:C	1:F:183:PRO:HD2	2.37	0.49
1:I:221:CYS:O	1:I:260:SER:HA	2.11	0.49
1:C:88:THR:O	1:C:92:ARG:HG3	2.12	0.49
1:F:49:VAL:HG21	1:F:91:LEU:HD22	1.93	0.49
1:C:94:LYS:NZ	1:C:177:PHE:HD2	2.10	0.49
1:C:237:ARG:HB2	1:C:242:ALA:HB2	1.94	0.49
3:E:457:LEU:HG	3:E:610:GLU:HB3	1.94	0.49
1:A:28:LEU:HD12	1:A:190:LEU:HD11	1.94	0.49
3:E:522:LYS:HD2	3:E:523:GLN:H	1.77	0.49
1:I:152:GLY:CA	3:L:512:ILE:HG22	2.37	0.49
2:D:36:GLU:OE1	2:D:39:LYS:HD2	2.13	0.49
2:J:59:LEU:HD13	2:J:88:THR:HG22	1.95	0.49
3:L:522:LYS:HD2	3:L:523:GLN:H	1.77	0.49
2:G:60:LEU:HD21	2:G:101:ARG:NH2	2.27	0.49
2:D:65:ARG:NH2	2:D:67:GLU:HG2	2.27	0.49
3:E:558:ARG:HD2	3:E:567:THR:HG23	1.95	0.49
3:K:466:VAL:HB	3:K:478:MET:HB3	1.94	0.49
1:C:93:ILE:HD13	1:C:173:LYS:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:VAL:HG23	1:A:83:TYR:HB2	1.95	0.49
1:F:124:ASP:O	1:F:125:ASN:ND2	2.46	0.49
1:C:100:GLU:O	1:C:103:LYS:HB2	2.13	0.49
1:F:32:TYR:CE1	1:F:177:PHE:HZ	2.31	0.48
1:F:260:SER:OG	2:G:119:MET:HG3	2.11	0.48
3:H:527:ALA:HB3	3:K:530:ASN:HD21	1.71	0.48
1:F:30:LEU:HB2	1:F:186:LEU:HD13	1.95	0.48
2:J:33:HIS:HB2	2:J:41:ASN:HD21	1.78	0.48
1:C:194:ARG:HH22	1:C:197:LEU:CD1	2.23	0.48
3:E:460:PRO:HD2	3:E:550:ASN:O	2.12	0.48
1:F:153:ASP:HB2	3:H:509:LEU:HD21	1.95	0.48
2:J:101:ARG:HG2	2:J:112:ILE:HB	1.94	0.48
1:C:150:TRP:CE2	1:C:164:TRP:HE3	2.31	0.48
1:F:237:ARG:HG3	1:F:242:ALA:CB	2.40	0.48
2:J:84:LEU:HD23	2:J:84:LEU:HA	1.68	0.48
3:E:510:VAL:HG23	3:E:515:LYS:HG3	1.96	0.48
3:K:503:ILE:CG2	3:K:506:LEU:HD23	2.44	0.48
1:C:80:VAL:HG11	1:C:82:TRP:CH2	2.48	0.48
1:F:229:PRO:HB3	1:F:257:PHE:CZ	2.49	0.47
1:I:143:PHE:CE2	1:I:175:LEU:HD22	2.49	0.47
1:C:53:LEU:HD13	1:C:53:LEU:HA	1.74	0.47
2:D:42:PHE:CE2	2:D:89:GLU:HG2	2.49	0.47
1:A:133:PHE:HE2	1:A:150:TRP:HD1	1.60	0.47
1:C:85:GLU:O	1:C:89:THR:HG23	2.14	0.47
3:L:531:ASN:HB2	3:L:598:GLY:H	1.80	0.47
1:F:101:ALA:HB1	1:F:160:ILE:HD13	1.95	0.47
1:F:265:VAL:HG11	1:F:273:TYR:CE2	2.49	0.47
1:C:177:PHE:HA	1:C:181:SER:HB3	1.96	0.47
1:F:209:ALA:HB2	1:F:290:LEU:HD23	1.97	0.47
1:C:34:LEU:CD1	1:C:117:LEU:HD12	2.44	0.47
2:G:27:ILE:HG12	2:G:102:VAL:HG21	1.95	0.47
1:I:88:THR:O	1:I:92:ARG:HG3	2.14	0.47
