



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:29 AM UTC

PDB ID : 7KGV / pdb_00007kgv
Title : Crystal structure of sodium-coupled neutral amino acid transporter SLC38A9 in the N-terminal plugged form
Authors : Lei, H.; Mu, X.; Hattne, J.; Gonen, T.
Deposited on : 2020-10-19
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

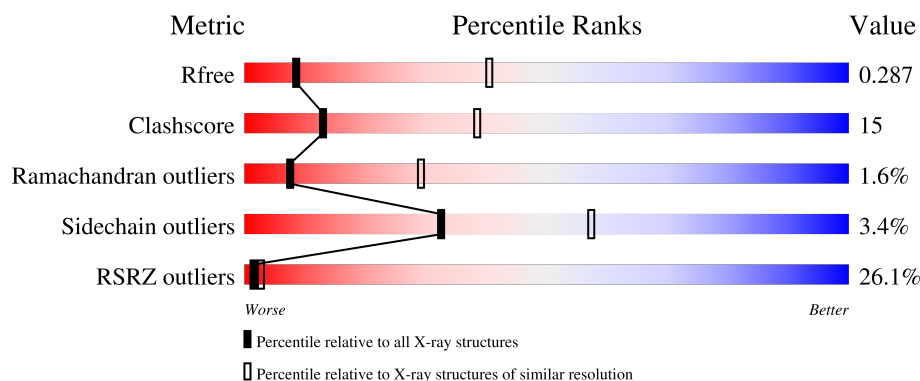
1 Overall quality at a glance

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	549	23% 46% 18% 34%
1	B	549	27% 47% 24% 26%
2	C	219	22% 72% 26%
2	D	219	15% 70% 26%
3	E	215	21% 66% 32%

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Mol	Chain	Length	Quality of chain
3	F	215	12% 71% 26% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12613 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 Sodium-coupled neutral amino acid transporter 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2905	1975	441	471	18			
1	B	404	Total	C	N	O	S	0	0	0
			3269	2211	508	531	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	227	GLN	ASN	engineered mutation	UNP Q08BA4
A	235	GLN	ASN	engineered mutation	UNP Q08BA4
A	252	GLN	ASN	engineered mutation	UNP Q08BA4
A	263	GLN	ASN	engineered mutation	UNP Q08BA4
B	227	GLN	ASN	engineered mutation	UNP Q08BA4
B	235	GLN	ASN	engineered mutation	UNP Q08BA4
B	252	GLN	ASN	engineered mutation	UNP Q08BA4
B	263	GLN	ASN	engineered mutation	UNP Q08BA4

- Molecule 2 is a protein called Monoclonal antibody Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	217	Total	C	N	O	S	0	0	0
			1574	987	261	319	7			
2	D	216	Total	C	N	O	S	0	0	0
			1569	984	260	318	7			

