



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:32 AM UTC

PDB ID : 6JJL / pdb_00006jjl
Title : Crystal structure of the DegP dodecamer with a modulator
Authors : Cho, H.; Choi, Y.; Lee, H.H.; Kim, S.
Deposited on : 2019-02-26
Resolution : 4.20 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

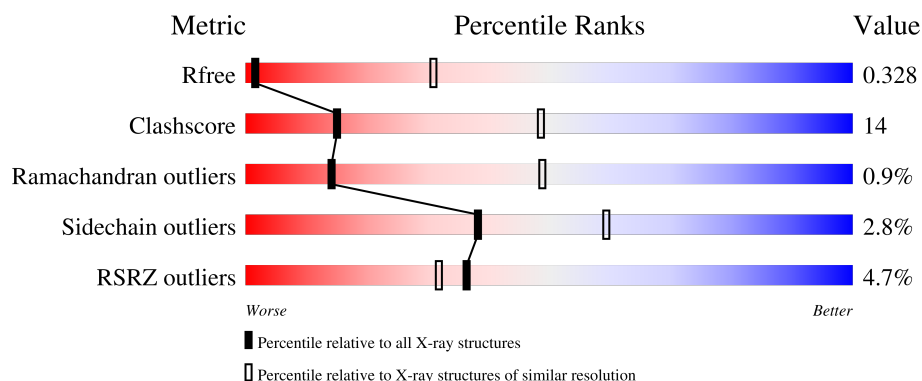
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	440	3% 63% 23% 13%
1	B	440	2% 63% 25% 11%
1	C	440	3% 57% 28% 13%
1	D	440	6% 57% 30% 12%
1	E	440	6% 64% 24% 12%

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Mol	Chain	Length	Quality of chain
1	F	440	% 63% 23% 14%
2	G	5	40% 100%
2	H	5	40% 80% 20%
2	I	5	40% 80% 20%
2	J	5	20% 100%
2	K	5	60% 80% 20%
2	L	5	60% 100%
2	M	5	100%
2	N	5	100%
2	O	5	20% 100%
2	P	5	40% 100%
2	Q	5	40% 100%
2	R	5	20% 100%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17212 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 Periplasmic serine endoprotease DegP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			2791	1741	493	544	13			
1	B	392	Total	C	N	O	S	0	0	0
			2867	1783	506	565	13			
1	C	382	Total	C	N	O	S	0	0	0
			2794	1742	493	546	13			
1	D	388	Total	C	N	O	S	0	0	0
			2835	1766	499	557	13			
1	E	388	Total	C	N	O	S	0	0	0
			2835	1765	500	557	13			
1	F	379	Total	C	N	O	S	0	0	0
			2777	1733	490	541	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	210	ALA	SER	conflict	UNP P0C0V0
B	210	ALA	SER	conflict	UNP P0C0V0
C	210	ALA	SER	conflict	UNP P0C0V0
D	210	ALA	SER	conflict	UNP P0C0V0
E	210	ALA	SER	conflict	UNP P0C0V0
F	210	ALA	SER	conflict	UNP P0C0V0

- Molecule 2 is a protein called CYS-TYR-ARG-LYS-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	M	5	Total	C	N	O	0	0	0
			32	21	5	6			
2	H	5	Total	C	N	O	0	0	0
			25	15	5	5			

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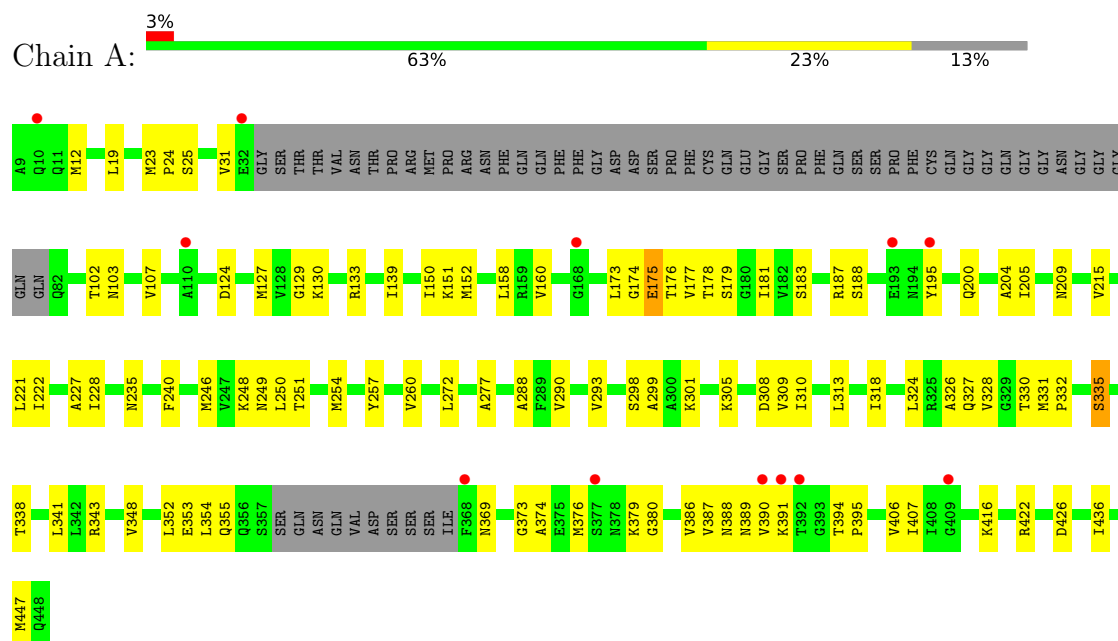
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	N	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	I	5	Total	C	N	O	0	0	0
			28	18	5	5			
2	Q	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	J	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	O	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	K	5	Total	C	N	O	0	0	0
			28	18	5	5			
2	R	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	L	5	Total	C	N	O	0	0	0
			25	15	5	5			
2	P	5	Total	C	N	O	0	0	0
			25	15	5	5			

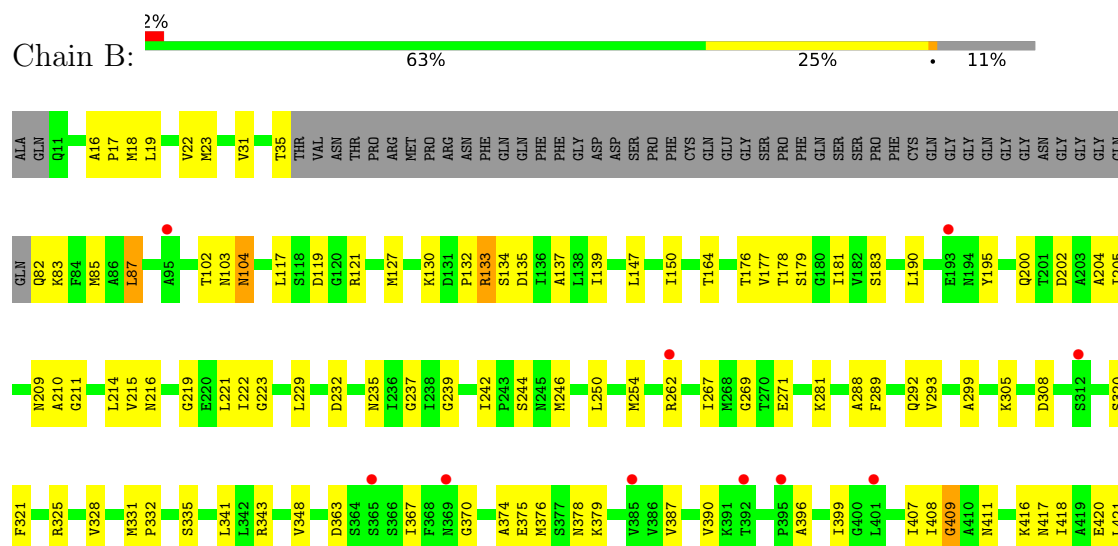
3 Residue-property plots [i](#)