2:B:58:ASP:HB3	2:B:65:ARG:HG2	1.97	0.47
2:D:58:ASP:HB3	2:D:65:ARG:HG2	1.97	0.47
1:I:147:GLN:HB3	1:I:149:THR:HG22	1.95	0.47
3:H:491:THR:HG23	3:H:495:GLN:O	2.15	0.47
1:A:70:PRO:HG3	1:A:84:TRP:CZ2	2.50	0.46
1:A:226:PHE:O	1:A:257:PHE:N	2.47	0.46
1:I:80:VAL:H	1:I:192:ARG:HH21	1.64	0.46
3:K:503:ILE:HG22	3:K:506:LEU:HD23	1.98	0.46
3:L:502:PRO:HG3	3:L:519:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:GLU:HG2	3:K:512:ILE:HD11	1.96	0.46
1:A:278:GLN:CG	1:A:285:PRO:HB3	2.45	0.46
1:F:59:LEU:HD23	1:F:60:SER:N	2.29	0.46
1:C:105:LEU:HD23	1:C:111:TYR:CE2	2.50	0.46
3:E:508:VAL:HB	3:E:516:ALA:HB3	1.96	0.46
2:B:76:PHE:C	2:B:83:TYR:HE1	2.24	0.46
1:C:121:LEU:HD22	1:C:186:LEU:HD23	1.96	0.46
3:L:528:GLN:NE2	3:L:595:ILE:HD12	2.30	0.46
1:C:80:VAL:HG22	1:C:192:ARG:HH12	1.81	0.46
1:C:94:LYS:NZ	1:C:177:PHE:CD2	2.80	0.46
1:C:105:LEU:HD12	1:C:105:LEU:HA	1.61	0.46
1:F:156:GLU:CD	1:F:156:GLU:H	2.23	0.46
1:F:266:LYS:HE3	1:F:266:LYS:HB2	1.41	0.46
1:I:154:TRP:CE2	3:L:509:LEU:HD13	2.50	0.46
3:H:433:LYS:HG2	3:H:639:GLU:HG3	1.96	0.46
3:E:446:ALA:O	3:E:629:PRO:HG2	2.16	0.46
3:K:502:PRO:HG3	3:K:519:TYR:CZ	2.51	0.46
1:I:77:GLU:OE2	1:I:79:GLN:OE1	2.34	0.46
3:H:508:VAL:HB	3:H:516:ALA:HB3	1.98	0.46
3:K:543:VAL:HG12	3:K:584:GLN:HA	1.98	0.46
1:I:80:VAL:N	1:I:192:ARG:HH21	2.13	0.46
1:C:234:ARG:HA	1:C:244:THR:HG22	1.97	0.46
1:A:150:TRP:HZ2	1:A:174:GLU:HG3	1.79	0.46
1:A:207:LEU:HB2	1:A:288:VAL:HG12	1.98	0.46
2:J:46:TYR:HE1	2:J:83:TYR:HD2	1.64	0.46
1:C:276:ILE:HD12	1:C:287:ARG:HG2	1.98	0.46
1:A:277:VAL:CG1	1:A:286:LEU:HB2	2.46	0.45
3:E:455:LYS:HE2	3:E:611:LEU:O	2.17	0.45
1:F:83:TYR:HD2	1:F:84:TRP:CD1	2.35	0.45
3:H:466:VAL:HB	3:H:478:MET:HB3	1.98	0.45
3:L:528:GLN:HE22	3:L:595:ILE:HD11	1.81	0.45
3:L:553:LEU:HD21	3:L:580:ILE:HD11	1.97	0.45
1:I:105:LEU:HD23	1:I:111:TYR:CD2	2.51	0.45
3:H:503:ILE:HD12	3:H:518:VAL:HG12	1.97	0.45
1:F:155:PRO:HD2	1:F:156:GLU:OE2	2.16	0.45
1:I:62:ASN:ND2	1:I:65:ARG:HB2	2.31	0.45
1:C:29:SER:HB3	1:C:120:GLU:HG3	1.98	0.45
3:L:611:LEU:HA	3:L:611:LEU:HD23	1.83	0.45
1:A:33:HIS:HB2	1:A:50:SER:OG	2.16	0.45
1:I:83:TYR:CD2	1:I:84:TRP:CD1	3.05	0.45