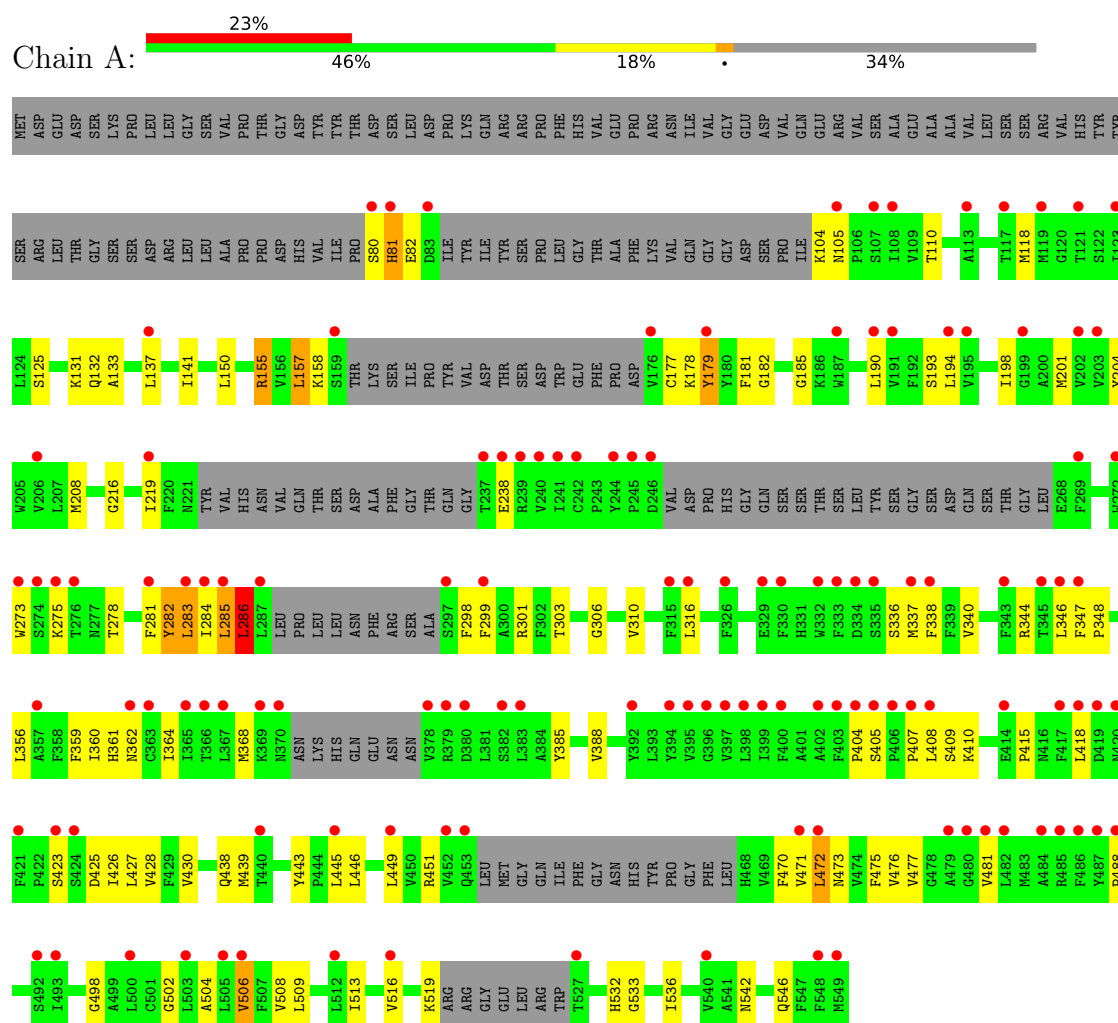
- Molecule 3 is a protein called Monoclonal antibody Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	215	Total	C	N	O	S	0	0	0
			1648	1036	273	335	4			
3	F	215	Total	C	N	O	S	0	0	0
			1648	1036	273	335	4			