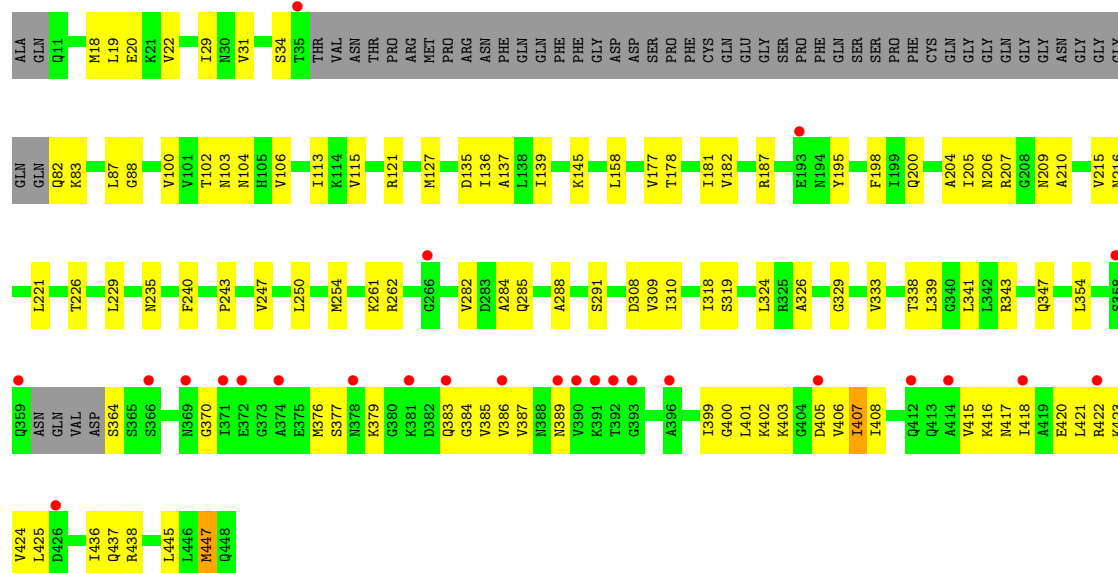
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Periplasmic serine endoprotease DegP

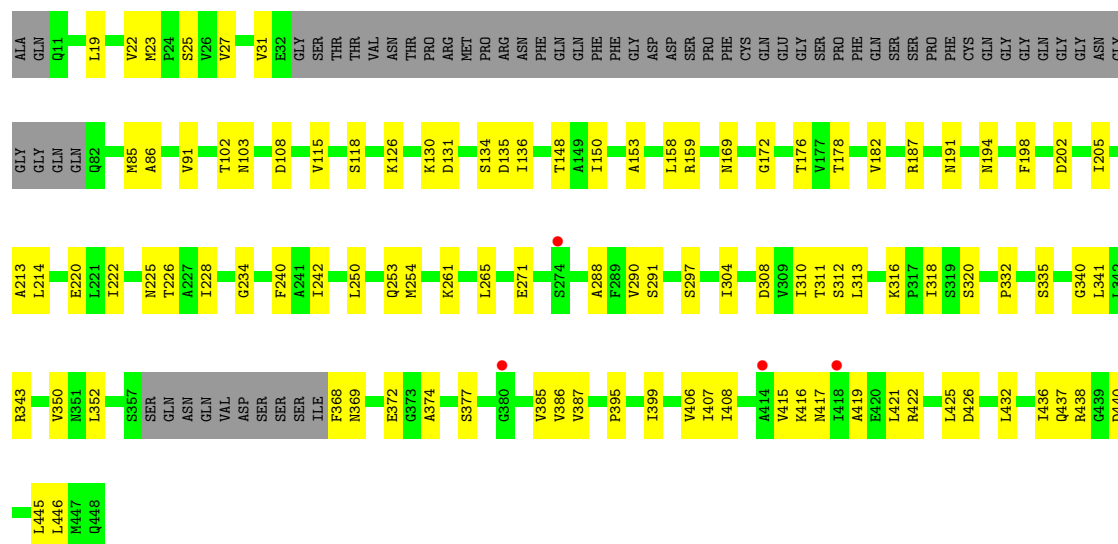


• Molecule 1: Periplasmic serine endoprotease DegP

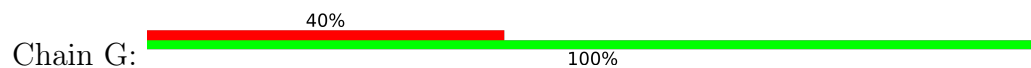




- Molecule 1: Periplasmic serine endoprotease DegP



- Molecule 2: CYS-TYR-ARG-LYS-LEU

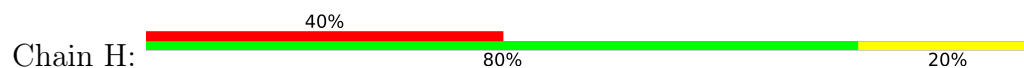


- Molecule 2: CYS-TYR-ARG-LYS-LEU



There are no outlier residues recorded for this chain.

- Molecule 2: CYS-TYR-ARG-LYS-LEU

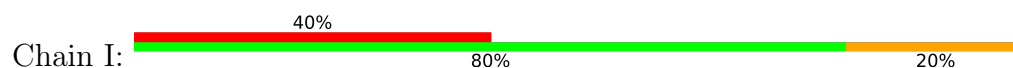


- Molecule 2: CYS-TYR-ARG-LYS-LEU

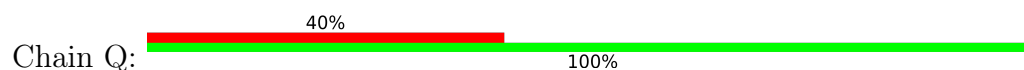


There are no outlier residues recorded for this chain.

- Molecule 2: CYS-TYR-ARG-LYS-LEU



- Molecule 2: CYS-TYR-ARG-LYS-LEU



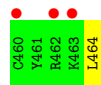
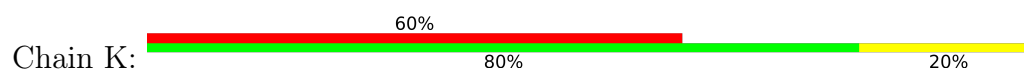
- Molecule 2: CYS-TYR-ARG-LYS-LEU



- Molecule 2: CYS-TYR-ARG-LYS-LEU



- Molecule 2: CYS-TYR-ARG-LYS-LEU



● Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain R:  20% 100%

●

C471
Y472
R473
K474
L475

● Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain L:  60% 100%

● ● ●

C460
Y461
R462
K463
L464

● Molecule 2: CYS-TYR-ARG-LYS-LEU

Chain P:  40% 100%

● ●

C471
Y472
R473
K474
L475

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	217.15Å 123.52Å 140.56Å 90.00° 118.00° 90.00°	Depositor
Resolution (Å)	50.00 – 4.20 50.00 – 4.20	Depositor EDS
% Data completeness (in resolution range)	98.5 (50.00-4.20) 99.7 (50.00-4.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.08 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.248 , 0.326 0.255 , 0.328	Depositor DCC
R_{free} test set	1262 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h +1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h- 1/2*k-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	17212	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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	0.42	0/2815	0.51	0/3798
1	B	0.39	0/2892	0.53	0/3904
1	C	0.44	0/2818	0.56	0/3802
1	D	0.36	0/2859	0.53	0/3858
1	E	0.37	0/2859	0.53	0/3857
1	F	0.39	0/2801	0.52	0/3779
2	G	0.79	0/24	0.56	0/32
2	H	0.53	0/24	0.39	0/32
2	I	0.48	0/27	0.62	0/36
2	J	0.51	0/24	0.46	0/32
2	K	0.43	0/27	0.47	0/36
2	L	0.43	0/24	0.30	0/32
2	M	0.47	0/32	0.42	0/43
2	N	0.47	0/24	0.38	0/32
2	O	0.32	0/24	0.39	0/32
2	P	0.37	0/24	0.29	0/32
2	Q	0.41	0/24	0.40	0/32
2	R	0.40	0/24	0.34	0/32
All	All	0.40	0/17346	0.53	0/23401

There are no bond length outliers.

There are no bond angle outliers.

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	2791	0	2888	66	1
1	B	2867	0	2957	79	0
1	C	2794	0	2890	103	0
1	D	2835	0	2929	113	0
1	E	2835	0	2929	86	0
1	F	2777	0	2875	53	0
2	G	25	0	9	0	0
2	H	25	0	9	1	0
2	I	28	0	18	1	0
2	J	25	0	9	0	0
2	K	28	0	18	5	0
2	L	25	0	9	0	0
2	M	32	0	16	0	0
2	N	25	0	9	0	0
2	O	25	0	9	0	0
2	P	25	0	9	0	0
2	Q	25	0	9	0	0
2	R	25	0	9	0	0
All	All	17212	0	17601	477	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 14.