3:K:550:ASN:HA	3:K:578:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:457:LEU:HG	3:L:610:GLU:HB3	1.99	0.45
1:C:210:ARG:HH21	2:D:118:ASP:HB2	1.81	0.45
1:F:180:PHE:O	1:F:183:PRO:HD2	2.16	0.45
2:G:59:LEU:HD13	2:G:88:THR:HG22	1.98	0.45
1:C:193:GLY:O	1:C:197:LEU:HG	2.17	0.45
1:A:94:LYS:HA	1:A:94:LYS:HD3	1.77	0.45
1:A:105:LEU:HD23	1:A:111:TYR:CE2	2.52	0.45
2:J:100:CYS:O	2:J:112:ILE:HA	2.17	0.45
3:H:600:MET:HE3	3:H:605:VAL:HG21	1.98	0.45
3:K:460:PRO:HA	3:K:552:TYR:OH	2.16	0.45
3:H:503:ILE:HG21	3:H:506:LEU:HD23	1.99	0.44
3:E:521:VAL:HG23	3:E:641:LEU:HD12	1.99	0.44
3:E:529:THR:HG23	3:E:532:LYS:HB2	1.99	0.44
1:A:182:CYS:HB3	1:A:183:PRO:HD3	1.99	0.44
1:A:253:SER:HB3	2:B:85:LEU:HD23	2.00	0.44
2:B:84:LEU:HA	2:B:84:LEU:HD23	1.71	0.44
1:F:192:ARG:H	1:F:192:ARG:HG2	1.36	0.44
3:K:460:PRO:HD2	3:K:550:ASN:O	2.17	0.44
2:G:75:SER:HB2	2:G:83:TYR:CZ	2.52	0.44
1:I:72:GLY:O	1:I:75:VAL:HG12	2.17	0.44
1:I:219:LEU:O	1:I:262:SER:HA	2.16	0.44
1:C:59:LEU:HD23	1:C:60:SER:N	2.32	0.44
3:E:543:VAL:HG12	3:E:584:GLN:HA	1.98	0.44
1:A:247:GLY:HA2	1:A:261:SER:HA	1.99	0.44
1:F:199:TRP:CD1	1:F:200:LYS:N	2.86	0.44
3:H:618:HIS:HA	3:E:628:MET:HE1	1.98	0.44
1:I:141:MET:HE2	1:I:150:TRP:CB	2.46	0.44
3:E:450:GLN:HG3	3:E:555:TYR:CG	2.52	0.44
2:B:94:GLU:CD	2:B:94:GLU:N	2.75	0.44
1:F:28:LEU:HD13	1:F:28:LEU:HA	1.83	0.44
2:G:42:PHE:CE2	2:G:89:GLU:HG2	2.53	0.44
2:J:49:GLY:HA2	2:J:81:SER:OG	2.17	0.44
1:A:55:PRO:HG2	1:A:227:TYR:OH	2.18	0.43
1:F:141:MET:N	3:H:512:ILE:HD13	2.32	0.43
1:F:231:LEU:HD12	1:F:279:HIS:HB2	1.99	0.43
1:I:180:PHE:O	1:I:183:PRO:HD2	2.17	0.43
3:K:493:ASP:OD2	3:K:495:GLN:HG2	2.18	0.43
1:A:147:GLN:O	1:A:149:THR:HG22	2.18	0.43
1:F:121:LEU:HD23	1:F:186:LEU:HD23	1.99	0.43
2:G:33:HIS:C	2:G:41:ASN:HD21	2.23	0.43
1:I:116:LEU:HD12	1:I:116:LEU:HA	1.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:HD2	1:C:84:TRP:CD1	2.36	0.43
2:D:49:GLY:HA2	2:D:81:SER:CB	2.48	0.43
1:A:117:LEU:HD23	1:A:131:ALA:HA	2.00	0.43
2:B:45:CYS:HB2	2:B:59:LEU:HD21	2.00	0.43
1:I:154:TRP:CZ3	3:L:472:VAL:HA	2.53	0.43
3:H:619:MET:CG	3:E:628:MET:HB2	2.48	0.43
3:K:566:THR:HG23	3:L:449:LYS:HA	2.00	0.43