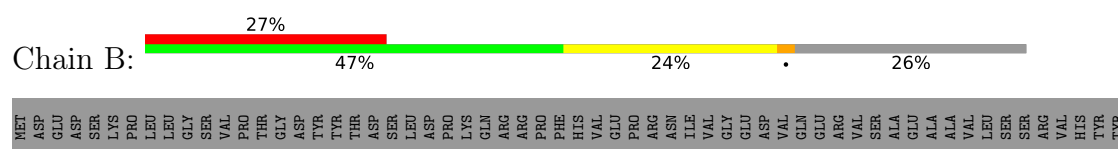
3 Residue-property plots

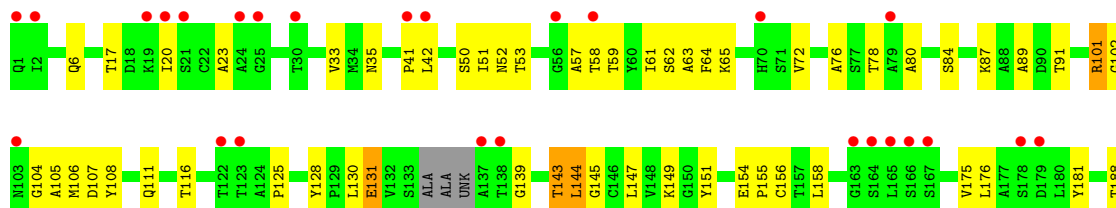
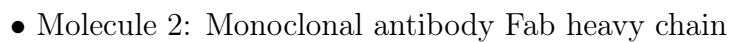
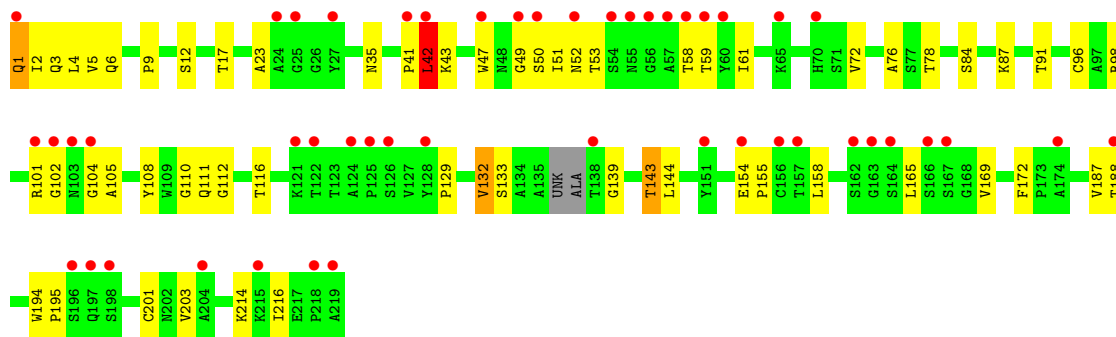
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

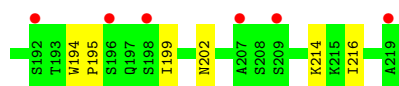
- Molecule 1: Sodium-coupled neutral amino acid transporter 9



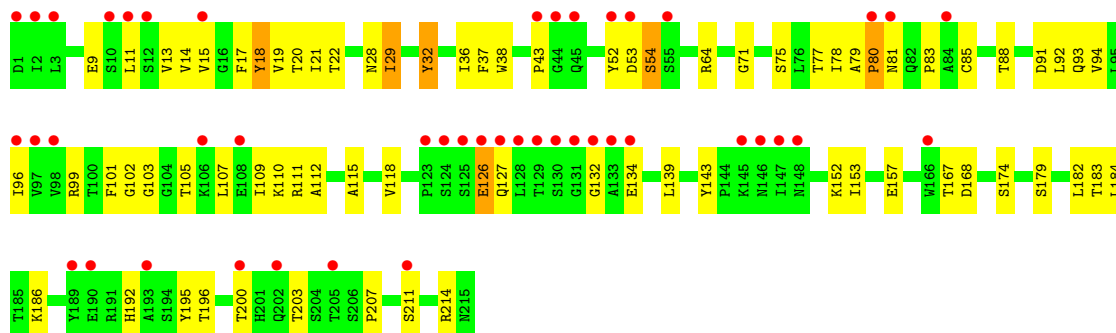
- Molecule 1: Sodium-coupled neutral amino acid transporter 9