All (477) 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:D:387:VAL:HG21	1:D:405:ASP:H	1.14	1.10
1:D:305:LYS:HD3	1:D:343:ARG:NH2	1.84	0.93
1:E:82:GLN:HG2	1:E:83:LYS:HA	1.56	0.88
1:B:408:ILE:H	1:B:409:GLY:HA3	1.37	0.88
1:B:409:GLY:HA2	1:B:435:ASN:HB3	1.57	0.87
1:D:407:ILE:HG13	1:D:408:ILE:HG22	1.57	0.85
1:D:246:MET:HG2	1:D:330:THR:HG21	1.58	0.84
1:D:387:VAL:HG13	1:D:406:VAL:HG23	1.62	0.82
1:D:374:ALA:HB1	1:D:389:ASN:HB2	1.61	0.82
1:D:187:ARG:NH1	1:D:200:GLN:OE1	2.15	0.80
1:C:436:ILE:HG22	1:C:437:GLN:H	1.45	0.79
1:C:435:ASN:ND2	1:C:443:ILE:O	2.16	0.79
1:E:318:ILE:HD11	1:E:324:LEU:HB2	1.64	0.78
1:E:34:SER:HA	1:E:82:GLN:HG3	1.63	0.78
1:C:318:ILE:HD12	1:C:324:LEU:HD13	1.66	0.76
1:C:435:ASN:CG	1:C:444:TYR:HA	2.11	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:LYS:HE3	1:E:438:ARG:HD3	1.68	0.76
1:B:215:VAL:HG12	1:B:221:LEU:HA	1.67	0.75
1:C:35:THR:HG22	1:C:84:PHE:HB3	1.69	0.74
1:D:387:VAL:HG21	1:D:405:ASP:N	1.98	0.73
1:C:407:ILE:HA	1:C:436:ILE:HG12	1.71	0.73
1:C:92:ILE:HG22	1:C:100:VAL:HB	1.71	0.73
1:B:22:VAL:HG21	1:B:219:GLY:HA3	1.72	0.71
1:D:308:ASP:OD1	1:D:343:ARG:HA	1.90	0.71
1:D:268:MET:HB2	1:D:292:GLN:HB3	1.72	0.71
1:D:32:GLU:HG3	1:D:85:MET:HG2	1.73	0.70
1:D:407:ILE:HD13	1:D:437:GLN:HG2	1.73	0.70
1:E:19:LEU:HD21	1:E:177:VAL:HG11	1.74	0.70
1:D:305:LYS:HD3	1:D:343:ARG:HH22	1.57	0.69
1:E:262:ARG:NH1	1:E:329:GLY:O	2.26	0.69
1:C:195:TYR:HD2	1:C:326:ALA:HA	1.58	0.68
1:E:215:VAL:HG12	1:E:221:LEU:HA	1.75	0.68
1:F:304:ILE:HG23	1:F:341:LEU:HD21	1.74	0.68
1:D:407:ILE:HB	1:D:436:ILE:HA	1.76	0.68
1:E:386:VAL:HA	1:E:406:VAL:HG23	1.75	0.68
1:D:31:VAL:HG23	1:D:113:ILE:HG12	1.76	0.68
1:C:169:ASN:HD21	1:C:172:GLY:HA2	1.58	0.67
1:C:380:GLY:O	1:C:383:GLN:NE2	2.28	0.67
1:C:386:VAL:HG22	1:C:406:VAL:HA	1.74	0.67
1:B:376:MET:HG2	1:B:387:VAL:HG22	1.75	0.67
1:A:187:ARG:NH1	1:A:200:GLN:OE1	2.27	0.67
1:B:328:VAL:HA	1:B:331:MET:HG3	1.76	0.67
1:C:265:LEU:HD11	1:C:352:LEU:HD13	1.77	0.66
1:B:374:ALA:H	1:B:396:ALA:HB3	1.61	0.66
1:A:129:GLY:HA3	1:A:254:MET:HG2	1.77	0.66
1:E:415:VAL:HG13	1:E:420:GLU:HB3	1.77	0.66
1:D:305:LYS:HB2	1:D:343:ARG:HH12	1.61	0.66
1:C:370:GLY:HA2	1:C:376:MET:HG2	1.79	0.65
1:C:411:ASN:N	1:C:434:LEU:HD11	2.12	0.65
1:E:288:ALA:HB3	1:E:310:ILE:HB	1.77	0.65
1:A:23:MET:HG2	1:A:175:GLU:OE1	1.96	0.65
1:E:206:ASN:C	2:K:464:LEU:HD12	2.20	0.65
1:E:384:GLY:HA3	1:E:416:LYS:O	1.96	0.65
1:C:103:ASN:HD22	1:C:104:ASN:N	1.94	0.65
1:B:408:ILE:N	1:B:409:GLY:HA3	2.11	0.65
1:C:178:THR:HG21	1:C:204:ALA:HB3	1.78	0.65
1:B:205:ILE:O	1:B:235:ASN:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:ARG:HA	1:E:425:LEU:HB3	1.79	0.64
1:C:158:LEU:HD11	1:C:222:ILE:HD12	1.80	0.64
1:C:136:ILE:HD13	1:C:247:VAL:HG13	1.80	0.64
1:C:407:ILE:HA	1:C:436:ILE:CG1	2.28	0.64
1:D:385:VAL:N	1:D:406:VAL:HG11	2.13	0.64
1:F:31:VAL:HB	1:F:86:ALA:HB3	1.81	0.64
1:A:379:LYS:HE2	1:A:406:VAL:HG22	1.80	0.63
1:D:178:THR:HG21	1:D:204:ALA:HB3	1.79	0.63
1:D:263:GLY:HA3	1:D:354:LEU:HD12	1.79	0.63
1:B:374:ALA:HB2	1:B:390:VAL:HG23	1.79	0.63
1:E:399:ILE:HD13	1:E:401:LEU:HG	1.80	0.63
1:A:178:THR:HG21	1:A:204:ALA:HB3	1.80	0.63
1:C:246:MET:HE3	1:C:330:THR:HG21	1.81	0.63
1:D:124:ASP:HB3	1:D:142:GLN:HG3	1.81	0.63
1:E:102:THR:HG23	1:E:137:ALA:HB3	1.81	0.63
1:C:435:ASN:ND2	1:C:444:TYR:HA	2.14	0.62
1:D:312:SER:HB3	1:D:340:GLY:HA3	1.80	0.62
1:D:103:ASN:HD21	1:D:226:THR:HG22	1.65	0.62
1:C:102:THR:OG1	1:C:103:ASN:N	2.32	0.62
1:A:298:SER:OG	1:A:355:GLN:NE2	2.32	0.62
1:C:385:VAL:HB	1:C:407:ILE:HD12	1.81	0.62
1:A:205:ILE:HG23	1:A:209:ASN:HB2	1.82	0.62
1:C:411:ASN:H	1:C:434:LEU:HD11	1.62	0.62
1:A:422:ARG:O	1:A:426:ASP:N	2.28	0.61
1:E:408:ILE:HG12	1:E:421:LEU:HD21	1.81	0.61
1:F:19:LEU:HA	1:F:22:VAL:HG12	1.81	0.61
1:C:29:ILE:HG22	1:C:30:ASN:H	1.64	0.61
1:F:91:VAL:HG21	1:F:213:ALA:HB2	1.81	0.61
1:F:265:LEU:HD22	1:F:352:LEU:HD13	1.82	0.61
1:A:332:PRO:O	1:A:335:SER:OG	2.17	0.61
1:B:19:LEU:HB3	1:B:23:MET:HG3	1.82	0.61
1:B:202:ASP:HA	1:B:237:GLY:O	2.00	0.61
1:C:408:ILE:HB	1:C:436:ILE:HG23	1.82	0.61
1:D:405:ASP:OD1	1:D:437:GLN:N	2.34	0.60
1:E:261:LYS:HE2	1:E:333:VAL:HB	1.82	0.60
1:B:178:THR:HG22	1:C:202:ASP:HB3	1.83	0.60
1:B:407:ILE:HD13	1:B:434:LEU:HD22	1.84	0.60
1:C:408:ILE:N	1:C:436:ILE:HG12	2.17	0.60
1:D:12:MET:SD	1:E:216:ASN:ND2	2.73	0.60
1:D:305:LYS:HB2	1:D:343:ARG:NH1	2.16	0.60
1:D:290:VAL:HG13	1:D:310:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:THR:HG22	1:E:187:ARG:HH12	1.67	0.59
1:D:158:LEU:HD11	1:D:222:ILE:HD12	1.84	0.59
1:D:310:ILE:HG21	1:D:339:LEU:HD22	1.83	0.59
1:C:103:ASN:HB3	1:C:106:VAL:HG23	1.85	0.59
1:C:86:ALA:HB1	1:C:207:ARG:HH22	1.68	0.58
1:C:341:LEU:HB3	1:C:348:VAL:HG23	1.84	0.58
1:A:328:VAL:HA	1:A:331:MET:HG3	1.84	0.58
1:A:388:ASN:O	1:A:389:ASN:ND2	2.36	0.58
1:C:411:ASN:H	1:C:434:LEU:CD1	2.16	0.58
1:F:108:ASP:OD1	1:F:130:LYS:NZ	2.36	0.58
1:D:143:ASN:HB3	1:D:145:LYS:HE2	1.86	0.58
1:C:389:ASN:HA	1:C:403:LYS:HG2	1.86	0.58
1:D:407:ILE:HG21	1:D:435:ASN:C	2.28	0.58
1:C:408:ILE:H	1:C:436:ILE:HG12	1.68	0.58
1:B:127:MET:HA	1:B:139:ILE:HG22	1.86	0.57
1:B:367:ILE:O	1:B:422:ARG:NH1	2.37	0.57
1:C:160:VAL:HG23	1:C:185:LEU:HG	1.85	0.57
1:A:150:ILE:HD13	1:A:221:LEU:HB2	1.85	0.57
1:E:20:GLU:OE1	1:F:159:ARG:NH2	2.37	0.57
1:E:178:THR:HG22	1:F:202:ASP:HB3	1.85	0.57
1:E:187:ARG:NH1	1:E:200:GLN:OE1	2.36	0.57
1:F:304:ILE:HD11	1:F:352:LEU:HD11	1.85	0.57
1:B:210:ALA:HB2	2:H:464:LEU:O	2.04	0.57
1:A:181:ILE:HD13	1:C:179:SER:HB3	1.87	0.57
1:E:399:ILE:HD12	1:E:400:GLY:N	2.19	0.57
1:E:243:PRO:O	1:E:247:VAL:HG23	2.05	0.57
1:F:408:ILE:HD13	1:F:437:GLN:HG3	1.85	0.57
1:A:407:ILE:HG12	1:A:436:ILE:HG22	1.86	0.56
1:D:390:VAL:HG22	1:D:403:LYS:HB3	1.86	0.56
1:E:408:ILE:HD13	1:E:416:LYS:HA	1.87	0.56
1:D:407:ILE:HG21	1:D:435:ASN:HB3	1.87	0.56
1:E:103:ASN:O	1:E:106:VAL:HG12	2.05	0.56
1:E:261:LYS:HG3	1:E:333:VAL:H	1.69	0.56
1:A:215:VAL:HG12	1:A:221:LEU:HA	1.87	0.56
1:A:183:SER:HB2	1:A:200:GLN:HG2	1.87	0.56
1:D:385:VAL:HG12	1:D:386:VAL:H	1.70	0.56
1:A:179:SER:HB2	1:B:181:ILE:HD13	1.88	0.56
1:F:288:ALA:HB3	1:F:310:ILE:HB	1.87	0.56
1:D:215:VAL:HG12	1:D:221:LEU:HA	1.86	0.56
1:A:379:LYS:HD3	1:A:386:VAL:HB	1.87	0.56
1:B:246:MET:O	1:B:250:LEU:HD12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:386:VAL:HA	1:E:406:VAL:CG2	2.35	0.55
1:A:12:MET:HE1	1:B:216:ASN:HB2	1.87	0.55
1:D:179:SER:HB3	1:E:181:ILE:HD13	1.89	0.55
1:C:30:ASN:HA	1:C:87:LEU:HD13	1.89	0.55
1:E:379:LYS:HA	1:E:384:GLY:HA2	1.89	0.55
1:D:313:LEU:HB2	1:D:318:ILE:HD11	1.89	0.55
1:E:407:ILE:HG13	1:E:436:ILE:HA	1.88	0.55
1:B:281:LYS:HE2	1:D:412:GLN:HG3	1.89	0.54
1:B:292:GLN:HB3	1:D:443:ILE:HB	1.89	0.54
1:F:407:ILE:HG12	1:F:436:ILE:HG22	1.90	0.54
1:F:386:VAL:HG22	1:F:406:VAL:HG22	1.90	0.54
1:A:205:ILE:HG23	1:A:209:ASN:CB	2.37	0.54
1:C:406:VAL:O	1:C:436:ILE:HD13	2.07	0.54
1:B:363:ASP:OD1	1:B:375:GLU:HB3	2.08	0.54
1:F:253:GLN:OE1	1:F:261:LYS:N	2.41	0.54
1:C:371:ILE:HD13	1:C:421:LEU:HD21	1.90	0.54
1:D:183:SER:N	1:D:200:GLN:O	2.41	0.54
1:E:29:ILE:HG22	1:E:115:VAL:HG22	1.90	0.54