2:D:60:LEU:HD23	2:D:64:GLU:C	2.44	0.43
1:A:207:LEU:HB3	1:A:290:LEU:HA	2.01	0.43
1:F:150:TRP:HZ2	1:F:174:GLU:HG3	1.83	0.43
1:F:210:ARG:O	1:F:218:VAL:N	2.49	0.43
1:I:181:SER:O	1:I:185:ARG:HB2	2.19	0.43
3:K:493:ASP:OD1	3:K:493:ASP:N	2.51	0.43
1:I:105:LEU:HD12	1:I:105:LEU:HA	1.91	0.43
3:K:468:ILE:HG21	3:K:539:PHE:CD2	2.54	0.43
3:E:621:LYS:O	3:E:621:LYS:HG3	2.19	0.43
1:F:141:MET:HE3	1:F:157:ALA:HA	2.00	0.43
3:K:433:LYS:HG2	3:K:639:GLU:CG	2.48	0.43
3:K:469:ALA:HB2	3:K:475:TYR:HB2	2.00	0.43
1:A:249:PHE:CD1	1:A:259:ALA:HB2	2.47	0.43
1:F:290:LEU:HD12	1:F:290:LEU:H	1.84	0.43
2:G:84:LEU:HA	2:G:84:LEU:HD23	1.71	0.43
1:I:79:GLN:HA	1:I:192:ARG:HH21	1.84	0.43
1:I:143:PHE:HE2	1:I:175:LEU:HD22	1.84	0.43
2:J:43:LEU:HD11	2:J:115:TRP:CG	2.53	0.43
1:C:121:LEU:HD13	1:C:121:LEU:HA	1.66	0.43
2:D:84:LEU:HD13	2:D:86:TYR:CE1	2.51	0.43
1:I:228:PRO:HD2	1:I:279:HIS:CE1	2.53	0.43
3:L:528:GLN:OE1	3:L:595:ILE:HD12	2.18	0.43
3:E:535:VAL:HG11	3:E:605:VAL:HB	2.00	0.43
3:H:435:VAL:HG22	3:H:637:CYS:HB3	2.01	0.43
3:K:518:VAL:HG22	3:K:541:VAL:HG12	2.01	0.43
1:C:105:LEU:HD13	1:C:160:ILE:HD11	2.00	0.43
1:A:172:ASN:OD1	1:A:172:ASN:N	2.51	0.42
1:I:184:HIS:O	1:I:188:GLU:HG2	2.19	0.42
1:I:224:PHE:HB3	2:J:32:ARG:O	2.19	0.42
3:K:549:VAL:O	3:K:579:GLY:HA2	2.18	0.42
3:H:537:SER:O	3:H:591:THR:HA	2.19	0.42
3:K:476:LEU:HA	3:K:608:ASN:OD1	2.19	0.42
1:C:58:TYR:O	1:C:71:CYS:N	2.52	0.42
3:E:532:LYS:HE3	3:E:532:LYS:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LEU:HA	1:F:186:LEU:HD12	1.75	0.42
3:H:550:ASN:HA	3:H:578:ALA:O	2.19	0.42
1:C:79:GLN:HG2	1:C:83:TYR:CD2	2.55	0.42
1:F:53:LEU:HD13	1:F:53:LEU:HA	1.57	0.42
1:F:119:CYS:HA	1:F:128:VAL:O	2.20	0.42
1:F:207:LEU:HD13	1:F:275:CYS:HB2	2.01	0.42
1:I:45:PRO:HD3	1:I:64:LEU:HD11	2.00	0.42
2:J:21:ILE:HD13	2:J:23:ARG:HE	1.84	0.42
3:K:636:MET:HE3	3:K:636:MET:HB3	1.87	0.42
3:L:460:PRO:HG3	3:L:552:TYR:CE1	2.55	0.42
3:L:480:GLY:O	3:L:590:LEU:HA	2.18	0.42
3:L:528:GLN:CD	3:L:595:ILE:HD12	2.45	0.42
3:L:636:MET:HE3	3:L:636:MET:HB3	1.70	0.42
3:E:503:ILE:CG2	3:E:506:LEU:HD23	2.49	0.42
1:A:237:ARG:HG3	1:A:240:LEU:HB2	2.01	0.42
1:I:224:PHE:HB3	2:J:33:HIS:HA	2.00	0.42