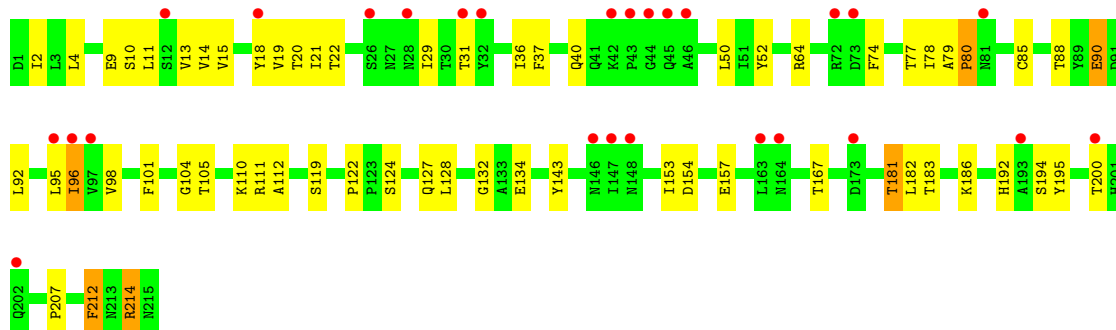




• Molecule 3: Monoclonal antibody Fab light chain



• Molecule 3: Monoclonal antibody Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	157.80Å 82.51Å 158.59Å 90.00° 106.02° 90.00°	Depositor
Resolution (Å)	49.37 – 3.40 49.37 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.37-3.40) 99.8 (49.37-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.251 , 0.284 0.252 , 0.287	Depositor DCC
R_{free} test set	1699 reflections (2.62%)	wwPDB-VP
Wilson B-factor (Å ²)	97.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12613	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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	0.39	0/2989	0.63	2/4059 (0.0%)
1	B	0.44	0/3367	0.73	1/4575 (0.0%)
2	C	0.54	0/1610	0.80	1/2198 (0.0%)
2	D	0.51	0/1605	0.77	0/2191
3	E	0.53	0/1685	0.80	1/2296 (0.0%)
3	F	0.55	0/1685	0.75	0/2296
All	All	0.48	0/12941	0.74	5/17615 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	C	0	1
All	All	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	LEU	CD1-CG-CD2	11.31	135.69	110.80
1	A	286	LEU	CA-CB-CG	6.93	140.55	116.30
1	B	82	GLU	CB-CA-C	-5.30	108.80	116.54
2	C	49	GLY	CA-C-O	-5.22	118.56	122.37
3	E	18	TYR	CA-CB-CG	5.03	122.96	113.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	104	LYS	Peptide
2	C	1	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2905	0	2970	87	0
1	B	3269	0	3333	99	1
2	C	1574	0	1533	47	0
2	D	1569	0	1528	49	0
3	E	1648	0	1590	61	0
3	F	1648	0	1590	54	0
All	All	12613	0	12544	376	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 15.