1:E:384:GLY:C	1:E:408:ILE:HD11	2.32	0.54
1:E:31:VAL:HG12	1:E:113:ILE:HG12	1.90	0.53
1:A:205:ILE:O	1:A:235:ASN:HB2	2.08	0.53
1:F:103:ASN:ND2	1:F:135:ASP:O	2.39	0.53
1:C:407:ILE:HA	1:C:436:ILE:CD1	2.37	0.53
1:E:102:THR:OG1	1:E:103:ASN:N	2.41	0.53
1:F:169:ASN:OD1	1:F:172:GLY:HA2	2.09	0.53
1:B:104:ASN:ND2	1:B:135:ASP:HA	2.24	0.53
1:D:399:ILE:HB	1:D:445:LEU:HD21	1.91	0.53
1:E:399:ILE:HD12	1:E:400:GLY:H	1.74	0.53
1:E:364:SER:N	1:E:376:MET:HG2	2.24	0.53
1:C:406:VAL:HG12	1:C:407:ILE:H	1.74	0.53
1:A:133:ARG:HB3	1:A:195:TYR:CE2	2.44	0.52
1:D:436:ILE:O	1:D:443:ILE:HG12	2.08	0.52
1:D:354:LEU:HD23	1:D:354:LEU:H	1.74	0.52
1:F:158:LEU:HD22	1:F:182:VAL:HG21	1.90	0.52
1:B:121:ARG:HA	1:C:285:GLN:HG2	1.91	0.52
1:D:408:ILE:CG1	1:D:414:ALA:HA	2.39	0.52
1:D:299:ALA:HA	1:D:352:LEU:HD21	1.89	0.52
1:B:35:THR:N	1:B:82:GLN:O	2.43	0.52
1:E:18:MET:SD	1:E:19:LEU:HD12	2.50	0.52
1:E:379:LYS:HE3	1:E:417:ASN:HB2	1.92	0.52
1:D:286:ARG:NH2	1:F:118:SER:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ASP:HB2	1:B:121:ARG:HG3	1.91	0.52
1:E:387:VAL:HG13	1:E:406:VAL:HG21	1.92	0.51
1:D:22:VAL:HG21	1:D:219:GLY:HA3	1.92	0.51
1:D:368:PHE:CG	1:D:372:GLU:HA	2.46	0.51
1:A:391:LYS:O	1:A:394:THR:OG1	2.28	0.51
1:D:382:ASP:O	1:D:416:LYS:HB2	2.11	0.51
1:D:33:GLY:HA2	1:D:110:ALA:HA	1.91	0.51
1:F:432:LEU:O	1:F:446:LEU:HA	2.10	0.51
1:A:272:LEU:HD11	1:A:277:ALA:HB2	1.91	0.51
1:A:353:GLU:HG3	1:A:354:LEU:O	2.10	0.51
1:E:104:ASN:HA	1:E:137:ALA:HB2	1.92	0.51
1:E:210:ALA:HB2	2:K:464:LEU:C	2.36	0.51
1:D:399:ILE:O	1:D:445:LEU:HD11	2.11	0.51
1:D:406:VAL:CG1	1:D:407:ILE:N	2.74	0.51
1:E:178:THR:HG21	1:E:204:ALA:HB3	1.91	0.51
1:F:332:PRO:O	1:F:335:SER:OG	2.26	0.51
1:D:24:PRO:HA	1:D:118:SER:HB3	1.92	0.50
1:D:126:LYS:H	1:D:126:LYS:HD2	1.76	0.50
1:C:438:ARG:CZ	1:C:443:ILE:HD11	2.41	0.50
1:E:207:ARG:HA	2:K:464:LEU:HB2	1.93	0.50
1:B:443:ILE:HG22	1:B:444:TYR:N	2.25	0.50
1:E:100:VAL:HB	1:E:139:ILE:HG13	1.93	0.50
1:B:288:ALA:HB1	1:B:321:PHE:HD1	1.76	0.50
1:D:186:GLY:HA2	1:D:197:ASN:OD1	2.11	0.50
1:A:152:MET:HE2	1:A:248:LYS:HB2	1.92	0.50
1:A:250:LEU:HG	1:A:330:THR:HG23	1.93	0.50
1:C:32:GLU:HB2	1:C:112:VAL:HG12	1.93	0.50
1:D:407:ILE:HG23	1:D:408:ILE:C	2.37	0.50
1:B:222:ILE:O	1:B:244:SER:N	2.44	0.50
1:D:420:GLU:HA	1:D:423:LYS:HE2	1.93	0.50
1:E:423:LYS:HE2	1:E:424:VAL:HG23	1.94	0.50
1:B:164:THR:HB	1:B:214:LEU:HD21	1.93	0.50
1:C:155:SER:N	1:C:245:ASN:OD1	2.45	0.50
1:C:379:LYS:HD3	1:C:386:VAL:HB	1.94	0.50
1:C:86:ALA:HB1	1:C:207:ARG:NH2	2.26	0.50
1:D:408:ILE:HG23	1:D:409:GLY:H	1.77	0.50
1:A:257:TYR:CD1	1:A:257:TYR:N	2.80	0.49
1:D:406:VAL:HG12	1:D:407:ILE:N	2.28	0.49
1:A:127:MET:SD	1:A:130:LYS:HE3	2.52	0.49
1:B:431:VAL:HA	1:B:448:GLN:CD	2.37	0.49
1:D:374:ALA:HB1	1:D:389:ASN:CB	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:405:ASP:O	1:E:406:VAL:HG13	2.11	0.49
1:A:249:ASN:HB2	1:A:330:THR:CG2	2.42	0.49
1:C:261:LYS:HB3	1:C:333:VAL:HG23	1.93	0.49
1:C:435:ASN:C	1:C:436:ILE:HG13	2.36	0.49
1:D:402:LYS:HD2	1:D:402:LYS:C	2.37	0.49
1:E:226:THR:O	2:K:464:LEU:HD23	2.13	0.49
1:E:407:ILE:HG12	1:E:437:GLN:HG2	1.93	0.49
1:F:131:ASP:OD2	1:F:134:SER:OG	2.18	0.49
1:C:88:GLY:HA2	1:C:208:GLY:HA2	1.94	0.49
1:C:422:ARG:O	1:C:426:ASP:N	2.45	0.49
1:D:272:LEU:HD22	1:D:309:VAL:HG11	1.95	0.49
1:D:313:LEU:HD11	1:D:337:LEU:HD23	1.95	0.49
1:E:121:ARG:NH1	1:E:145:LYS:O	2.36	0.49
1:D:178:THR:HG21	1:D:204:ALA:H	1.78	0.49
1:C:29:ILE:HG22	1:C:30:ASN:N	2.26	0.48
1:C:100:VAL:HG13	1:C:139:ILE:HG13	1.94	0.48
1:A:102:THR:OG1	1:A:103:ASN:N	2.47	0.48
1:C:385:VAL:N	1:C:407:ILE:HB	2.28	0.48
1:A:327:GLN:O	1:A:330:THR:HB	2.13	0.48
1:B:104:ASN:HD22	1:B:135:ASP:HA	1.78	0.48
1:B:127:MET:HB2	1:B:127:MET:HE2	1.67	0.48
1:D:27:VAL:HG12	1:D:117:LEU:HA	1.95	0.48
1:D:408:ILE:HG13	1:D:414:ALA:HA	1.96	0.48
1:D:435:ASN:O	1:D:435:ASN:ND2	2.46	0.48
1:A:290:VAL:HG22	1:A:308:ASP:O	2.14	0.48
1:B:378:ASN:HD21	1:B:418:ILE:H	1.62	0.48
1:E:136:ILE:HD11	1:E:247:VAL:HG22	1.96	0.48
1:A:127:MET:HA	1:A:139:ILE:HG22	1.95	0.47
1:D:373:GLY:HA3	1:D:396:ALA:HB3	1.96	0.47
1:D:385:VAL:H	1:D:406:VAL:HG11	1.78	0.47
1:C:166:ALA:N	1:C:178:THR:O	2.33	0.47
1:D:155:SER:N	1:D:245:ASN:OD1	2.46	0.47
1:C:162:ASP:O	1:C:182:VAL:HG23	2.14	0.47
1:E:405:ASP:C	1:E:406:VAL:HG13	2.40	0.47
1:C:410:ALA:HA	1:C:434:LEU:HD12	1.97	0.47
1:C:433:ALA:N	1:C:434:LEU:HD22	2.29	0.47
1:B:179:SER:HB3	1:C:181:ILE:HD13	1.97	0.47
1:C:396:ALA:HA	1:C:399:ILE:HD12	1.97	0.47
1:D:119:ASP:HB3	1:D:121:ARG:HG3	1.95	0.47
1:A:318:ILE:HD11	1:A:324:LEU:HD13	1.96	0.47
1:B:242:ILE:HG23	1:B:246:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASP:OD2	1:B:343:ARG:NH2	2.48	0.47
1:C:150:ILE:HD13	1:C:221:LEU:HB2	1.96	0.47
1:C:407:ILE:HA	1:C:436:ILE:HD13	1.97	0.47
1:E:250:LEU:O	1:E:254:MET:HG3	2.14	0.47
1:E:387:VAL:HG23	1:E:403:LYS:HA	1.97	0.47
1:F:187:ARG:HA	1:F:187:ARG:HD3	1.56	0.47
1:B:150:ILE:HD11	1:B:215:VAL:HG11	1.97	0.47
1:C:29:ILE:C	1:C:87:LEU:HD11	2.40	0.47
1:D:93:ILE:HD12	1:D:152:MET:HE2	1.97	0.47
1:A:23:MET:N	1:A:24:PRO:HD2	2.30	0.46
1:F:308:ASP:OD1	1:F:343:ARG:HB3	2.14	0.46
1:A:25:SER:OG	1:A:150:ILE:HB	2.15	0.46
1:C:293:VAL:HG11	1:C:304:ILE:O	2.15	0.46
1:C:391:LYS:HG2	1:C:394:THR:HG23	1.97	0.46
1:E:282:VAL:HG12	1:E:284:ALA:H	1.80	0.46
1:E:308:ASP:CG	1:E:343:ARG:HG2	2.39	0.46
1:C:266:GLY:HA3	1:C:297:SER:OG	2.15	0.46
1:B:178:THR:HG21	1:B:204:ALA:HB3	1.98	0.46
1:B:332:PRO:O	1:B:335:SER:OG	2.29	0.46
1:D:407:ILE:HG12	1:D:435:ASN:O	2.15	0.46
1:B:271:GLU:HG3	1:B:321:PHE:H	1.79	0.46
1:C:153:ALA:HB2	1:C:220:GLU:HB2	1.98	0.46
1:E:195:TYR:HB3	1:E:326:ALA:HA	1.96	0.46
1:C:103:ASN:ND2	1:C:135:ASP:O	2.49	0.46
1:D:387:VAL:HG11	1:D:405:ASP:O	2.16	0.46
1:B:19:LEU:HD11	1:B:177:VAL:HG11	1.97	0.46
1:B:440:ASP:N	1:B:440:ASP:OD1	2.48	0.46
1:C:324:LEU:O	1:C:328:VAL:HG22	2.16	0.46
1:E:127:MET:HA	1:E:139:ILE:HG22	1.98	0.46
1:D:335:SER:H	1:D:354:LEU:HD21	1.80	0.46
1:C:262:ARG:HD3	1:C:329:GLY:O	2.16	0.46
1:E:377:SER:N	1:E:386:VAL:O	2.43	0.46
1:E:401:LEU:HD22	1:E:445:LEU:HD13	1.97	0.46
1:C:288:ALA:HB1	1:C:321:PHE:HD2	1.81	0.46
1:D:297:SER:O	1:D:301:LYS:HG3	2.16	0.46
1:D:365:SER:HA	1:D:368:PHE:HD2	1.80	0.46
1:A:187:ARG:HA	1:A:187:ARG:HD3	1.77	0.45
1:C:183:SER:N	1:C:200:GLN:O	2.48	0.45
1:C:436:ILE:HG22	1:C:437:GLN:N	2.22	0.45
1:D:183:SER:HB3	1:F:176:THR:HG23	1.98	0.45
1:B:267:ILE:HD13	1:B:299:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:338:THR:O	1:E:339:LEU:HD23	2.17	0.45
1:A:298:SER:HA	1:A:301:LYS:HE2	1.98	0.45
1:A:288:ALA:HB3	1:A:310:ILE:HB	1.99	0.45
1:A:288:ALA:O	1:A:309:VAL:HA	2.17	0.45
1:D:234:GLY:O	1:D:236:ILE:HG23	2.17	0.45
1:D:202:ASP:HB3	1:F:178:THR:HG22	1.98	0.45
1:E:399:ILE:HG22	1:E:447:MET:HE1	1.99	0.45
1:B:204:ALA:HA	1:B:235:ASN:OD1	2.17	0.45
1:C:92:ILE:HA	1:C:100:VAL:HA	1.99	0.45
1:D:83:LYS:HB2	1:D:83:LYS:HE3	1.79	0.45
1:C:19:LEU:HD21	1:C:165:VAL:HG11	1.99	0.45
1:C:272:LEU:HD21	1:C:284:ALA:O	2.17	0.45
1:D:387:VAL:CG2	1:D:405:ASP:H	2.04	0.45
1:F:102:THR:OG1	1:F:103:ASN:N	2.50	0.45
1:A:173:LEU:HD11	1:B:229:LEU:HD23	1.99	0.44
1:C:433:ALA:C	1:C:434:LEU:HD13	2.42	0.44