3:H:558:ARG:O	3:E:557:TYR:HB2	2.19	0.42
3:L:446:ALA:O	3:L:629:PRO:HG2	2.19	0.42
1:F:167:GLN:HG3	1:F:168:ASP:N	2.34	0.42
1:F:254:ASP:CG	2:G:32:ARG:NH1	2.75	0.42
2:G:43:LEU:HD12	2:G:43:LEU:HA	1.75	0.42
1:C:193:GLY:HA2	1:C:196:ASN:HD22	1.85	0.42
1:A:235:PHE:O	1:A:236:LEU:HD23	2.18	0.42
3:H:503:ILE:CG2	3:H:506:LEU:HD23	2.49	0.42
1:C:256:SER:OG	1:C:257:PHE:N	2.52	0.42
2:D:39:LYS:O	2:D:92:PRO:HD2	2.19	0.42
3:K:453:VAL:HG12	3:K:480:GLY:HA2	2.02	0.42
3:L:507:GLN:OE1	3:L:514:LYS:HD3	2.20	0.42
1:I:94:LYS:NZ	1:I:174:GLU:HG2	2.35	0.42
1:I:146:LYS:O	1:C:128:VAL:HG13	2.20	0.42
1:A:33:HIS:O	1:A:49:VAL:HA	2.19	0.41
3:H:624:VAL:HB	3:E:624:VAL:HB	2.01	0.41
3:K:470:LYS:HA	3:K:505:GLY:O	2.20	0.41
3:L:472:VAL:H	3:L:472:VAL:HG22	1.63	0.41
1:A:28:LEU:HD23	1:A:28:LEU:HA	1.87	0.41
1:A:105:LEU:HD23	1:A:111:TYR:CD2	2.55	0.41
1:F:101:ALA:HB1	1:F:160:ILE:CD1	2.51	0.41
2:G:61:LYS:HG3	2:G:98:TYR:CE1	2.54	0.41
1:I:256:SER:OG	1:I:257:PHE:N	2.52	0.41
2:B:22:GLN:HA	2:B:51:HIS:O	2.20	0.41
1:F:32:TYR:CD1	1:F:177:PHE:HZ	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:GLU:HG2	1:F:79:GLN:HG2	2.02	0.41
2:J:84:LEU:HD13	2:J:86:TYR:CE1	2.56	0.41
3:H:628:MET:HE2	3:H:628:MET:HB3	1.72	0.41
3:L:555:TYR:CZ	3:L:572:ARG:HD3	2.54	0.41
1:F:105:LEU:HD21	1:F:135:LEU:HD21	2.02	0.41
3:L:528:GLN:OE1	3:L:532:LYS:CE	2.57	0.41
1:C:34:LEU:HD11	1:C:117:LEU:HD12	2.03	0.41
2:D:90:PHE:HD2	2:D:98:TYR:CE2	2.36	0.41
3:E:436:LEU:HD22	3:E:484:ILE:HG21	2.03	0.41
2:G:54:ASP:OD1	2:G:54:ASP:N	2.48	0.41
1:C:140:PHE:CZ	1:C:141:MET:HE3	2.54	0.41
1:A:206:ARG:HD3	1:A:206:ARG:HA	1.61	0.41
2:G:74:LEU:HA	2:G:74:LEU:HD23	1.56	0.41
2:D:59:LEU:HD13	2:D:88:THR:CG2	2.50	0.41
2:B:62:ASN:HD21	2:B:96:ASP:HB3	1.86	0.41
1:F:105:LEU:HD12	1:F:105:LEU:HA	1.74	0.41
3:K:529:THR:HG23	3:K:532:LYS:HB2	2.02	0.41
3:L:469:ALA:HA	3:L:475:TYR:HA	2.03	0.41
3:K:556:PHE:CE1	3:K:571:VAL:HG22	2.56	0.41
2:B:78:LYS:H	2:B:78:LYS:HG2	1.35	0.40
3:E:466:VAL:HB	3:E:478:MET:HB3	2.02	0.40
1:F:62:ASN:ND2	1:F:64:LEU:HB2	2.36	0.40
1:I:100:GLU:OE2	1:I:163:ARG:NH1	2.50	0.40
1:A:53:LEU:HD22	1:A:58:TYR:CD1	2.56	0.40
1:F:37:VAL:HG23	1:F:40:PRO:HB3	2.04	0.40