All (376) 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)
3:F:18:TYR:HE1	3:F:77:THR:HB	1.30	0.94
3:F:64:ARG:HB2	3:F:80:PRO:HD2	1.47	0.93
3:E:18:TYR:HE1	3:E:77:THR:HB	1.34	0.92
3:F:18:TYR:CE1	3:F:77:THR:HB	2.09	0.87
1:A:81:HIS:CD2	1:A:82:GLU:HG2	2.08	0.87
1:B:80:SER:O	1:B:81:HIS:ND1	2.07	0.87
2:C:129:PRO:HG3	2:C:214:LYS:HB3	1.56	0.87
1:B:118:MET:HE3	1:B:388:VAL:HG21	1.55	0.85
3:F:13:VAL:HG21	3:F:19:VAL:HB	1.60	0.83
3:E:18:TYR:CE1	3:E:77:THR:HB	2.17	0.80
1:A:81:HIS:CG	1:A:82:GLU:H	2.01	0.79
1:B:81:HIS:HB2	1:B:122:SER:HB3	1.66	0.78
2:C:144:LEU:HD22	2:C:216:ILE:HG21	1.66	0.78
1:A:306:GLY:HA2	1:A:438:GLN:HG3	1.66	0.77
1:B:508:VAL:HA	1:B:536:ILE:HD13	1.65	0.77
2:C:53:THR:HG22	2:C:72:VAL:HG11	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:SER:O	1:A:81:HIS:ND1	2.18	0.76
3:E:64:ARG:HB2	3:E:80:PRO:HD2	1.68	0.75
3:E:64:ARG:NH2	3:E:85:CYS:SG	2.59	0.75
2:C:91:THR:HG23	2:C:116:THR:HA	1.69	0.74
3:E:37:PHE:HD1	3:E:52:TYR:HA	1.52	0.74
1:A:80:SER:HG	1:A:204:TYR:HH	1.33	0.74
3:F:127:GLN:HE22	3:F:134:GLU:CD	1.97	0.72
1:A:470:PHE:CD1	1:A:473:ASN:HB2	2.24	0.72
1:B:105:ASN:HB2	1:B:371:ASN:H	1.55	0.72
3:F:153:ILE:HD11	3:F:182:LEU:HD21	1.71	0.71
3:E:92:LEU:HD13	3:E:101:PHE:CE1	2.26	0.70
2:D:176:LEU:HG	2:D:181:TYR:CE1	2.27	0.69
2:D:53:THR:HG22	2:D:72:VAL:HG11	1.73	0.69
1:A:356:LEU:HD13	1:A:498:GLY:HA2	1.75	0.69
1:B:208:MET:HE2	1:B:439:MET:HB3	1.76	0.68
1:A:181:PHE:HB2	1:A:185:GLY:HA3	1.76	0.67
3:F:29:ILE:HD11	3:F:74:PHE:CE1	2.29	0.67
2:C:35:ASN:ND2	2:C:50:SER:OG	2.27	0.67
1:A:502:GLY:O	1:A:506:VAL:HG12	1.96	0.66
2:D:91:THR:HG23	2:D:116:THR:HA	1.77	0.66
1:A:177:CYS:SG	1:A:178:LYS:N	2.69	0.66
1:A:281:PHE:HA	1:A:284:ILE:HD13	1.77	0.66
3:F:92:LEU:HD13	3:F:101:PHE:CE2	2.31	0.66
3:E:192:HIS:O	3:E:214:ARG:NE	2.21	0.66
1:B:194:LEU:HD21	1:B:454:LEU:HG	1.76	0.66
1:B:216:GLY:HA2	1:B:219:ILE:HG12	1.77	0.65
1:B:306:GLY:HA2	1:B:438:GLN:HG3	1.77	0.65
3:E:118:VAL:HG22	3:E:139:LEU:HG	1.80	0.64
3:F:212:PHE:C	3:F:212:PHE:HD1	2.04	0.64
3:F:200:THR:HG22	3:F:207:PRO:HB3	1.78	0.64
1:A:285:LEU:HD11	1:A:477:VAL:HG23	1.80	0.64
1:B:404:PRO:HG3	3:E:32:TYR:HE2	1.62	0.64
1:A:470:PHE:CE1	1:A:473:ASN:HB2	2.31	0.64
2:C:2:ILE:HD13	2:C:98:ARG:NH1	2.12	0.64
1:A:425:ASP:HB3	1:A:428:VAL:HB	1.79	0.64
1:B:471:VAL:HA	1:B:474:VAL:HG12	1.80	0.63