1:F:103:ASN:HD21	1:F:226:THR:HG23	1.82	0.44
1:F:395:PRO:O	1:F:399:ILE:HG23	2.17	0.44
1:B:378:ASN:HD21	1:B:417:ASN:HB2	1.82	0.44
1:C:271:GLU:OE2	1:C:320:SER:HB2	2.17	0.44
1:D:19:LEU:HB3	1:D:23:MET:SD	2.57	0.44
1:C:235:ASN:CG	1:C:237:GLY:H	2.25	0.44
1:B:176:THR:HG23	1:C:183:SER:HB3	2.00	0.44
1:C:304:ILE:HA	1:C:343:ARG:HH22	1.82	0.44
1:C:131:ASP:HB2	1:C:260:VAL:HG21	1.98	0.44
1:E:136:ILE:HD12	1:E:250:LEU:HD12	1.99	0.44
1:B:130:LYS:O	1:B:132:PRO:HD3	2.18	0.44
1:C:328:VAL:HG12	1:C:331:MET:SD	2.57	0.44
1:D:226:THR:HG21	1:D:242:ILE:HD12	2.00	0.44
1:E:198:PHE:CD2	1:E:240:PHE:HB3	2.53	0.44
1:F:374:ALA:HB1	1:F:387:VAL:HG13	2.00	0.44
1:F:440:ASP:OD1	1:F:440:ASP:N	2.48	0.44
1:B:150:ILE:HD13	1:B:221:LEU:HB2	2.00	0.44
1:B:223:GLY:HA2	1:B:242:ILE:O	2.18	0.44
1:B:416:LYS:HE3	1:B:420:GLU:OE2	2.18	0.44
1:C:425:LEU:HD21	1:C:432:LEU:HD11	1.99	0.44
1:A:195:TYR:HD1	1:A:326:ALA:HA	1.83	0.43
1:B:18:MET:SD	1:B:18:MET:C	3.01	0.43
1:C:168:GLY:O	1:C:175:GLU:HA	2.18	0.43
1:C:415:VAL:HG23	1:C:420:GLU:HB2	2.00	0.43
1:D:387:VAL:HG23	1:D:404:GLY:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LYS:NZ	1:E:418:ILE:HB	2.32	0.43
1:F:311:THR:O	1:F:318:ILE:HG22	2.17	0.43
1:B:435:ASN:HB2	1:B:444:TYR:CZ	2.53	0.43
1:E:308:ASP:OD1	1:E:343:ARG:HG2	2.19	0.43
1:A:373:GLY:HA2	1:A:395:PRO:HD2	2.00	0.43
1:E:104:ASN:HB3	1:E:135:ASP:HA	1.99	0.43
1:D:280:MET:HB3	1:D:282:VAL:HG23	1.99	0.43
1:F:445:LEU:HD23	1:F:445:LEU:HA	1.79	0.43
1:C:92:ILE:HG13	1:C:149:ALA:HA	1.99	0.43
1:E:158:LEU:HD22	1:E:182:VAL:HG21	2.01	0.43
1:F:417:ASN:ND2	1:F:419:ALA:HB3	2.34	0.43
1:B:205:ILE:HG23	1:B:209:ASN:HB3	2.01	0.43
1:F:205:ILE:HD13	1:F:225:ASN:HB3	1.99	0.43
1:F:415:VAL:HG21	1:F:421:LEU:HB2	2.01	0.43
1:A:158:LEU:HD11	1:A:222:ILE:HD12	2.00	0.43
1:A:183:SER:N	1:A:200:GLN:O	2.51	0.43
1:A:251:THR:HA	1:A:254:MET:HB2	2.00	0.43
1:B:379:LYS:HD3	1:B:379:LYS:HA	1.72	0.43
1:E:205:ILE:HG23	1:E:209:ASN:HB3	2.01	0.43
1:E:389:ASN:HA	1:E:403:LYS:HD2	2.00	0.43
1:C:169:ASN:O	1:C:169:ASN:ND2	2.52	0.43
1:D:409:GLY:O	1:D:435:ASN:HB2	2.19	0.43
1:F:312:SER:OG	1:F:340:GLY:HA3	2.19	0.43
1:B:281:LYS:HE3	1:B:281:LYS:HB2	1.92	0.43
1:C:435:ASN:O	1:C:436:ILE:HG13	2.19	0.43
1:A:249:ASN:HB2	1:A:330:THR:HG22	1.99	0.43
1:A:272:LEU:HD22	1:A:309:VAL:HG11	1.99	0.43
1:D:343:ARG:HG3	1:D:344:ASP:H	1.83	0.43
1:F:126:LYS:HE2	1:F:126:LYS:HB3	1.87	0.43
1:A:313:LEU:HD22	1:A:324:LEU:HD12	2.00	0.42
1:A:343:ARG:HD2	1:A:348:VAL:HG21	2.01	0.42
1:B:232:ASP:OD1	1:B:232:ASP:N	2.50	0.42
1:A:308:ASP:OD2	1:A:343:ARG:NH1	2.52	0.42
1:B:250:LEU:O	1:B:254:MET:HG3	2.19	0.42
1:B:269:GLY:HA3	1:B:289:PHE:O	2.20	0.42
1:C:119:ASP:OD1	1:C:119:ASP:N	2.50	0.42
1:C:197:ASN:O	1:C:197:ASN:ND2	2.51	0.42
1:F:416:LYS:HB2	1:F:417:ASN:H	1.74	0.42
1:B:104:ASN:CB	1:B:137:ALA:HB2	2.49	0.42
1:C:103:ASN:HD22	1:C:103:ASN:C	2.27	0.42
1:F:153:ALA:HB2	1:F:220:GLU:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:HG21	1:B:200:GLN:HE22	1.85	0.42
1:C:99:TYR:HE1	1:C:140:GLN:OE1	2.01	0.42
1:C:274:SER:HA	1:C:285:GLN:HG3	2.01	0.42
1:E:309:VAL:O	1:E:341:LEU:HA	2.20	0.42
1:E:436:ILE:HD11	1:E:438:ARG:HE	1.83	0.42
1:A:374:ALA:HB1	1:A:390:VAL:HA	2.00	0.42
1:B:87:LEU:HD12	1:B:87:LEU:O	2.20	0.42
1:A:246:MET:HB3	1:A:246:MET:HE3	1.79	0.42
1:B:443:ILE:CG2	1:B:444:TYR:N	2.83	0.42
1:C:210:ALA:HB2	2:I:464:LEU:O	2.19	0.42
1:D:264:GLU:HB2	1:D:357:SER:HA	2.01	0.42
1:E:205:ILE:HG22	2:K:464:LEU:HD11	2.02	0.42
1:B:31:VAL:O	1:B:85:MET:HA	2.19	0.42
1:B:399:ILE:HD12	1:B:447:MET:HE2	2.02	0.42
1:D:156:ASP:HB3	1:D:316:LYS:HE2	2.01	0.42
1:D:385:VAL:HG12	1:D:386:VAL:N	2.35	0.42
1:D:267:ILE:HD12	1:D:290:VAL:HG12	2.01	0.42
1:B:421:LEU:HG	1:B:425:LEU:HD11	2.02	0.42
1:C:30:ASN:OD1	1:C:87:LEU:HD22	2.20	0.42
1:D:121:ARG:HG2	1:E:285:GLN:HG2	2.01	0.42
1:D:352:LEU:HD23	1:D:352:LEU:HA	1.89	0.42
1:E:205:ILE:O	1:E:235:ASN:HB2	2.20	0.42
1:A:31:VAL:HG21	1:A:107:VAL:HG23	2.02	0.41
1:A:133:ARG:HB3	1:A:195:TYR:CD2	2.55	0.41
1:B:341:LEU:HB3	1:B:348:VAL:HG23	2.02	0.41
1:D:323:ALA:O	1:D:327:GLN:N	2.47	0.41
1:D:326:ALA:O	1:D:330:THR:HG22	2.19	0.41
1:E:399:ILE:HG22	1:E:447:MET:CE	2.50	0.41
1:B:16:ALA:N	1:B:17:PRO:HD2	2.35	0.41
1:B:19:LEU:CD1	1:B:177:VAL:HG11	2.50	0.41
1:C:407:ILE:HG12	1:C:436:ILE:HD13	2.01	0.41
1:D:150:ILE:HD13	1:D:221:LEU:HB2	2.02	0.41
1:D:168:GLY:HA3	1:D:209:ASN:HD22	1.86	0.41
1:D:379:LYS:HE2	1:D:383:GLN:HB2	2.01	0.41
1:E:385:VAL:HG22	1:E:418:ILE:HG12	2.02	0.41
1:B:183:SER:HB2	1:B:200:GLN:HG2	2.02	0.41
1:D:163:TYR:HB2	1:D:217:LEU:HD11	2.02	0.41
1:D:407:ILE:HG13	1:D:408:ILE:H	1.85	0.41
1:A:150:ILE:HG12	1:A:151:LYS:O	2.21	0.41
1:C:250:LEU:O	1:C:254:MET:HG3	2.19	0.41
1:C:342:LEU:HD12	1:C:342:LEU:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:ASN:C	1:C:436:ILE:CG1	2.92	0.41
1:E:88:GLY:HA3	1:E:106:VAL:HG21	2.02	0.41
1:E:387:VAL:CG2	1:E:403:LYS:HA	2.50	0.41
1:F:290:VAL:HG23	1:F:308:ASP:O	2.18	0.41
1:A:227:ALA:O	1:A:240:PHE:N	2.54	0.41
1:B:133:ARG:HG3	1:B:262:ARG:HH21	1.86	0.41
1:D:160:VAL:HG11	1:F:23:MET:HE1	2.03	0.41
1:F:422:ARG:O	1:F:426:ASP:N	2.40	0.41
1:A:152:MET:CE	1:A:248:LYS:HB2	2.51	0.41
1:B:117:LEU:HD11	1:B:147:LEU:HD22	2.03	0.41
1:D:407:ILE:HG13	1:D:408:ILE:N	2.36	0.41
1:E:379:LYS:CA	1:E:384:GLY:HA2	2.51	0.41
1:E:405:ASP:OD1	1:E:406:VAL:N	2.53	0.41
1:D:173:LEU:HD11	1:E:229:LEU:HD23	2.02	0.41
1:F:191:ASN:HB3	1:F:194:ASN:HB2	2.02	0.41
1:A:174:GLY:O	1:A:176:THR:HG23	2.21	0.41
1:A:228:ILE:O	1:A:228:ILE:HG13	2.21	0.41
1:D:341:LEU:HB2	1:D:348:VAL:O	2.21	0.41
1:F:368:PHE:CE2	1:F:422:ARG:HD3	2.56	0.41
1:A:305:LYS:H	1:A:343:ARG:HH12	1.67	0.41
1:B:411:ASN:OD1	1:B:433:ALA:N	2.39	0.41
1:D:385:VAL:C	1:D:406:VAL:HG21	2.46	0.41
1:E:261:LYS:HG3	1:E:333:VAL:HG23	2.03	0.41
1:E:399:ILE:H	1:E:399:ILE:HG13	1.68	0.41
1:F:198:PHE:CD2	1:F:240:PHE:HB3	2.56	0.41
1:F:250:LEU:O	1:F:254:MET:HG3	2.21	0.41
1:F:271:GLU:OE2	1:F:320:SER:HB2	2.21	0.41
1:A:299:ALA:HA	1:A:352:LEU:HD13	2.03	0.40
1:B:195:TYR:HE1	1:B:325:ARG:HE	1.69	0.40
1:D:28:SER:HB3	1:D:169:ASN:HD22	1.86	0.40
1:F:25:SER:HB3	1:F:150:ILE:HB	2.03	0.40
1:F:136:ILE:HD11	1:F:242:ILE:HG21	2.02	0.40
1:B:200:GLN:HA	1:B:239:GLY:O	2.22	0.40
1:C:204:ALA:HA	1:C:235:ASN:ND2	2.36	0.40
1:C:376:MET:HB3	1:C:385:VAL:HG11	2.03	0.40
1:C:433:ALA:HA	1:C:446:LEU:HA	2.04	0.40
1:D:236:ILE:HG21	1:F:234:GLY:HA3	2.03	0.40
1:D:288:ALA:O	1:D:309:VAL:HA	2.20	0.40
1:D:415:VAL:CG1	1:D:421:LEU:HB2	2.51	0.40
1:F:313:LEU:N	1:F:316:LYS:O	2.47	0.40
1:A:376:MET:HG2	1:A:387:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:LEU:HD13	1:E:421:LEU:HA	1.88	0.40
1:A:19:LEU:HD21	1:A:177:VAL:HG11	2.04	0.40
1:D:250:LEU:HD13	1:D:330:THR:OG1	2.21	0.40
1:D:305:LYS:CD	1:D:343:ARG:HH22	2.29	0.40
1:E:385:VAL:O	1:E:385:VAL:HG12	2.21	0.40
1:F:27:VAL:HG21	1:F:115:VAL:HG13	2.04	0.40
1:B:103:ASN:OD1	1:B:211:GLY:N	2.54	0.40
1:B:305:LYS:HB2	1:B:343:ARG:HH12	1.87	0.40
1:D:205:ILE:O	1:D:235:ASN:HB2	2.22	0.40
1:F:214:LEU:O	1:F:222:ILE:HG12	2.21	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:A:257:TYR:OH	1:A:257:TYR:OH[2_555]	2.05	0.15