1:I:254:ASP:HB3	2:J:32:ARG:NH2	2.28	0.40
1:C:150:TRP:HZ2	1:C:174:GLU:HG3	1.86	0.40
1:C:279:HIS:CD2	1:C:280:ALA:H	2.39	0.40
2:D:22:GLN:HG2	2:D:106:THR:CG2	2.51	0.40
2:D:49:GLY:HA2	2:D:81:SER:HB2	2.04	0.40
1:A:290:LEU:H	1:A:290:LEU:HD12	1.87	0.40
2:B:43:LEU:HD23	2:B:59:LEU:HD22	2.03	0.40
1:F:252:ASN:HB2	1:F:256:SER:O	2.21	0.40
2:G:116:ASP:OD2	2:G:118:ASP:HB2	2.21	0.40
1:C:83:TYR:CD2	1:C:83:TYR:C	2.99	0.40
1:A:237:ARG:HB3	1:A:273:TYR:CE1	2.56	0.40
1:F:77:GLU:CD	1:F:79:GLN:HG2	2.47	0.40
1:I:74:TRP:HA	1:I:77:GLU:HG2	2.03	0.40
3:K:478:MET:HG3	3:K:590:LEU:HB3	2.04	0.40
3:K:522:LYS:HD2	3:K:523:GLN:H	1.87	0.40
3:E:523:GLN:HE21	3:E:523:GLN:HB3	1.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/278 (94%)	249 (95%)	12 (5%)	1 (0%)	30	59
1	C	261/278 (94%)	254 (97%)	7 (3%)	0	100	100
1	F	264/278 (95%)	252 (96%)	12 (4%)	0	100	100
1	I	207/278 (74%)	199 (96%)	8 (4%)	0	100	100
2	B	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	D	97/99 (98%)	94 (97%)	3 (3%)	0	100	100
2	G	97/99 (98%)	93 (96%)	4 (4%)	0	100	100
2	J	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
3	E	213/228 (93%)	206 (97%)	7 (3%)	0	100	100
3	H	213/228 (93%)	203 (95%)	10 (5%)	0	100	100
3	K	213/228 (93%)	205 (96%)	8 (4%)	0	100	100
3	L	213/228 (93%)	206 (97%)	6 (3%)	1 (0%)	24	54
All	All	2218/2420 (92%)	2132 (96%)	84 (4%)	2 (0%)	48	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	PRO
3	L	602	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/230 (95%)	198 (91%)	20 (9%)	8	29
1	C	217/230 (94%)	191 (88%)	26 (12%)	5	19
1	F	220/230 (96%)	198 (90%)	22 (10%)	7	26
1	I	179/230 (78%)	155 (87%)	24 (13%)	4	15
2	B	94/94 (100%)	82 (87%)	12 (13%)	4	17
2	D	94/94 (100%)	83 (88%)	11 (12%)	5	20
2	G	94/94 (100%)	80 (85%)	14 (15%)	3	12
2	J	84/94 (89%)	75 (89%)	9 (11%)	6	23
3	E	187/195 (96%)	176 (94%)	11 (6%)	18	44
3	H	187/195 (96%)	176 (94%)	11 (6%)	18	44
3	K	187/195 (96%)	174 (93%)	13 (7%)	14	40
3	L	187/195 (96%)	178 (95%)	9 (5%)	23	50
All	All	1948/2076 (94%)	1766 (91%)	182 (9%)	8	29

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	LEU
1	A	76	TRP
1	A	77	GLU
1	A	79	GLN