2:D:194:TRP:CG	2:D:195:PRO:HA	2.33	0.63
1:A:446:LEU:HA	1:A:449:LEU:HB2	1.80	0.63
3:F:212:PHE:C	3:F:212:PHE:CD1	2.78	0.62
3:F:122:PRO:HB3	3:F:212:PHE:CE2	2.35	0.62
3:E:111:ARG:NH1	3:E:112:ALA:O	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:CE1	1:A:473:ASN:CB	2.82	0.61
1:B:75:ASP:HB2	1:B:86:ILE:HD12	1.81	0.61
3:F:64:ARG:NH2	3:F:85:CYS:SG	2.73	0.61
2:D:35:ASN:HD22	2:D:106:MET:HE2	1.65	0.61
1:B:275:LYS:C	1:B:277:ASN:H	2.09	0.61
2:D:52:ASN:ND2	2:D:101:ARG:HH21	1.99	0.61
1:B:335:SER:HB3	1:B:341:PRO:HD3	1.82	0.60
3:F:37:PHE:HD1	3:F:52:TYR:HA	1.66	0.60
1:A:81:HIS:CG	1:A:82:GLU:N	2.65	0.60
3:E:14:VAL:HG22	3:E:110:LYS:HG2	1.82	0.60
1:A:201:MET:SD	1:A:476:VAL:HG11	2.42	0.60
1:A:208:MET:HE2	1:A:439:MET:HB3	1.82	0.60
1:B:178:LYS:HE2	1:B:509:LEU:HD13	1.83	0.60
2:C:2:ILE:HD13	2:C:98:ARG:CZ	2.31	0.60
2:C:52:ASN:HB2	2:C:101:ARG:NH2	2.16	0.60
2:D:23:ALA:HA	2:D:78:THR:HG22	1.83	0.60
2:C:87:LYS:HE3	2:D:63:ALA:O	2.01	0.60
3:E:17:PHE:O	3:E:81:ASN:ND2	2.35	0.59
3:E:152:LYS:HB2	3:E:196:THR:OG1	2.02	0.59
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.85	0.59
3:F:90:GLU:HG3	3:F:104:GLY:HA2	1.83	0.59
1:B:80:SER:C	1:B:82:GLU:H	2.10	0.59
3:F:11:LEU:HD21	3:F:19:VAL:HG23	1.85	0.59
1:A:338:PHE:HB3	1:A:405:SER:O	2.03	0.58
3:E:79:ALA:HB3	3:E:80:PRO:HD3	1.85	0.58
3:F:79:ALA:HB3	3:F:80:PRO:HD3	1.85	0.58
1:B:310:VAL:O	1:B:314:ILE:HG12	2.03	0.58
1:B:85:TYR:C	1:B:85:TYR:HD2	2.11	0.58
3:F:9:GLU:HG2	3:F:10:SER:H	1.67	0.58
3:E:13:VAL:HG12	3:E:107:LEU:HD11	1.86	0.58
1:B:425:ASP:HB3	1:B:428:VAL:HB	1.84	0.58
3:E:94:VAL:HG13	3:E:99:ARG:HH12	1.68	0.58
1:A:282:TYR:HB2	1:A:477:VAL:HG11	1.86	0.57
3:E:14:VAL:HA	3:E:110:LYS:HB3	1.85	0.57
1:B:131:LYS:HD2	1:B:410:LYS:O	2.04	0.57
2:C:143:THR:HB	2:C:188:THR:HG22	1.87	0.57
1:B:85:TYR:C	1:B:85:TYR:CD2	2.83	0.56
1:B:177:CYS:C	1:B:179:TYR:H	2.13	0.56
1:B:137:LEU:O	1:B:141:ILE:HG12	2.05	0.56
2:C:169:VAL:HG22	2:C:187:VAL:HG22	1.86	0.56
2:D:87:LYS:HG3	2:D:89:ALA:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:THR:HB	2:D:188:THR:HG22	1.87	0.56
3:F:195:TYR:HB2	3:F:212:PHE:CE1	2.40	0.56
2:D:35:ASN:ND2	2:D:106:MET:HE2	2.21	0.56
3:E:21:ILE:HG12	3:E:105:THR:HG21	1.89	0.56
1:B:516:VAL:O	1:B:519:LYS:HG3	2.06	0.55
3:F:111:ARG:NH1	3:F:112:ALA:O	2.40	0.55
1:A:316:LEU:HD13	1:A:427:LEU:HB3	1.88	0.55