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	375/440 (85%)	342 (91%)	28 (8%)	5 (1%)	9	41
1	B	388/440 (88%)	358 (92%)	27 (7%)	3 (1%)	16	52
1	C	376/440 (86%)	345 (92%)	29 (8%)	2 (0%)	24	62
1	D	382/440 (87%)	339 (89%)	40 (10%)	3 (1%)	16	52
1	E	382/440 (87%)	353 (92%)	25 (6%)	4 (1%)	12	47
1	F	373/440 (85%)	352 (94%)	17 (5%)	4 (1%)	11	45
2	G	3/5 (60%)	3 (100%)	0	0	100	100
2	H	3/5 (60%)	3 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I	3/5 (60%)	3 (100%)	0	0	100	100
2	J	3/5 (60%)	3 (100%)	0	0	100	100
2	K	3/5 (60%)	3 (100%)	0	0	100	100
2	L	3/5 (60%)	3 (100%)	0	0	100	100
2	M	3/5 (60%)	3 (100%)	0	0	100	100
2	N	3/5 (60%)	3 (100%)	0	0	100	100
2	O	3/5 (60%)	3 (100%)	0	0	100	100
2	P	3/5 (60%)	3 (100%)	0	0	100	100
2	Q	3/5 (60%)	3 (100%)	0	0	100	100
2	R	3/5 (60%)	3 (100%)	0	0	100	100
All	All	2312/2700 (86%)	2125 (92%)	166 (7%)	21 (1%)	14	49