1	A	121	LEU
1	A	124	ASP
1	A	125	ASN
1	A	127	SER
1	A	156	GLU
1	A	176	THR
1	A	190	LEU
1	A	192	ARG
1	A	200	LYS
1	A	206	ARG
1	A	213	SER
1	A	240	LEU
1	A	244	THR
1	A	256	SER
1	A	289	GLU

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Mol	Chain	Res	Type
1	A	290	LEU
2	B	28	GLN
2	B	48	SER
2	B	53	SER
2	B	54	ASP
2	B	70	GLU
2	B	75	SER
2	B	78	LYS
2	B	93	THR
2	B	94	GLU
2	B	96	ASP
2	B	112	ILE
2	B	116	ASP
1	F	28	LEU
1	F	31	LEU
1	F	53	LEU
1	F	64	LEU
1	F	121	LEU
1	F	124	ASP
1	F	125	ASN
1	F	156	GLU
1	F	175	LEU
1	F	190	LEU
1	F	192	ARG
1	F	206	ARG
1	F	218	VAL
1	F	236	LEU
1	F	244	THR
1	F	253	SER
1	F	266	LYS
1	F	270	GLU
1	F	274	CYS
1	F	277	VAL
1	F	282	LEU
1	F	286	LEU
2	G	21	ILE
2	G	28	GLN
2	G	53	SER
2	G	54	ASP
2	G	56	GLU
2	G	75	SER
2	G	77	SER

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Mol	Chain	Res	Type
2	G	78	LYS
2	G	93	THR
2	G	96	ASP
2	G	107	LEU
2	G	108	SER
2	G	109	GLN
2	G	112	ILE
1	I	28	LEU
1	I	39	SER
1	I	53	LEU
1	I	60	SER
1	I	62	ASN
1	I	75	VAL
1	I	77	GLU
1	I	79	GLN
1	I	80	VAL
1	I	121	LEU
1	I	124	ASP
1	I	125	ASN
1	I	147	GLN
1	I	156	GLU
1	I	168	ASP
1	I	175	LEU
1	I	179	LEU
1	I	184	HIS
1	I	190	LEU
1	I	192	ARG
1	I	194	ARG
1	I	199	TRP
1	I	219	LEU
1	I	256	SER
2	J	21	ILE
2	J	32	ARG
2	J	53	SER
2	J	54	ASP
2	J	77	SER
2	J	107	LEU
2	J	112	ILE
2	J	118	ASP
2	J	119	MET
3	H	440	SER
3	H	455	LYS

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Mol	Chain	Res	Type
3	H	482	THR
3	H	497	SER
3	H	509	LEU
3	H	514	LYS
3	H	526	THR
3	H	538	LEU
3	H	542	LYS
3	H	581	SER
3	H	641	LEU
3	K	461	SER
3	K	493	ASP
3	K	497	SER
3	K	514	LYS
3	K	531	ASN
3	K	535	VAL
3	K	537	SER
3	K	548	GLN
3	K	564	ASP
3	K	583	THR
3	K	594	SER
3	K	613	THR
3	K	641	LEU
3	L	442	MET
3	L	493	ASP
3	L	513	SER
3	L	537	SER
3	L	570	LEU
3	L	583	THR
3	L	613	THR
3	L	639	GLU
3	L	641	LEU
1	C	53	LEU
1	C	57	GLN
1	C	60	SER
1	C	69	GLU
1	C	75	VAL
1	C	77	GLU
1	C	79	GLN
1	C	80	VAL
1	C	105	LEU
1	C	108	LYS
1	C	121	LEU

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Mol	Chain	Res	Type
1	C	124	ASP
1	C	127	SER
1	C	147	GLN
1	C	156	GLU
1	C	167	GLN
1	C	190	LEU
1	C	216	PHE
1	C	253	SER
1	C	256	SER
1	C	266	LYS
1	C	271	HIS