3:E:132:GLY:H	3:E:186:LYS:HB2	1.72	0.54
2:C:43:LYS:HD3	3:E:103:GLY:O	2.07	0.54
3:E:22:THR:HG22	3:E:75:SER:HB3	1.90	0.54
1:A:533:GLY:HA2	1:A:536:ILE:HD12	1.89	0.54
3:E:83:PRO:HB3	3:E:174:SER:OG	2.08	0.54
1:A:283:LEU:HA	1:A:286:LEU:HD13	1.89	0.54
1:A:337:MET:HB2	2:D:59:THR:CG2	2.37	0.54
1:B:281:PHE:HZ	1:B:443:TYR:HB3	1.72	0.54
2:D:62:SER:HA	2:D:65:LYS:HE3	1.89	0.54
1:A:137:LEU:O	1:A:141:ILE:HG12	2.08	0.54
3:E:36:ILE:HG22	3:E:54:SER:HB2	1.89	0.54
1:A:105:ASN:HB3	1:A:110:THR:OG1	2.07	0.54
2:D:52:ASN:HB2	2:D:101:ARG:NH2	2.23	0.54
1:B:174:PRO:C	1:B:176:VAL:H	2.16	0.53
1:A:404:PRO:O	1:A:408:LEU:HB2	2.09	0.53
2:C:51:ILE:HD13	2:C:72:VAL:HG13	1.90	0.53
3:F:19:VAL:CG1	3:F:78:ILE:HB	2.38	0.53
1:B:281:PHE:CZ	1:B:443:TYR:HB3	2.43	0.53
3:E:11:LEU:HD21	3:E:19:VAL:HG23	1.89	0.53
2:C:158:LEU:HD13	2:C:203:VAL:HG22	1.90	0.53
3:F:40:GLN:HB2	3:F:50:LEU:HD11	1.91	0.53
1:A:286:LEU:HG	1:A:470:PHE:CD1	2.44	0.53
2:C:214:LYS:NZ	3:E:126:GLU:OE2	2.39	0.53
1:A:82:GLU:OE1	1:A:359:PHE:HB3	2.08	0.52
2:D:128:TYR:HB3	3:F:124:SER:OG	2.08	0.52
1:A:516:VAL:O	1:A:519:LYS:HG3	2.08	0.52
3:E:20:THR:HG23	3:E:77:THR:HG22	1.91	0.52
3:F:110:LYS:HA	3:F:143:TYR:OH	2.09	0.52
2:C:154:GLU:N	2:C:155:PRO:HD2	2.24	0.52
2:D:33:VAL:HG12	2:D:35:ASN:OD1	2.08	0.52
1:B:237:THR:HG22	1:B:239:ARG:HG2	1.92	0.52
1:A:194:LEU:O	1:A:198:ILE:HG12	2.10	0.52
1:A:470:PHE:CE1	1:A:473:ASN:HB3	2.44	0.52
3:F:29:ILE:C	3:F:95:LEU:HD13	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:GLU:OE2	3:F:122:PRO:HG2	2.10	0.51
1:B:451:ARG:HG3	1:B:455:MET:HG3	1.92	0.51
1:A:316:LEU:HD21	1:A:428:VAL:HG22	1.92	0.51
2:D:158:LEU:HA	2:D:202:ASN:O	2.11	0.51
3:E:153:ILE:HG23	3:E:195:TYR:CE1	2.46	0.51
3:E:200:THR:HG22	3:E:207:PRO:HG3	1.93	0.51
1:A:360:ILE:HG23	1:A:364:ILE:HB	1.92	0.51
1:B:338:PHE:HB3	1:B:405:SER:O	2.10	0.51
3:F:20:THR:HG23	3:F:77:THR:HG22	1.92	0.51
1:B:133:ALA:C	1:B:344:ARG:HB2	2.35	0.51
2:C:17:THR:HG22	2:C:84:SER:HA	1.92	0.51
2:D:154:GLU:N	2:D:155:PRO:HD2	2.25	0.50
2:D:76:ALA:O	2:D:78:THR:HG23	2.12	0.50
3:F:128:LEU:O	3:F:186:LYS:HD2	2.11	0.50
1:B:337:MET:HB2	2:C:59:THR:OG1	2.11	0.50
2:C:129:PRO:HB3	2:C:216:ILE:HD13	1.94	0.50
1:B:273:TRP:HA	1:B:273:TRP:CE3	2.46	0.50
1:B:269:PHE:CD2	1:B:271:HIS:HB3	2.46	0.50
3:E:153:ILE:HD11	3:E:182:LEU:HD21	1.94	0.49