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	408	ILE
1	F	291	SER
1	F	369	ASN
1	A	335	SER
1	C	436	ILE
1	D	411	ASN
1	E	383	GLN
1	F	372	GLU
1	B	370	GLY
1	B	409	GLY
1	B	430	SER
1	E	370	GLY
1	A	175	GLU
1	A	369	ASN
1	D	434	LEU
1	E	347	GLN
1	E	407	ILE
1	F	438	ARG
1	A	380	GLY
1	C	408	ILE
1	A	160	VAL

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	301/350 (86%)	293 (97%)	8 (3%)	39	60
1	B	312/350 (89%)	302 (97%)	10 (3%)	34	56
1	C	302/350 (86%)	292 (97%)	10 (3%)	33	55
1	D	308/350 (88%)	299 (97%)	9 (3%)	37	58
1	E	308/350 (88%)	302 (98%)	6 (2%)	50	66
1	F	300/350 (86%)	292 (97%)	8 (3%)	39	60
2	I	1/5 (20%)	0	1 (100%)	0	0
2	K	1/5 (20%)	1 (100%)	0	100	100
2	M	1/5 (20%)	1 (100%)	0	100	100
All	All	1834/2115 (87%)	1782 (97%)	52 (3%)	38	59

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	ASP
1	A	188	SER
1	A	260	VAL
1	A	293	VAL
1	A	338	THR
1	A	341	LEU
1	A	416	LYS
1	A	447	MET
1	B	83	LYS
1	B	87	LEU
1	B	102	THR
1	B	104	ASN
1	B	133	ARG
1	B	134	SER
1	B	190	LEU
1	B	293	VAL
1	B	320	SER
1	B	440	ASP