1	C	272	HIS
1	C	274	CYS
1	C	286	LEU
1	C	289	GLU
2	D	21	ILE
2	D	28	GLN
2	D	53	SER
2	D	54	ASP
2	D	74	LEU
2	D	78	LYS
2	D	79	ASP
2	D	93	THR
2	D	107	LEU
2	D	112	ILE
2	D	119	MET
3	E	442	MET
3	E	455	LYS
3	E	482	THR
3	E	486	SER
3	E	513	SER
3	E	523	GLN
3	E	530	ASN
3	E	531	ASN
3	E	583	THR
3	E	613	THR
3	E	641	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN

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Mol	Chain	Res	Type
1	F	79	GLN
1	F	125	ASN
2	G	33	HIS
1	I	62	ASN
3	H	465	ASN
3	H	568	ASN
3	K	448	ASN
3	K	465	ASN
3	K	530	ASN
3	K	568	ASN
3	K	584	GLN
3	L	447	ASN
3	L	465	ASN
3	L	568	ASN
1	C	196	ASN
2	D	37	ASN
3	E	465	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 ⓘ

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	264/278 (94%)	0.13	10 (3%) 44 31	89, 119, 156, 169	0
1	C	263/278 (94%)	-0.04	5 (1%) 66 51	79, 119, 146, 161	0
1	F	266/278 (95%)	0.08	6 (2%) 61 46	72, 116, 151, 176	0
1	I	215/278 (77%)	-0.11	2 (0%) 81 68	85, 123, 173, 185	0
2	B	99/99 (100%)	0.00	1 (1%) 79 66	102, 131, 155, 160	0
2	D	99/99 (100%)	-0.17	0 100 100	92, 124, 160, 174	0
2	G	99/99 (100%)	-0.29	0 100 100	83, 116, 154, 162	0
2	J	87/99 (87%)	0.01	1 (1%) 78 65	100, 157, 176, 183	0
3	E	215/228 (94%)	-0.28	0 100 100	64, 86, 116, 153	1 (0%)
3	H	215/228 (94%)	-0.42	1 (0%) 87 78	61, 83, 122, 160	1 (0%)
3	K	215/228 (94%)	-0.14	1 (0%) 87 78	72, 100, 136, 161	2 (0%)
3	L	215/228 (94%)	-0.21	1 (0%) 87 78	72, 96, 122, 162	2 (0%)
All	All	2252/2420 (93%)	-0.11	28 (1%) 76 63	61, 110, 158, 185	6 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	148	GLY	4.2
1	A	143	PHE	3.4
1	C	238	ASN	3.3
1	I	218	VAL	3.2
1	I	101	ALA	3.1
1	A	145	LEU	2.9
1	F	145	LEU	2.9
1	C	28	LEU	2.9
3	H	509	LEU	2.9
1	F	238	ASN	2.8
1	F	175	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	238	ASN	2.7
1	A	28	LEU	2.6
1	F	272	HIS	2.6
2	J	91	THR	2.5
1	A	98	PHE	2.5
2	B	21	ILE	2.5
1	A	117	LEU	2.5
1	A	148	GLY	2.5
1	F	79	GLN	2.4
3	K	644	ILE	2.3
1	A	178	LEU	2.3
1	C	80	VAL	2.2
1	C	253	SER	2.1
1	C	214	PRO	2.1
1	A	133	PHE	2.1
1	A	290	LEU	2.1
3	L	644	ILE	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.