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Mol	Chain	Res	Type
1	C	101	VAL
1	C	145	LYS
1	C	178	THR
1	C	183	SER
1	C	214	LEU
1	C	319	SER
1	C	338	THR
1	C	385	VAL
1	C	434	LEU
1	C	445	LEU
1	D	25	SER
1	D	28	SER
1	D	34	SER
1	D	82	GLN
1	D	178	THR
1	D	182	VAL
1	D	185	LEU
1	D	290	VAL
1	D	443	ILE
1	E	22	VAL
1	E	87	LEU
1	E	291	SER
1	E	319	SER
1	E	354	LEU
1	E	447	MET
1	F	85	MET
1	F	148	THR
1	F	228	ILE
1	F	297	SER
1	F	350	VAL
1	F	377	SER
1	F	385	VAL
1	F	425	LEU
2	I	464	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	218	ASN
1	A	253	GLN
1	A	355	GLN

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Mol	Chain	Res	Type
1	B	103	ASN
1	B	104	ASN
1	B	109	ASN
1	B	200	GLN
1	B	206	ASN
1	B	369	ASN
1	B	388	ASN
1	C	103	ASN
1	C	169	ASN
1	C	327	GLN
1	C	383	GLN
1	C	389	ASN
1	C	435	ASN
1	D	296	ASN
1	D	355	GLN
1	D	369	ASN
1	D	398	GLN
1	D	412	GLN
1	E	109	ASN
1	E	194	ASN
1	E	209	ASN
1	E	285	GLN
1	F	109	ASN
1	F	116	GLN
1	F	388	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

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	381/440 (86%)	0.43	12 (3%) 51 39	2, 30, 97, 131	0
1	B	392/440 (89%)	0.50	10 (2%) 57 43	4, 50, 117, 166	0
1	C	382/440 (86%)	0.48	15 (3%) 43 36	2, 29, 128, 152	0
1	D	388/440 (88%)	0.72	25 (6%) 25 25	8, 69, 164, 208	0
1	E	388/440 (88%)	0.66	26 (6%) 24 24	6, 55, 134, 165	0
1	F	379/440 (86%)	0.43	4 (1%) 78 62	7, 35, 90, 119	0
2	G	5/5 (100%)	1.66	2 (40%) 1 2	24, 43, 44, 47	0
2	H	5/5 (100%)	1.75	2 (40%) 1 2	59, 67, 80, 85	0
2	I	5/5 (100%)	1.85	2 (40%) 1 2	24, 57, 76, 85	0
2	J	5/5 (100%)	1.49	1 (20%) 3 6	42, 60, 70, 73	0
2	K	5/5 (100%)	2.40	3 (60%) 0 1	60, 67, 79, 87	0
2	L	5/5 (100%)	2.33	3 (60%) 0 1	57, 80, 100, 104	0
2	M	5/5 (100%)	0.63	0 100 100	26, 33, 59, 59	0
2	N	5/5 (100%)	0.62	0 100 100	54, 65, 70, 72	0
2	O	5/5 (100%)	1.69	1 (20%) 3 6	82, 85, 107, 113	0
2	P	5/5 (100%)	1.72	2 (40%) 1 2	50, 71, 90, 98	0
2	Q	5/5 (100%)	1.35	2 (40%) 1 2	28, 42, 87, 94	0
2	R	5/5 (100%)	1.14	1 (20%) 3 6	61, 65, 79, 90	0
All	All	2370/2700 (87%)	0.56	111 (4%) 36 32	2, 45, 124, 208	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	392	THR	4.5
2	K	463	LYS	4.0
1	C	407	ILE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	442	THR	3.9
2	O	471	CYS	3.9
2	L	460	CYS	3.8
2	I	460	CYS	3.5
1	E	414	ALA	3.5
1	B	369	ASN	3.5
1	C	408	ILE	3.3
1	E	372	GLU	3.3
1	E	369	ASN	3.2
1	D	375	GLU	3.2
2	G	463	LYS	3.2
2	H	464	LEU	3.2
2	J	460	CYS	3.1
2	Q	471	CYS	3.1
1	C	266	GLY	3.0
1	D	392	THR	3.0
1	A	392	THR	3.0
2	P	471	CYS	3.0
1	D	292	GLN	2.9
1	E	390	VAL	2.9
1	C	34	SER	2.9
2	K	460	CYS	2.8
2	P	473	ARG	2.8
2	L	462	ARG	2.8
1	D	377	SER	2.8
1	C	369	ASN	2.7
1	C	409	GLY	2.7
1	C	148	THR	2.7
1	D	362	VAL	2.7
1	B	312	SER	2.6
1	D	438	ARG	2.6
1	E	266	GLY	2.6
1	D	405	ASP	2.6
2	I	463	LYS	2.6
1	E	35	THR	2.6
1	B	365	SER	2.6
1	A	409	GLY	2.5
1	F	380	GLY	2.5
1	E	374	ALA	2.5
1	D	296	ASN	2.5
1	B	95	ALA	2.5
1	A	193	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	414	ALA	2.5
1	D	390	VAL	2.4
1	E	366	SER	2.4
2	Q	472	TYR	2.4
2	R	473	ARG	2.4
1	E	383	GLN	2.4
1	B	392	THR	2.4
1	E	426	ASP	2.4
1	D	391	LYS	2.3
1	E	396	ALA	2.3
1	E	358	SER	2.3
1	B	262	ARG	2.3
1	C	278	LYS	2.3
1	E	412	GLN	2.3
1	D	414	ALA	2.3
1	B	385	VAL	2.3
1	A	110	ALA	2.3
1	D	293	VAL	2.3
2	H	460	CYS	2.3
1	E	405	ASP	2.3
1	E	359	GLN	2.3
1	C	388	ASN	2.2
1	E	378	ASN	2.2
2	K	462	ARG	2.2
1	D	372	GLU	2.2
1	A	195	TYR	2.2
1	A	368	PHE	2.2
1	E	193	GLU	2.2
1	E	371	ILE	2.2
1	E	389	ASN	2.2
1	D	439	GLY	2.2
1	C	395	PRO	2.2
1	C	392	THR	2.2
1	D	134	SER	2.2
1	E	386	VAL	2.2
1	A	390	VAL	2.2
1	D	115	VAL	2.2
1	E	391	LYS	2.1
1	A	391	LYS	2.1
1	D	84	PHE	2.1
1	E	393	GLY	2.1
1	F	418	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	460	CYS	2.1
1	D	331	MET	2.1
1	C	35	THR	2.1
1	D	35	THR	2.1
1	A	168	GLY	2.1
1	D	429	PRO	2.1
1	E	381	LYS	2.1
1	A	10	GLN	2.1
1	B	401	LEU	2.1
1	D	393	GLY	2.1
1	A	377	SER	2.1
1	C	406	VAL	2.1
1	E	422	ARG	2.0
1	B	395	PRO	2.0
1	D	388	ASN	2.0
1	D	436	ILE	2.0
1	B	193	GLU	2.0
1	F	274	SER	2.0
1	E	418	ILE	2.0
2	L	461	TYR	2.0
1	A	32	GLU	2.0
1	C	378	ASN	2.0
1	D	394	THR	2.0
1	D	366	SER	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.