1:B:278:THR:O	1:B:282:TYR:HD1	1.95	0.49
1:B:80:SER:C	1:B:82:GLU:N	2.71	0.49
2:D:194:TRP:CD1	2:D:199:ILE:HD12	2.47	0.49
1:A:508:VAL:HG22	1:A:536:ILE:HG23	1.95	0.49
2:C:6:GLN:NE2	2:C:96:CYS:SG	2.86	0.49
3:E:19:VAL:CG1	3:E:78:ILE:HB	2.43	0.49
1:A:284:ILE:HD12	1:A:284:ILE:H	1.77	0.49
1:A:131:LYS:HG3	1:A:410:LYS:O	2.13	0.49
1:B:211:PHE:CD1	1:B:432:ARG:HG2	2.48	0.49
3:E:19:VAL:HG12	3:E:78:ILE:HB	1.95	0.49
3:E:196:THR:HG22	3:E:211:SER:HB3	1.94	0.49
1:B:269:PHE:HD2	1:B:271:HIS:HB3	1.78	0.48
3:E:29:ILE:H	3:E:29:ILE:HD12	1.78	0.48
3:F:2:ILE:HG22	3:F:4:LEU:HD12	1.95	0.48
1:A:472:LEU:O	1:A:475:PHE:HB3	2.13	0.48
1:B:275:LYS:C	1:B:277:ASN:N	2.70	0.48
1:B:426:ILE:HD12	1:B:426:ILE:H	1.77	0.48
2:D:143:THR:HG22	2:D:188:THR:HB	1.95	0.48
1:B:157:LEU:HD21	1:B:368:MET:HG3	1.96	0.48
1:B:207:LEU:HG	1:B:490:ILE:HD11	1.95	0.48
3:F:192:HIS:O	3:F:214:ARG:NE	2.44	0.48
1:A:285:LEU:HD11	1:A:477:VAL:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:53:THR:CG2	2:C:72:VAL:HG11	2.41	0.48
3:F:132:GLY:H	3:F:186:LYS:HB2	1.78	0.48
3:F:154:ASP:HA	3:F:194:SER:HB3	1.94	0.48
3:E:183:THR:O	3:E:184:LEU:HD23	2.14	0.48
3:F:21:ILE:HG12	3:F:105:THR:HG21	1.95	0.48
1:B:509:LEU:O	1:B:513:ILE:HG12	2.14	0.48
2:C:3:GLN:HG3	2:C:5:VAL:HG23	1.96	0.48
3:E:111:ARG:HD2	3:E:174:SER:O	2.14	0.48
1:A:179:TYR:C	1:A:179:TYR:CD2	2.91	0.48
1:B:409:SER:O	1:B:412:CYS:HB2	2.14	0.48
3:E:38:TRP:CZ3	3:E:91:ASP:HB3	2.48	0.48
3:F:29:ILE:HA	3:F:95:LEU:HD13	1.96	0.48
2:D:17:THR:HG22	2:D:84:SER:HA	1.94	0.47
2:C:102:GLY:C	2:C:104:GLY:H	2.22	0.47
2:D:149:LYS:NZ	3:F:134:GLU:HG2	2.29	0.47
3:E:29:ILE:HG21	3:E:93:GLN:HB2	1.96	0.47
1:A:347:PHE:CG	1:A:348:PRO:HD3	2.49	0.47
1:B:288:LEU:HD13	1:B:297:SER:HA	1.95	0.47
1:B:320:LYS:HE3	1:B:421:PHE:CE1	2.49	0.47
2:D:105:ALA:HB2	3:F:37:PHE:CD1	2.50	0.47
1:A:542:ASN:O	1:A:546:GLN:HG2	2.14	0.47
1:A:273:TRP:HA	1:A:273:TRP:CE3	2.49	0.47
3:F:64:ARG:HD2	3:F:80:PRO:O	2.14	0.47
2:C:132:VAL:O	2:C:133:SER:HB2	2.15	0.47
1:A:125:SER:HA	1:A:415:PRO:O	2.14	0.47
1:A:201:MET:O	1:A:443:TYR:HE1	1.97	0.47
1:B:123:ILE:HG22	1:B:395:VAL:HG11	1.96	0.47
2:D:102:GLY:C	2:D:104:GLY:H	2.22	0.47
1:A:299:PHE:HB2	1:A:445:LEU:HD11	1.96	0.47
1:A:316:LEU:CD1	1:A:427:LEU:HB3	2.44	0.47
2:C:76:ALA:O	2:C:78:THR:HG23	2.15	0.47
3:F:134:GLU:HG3	3:F:183:THR:HG23	1.97	0.47
1:A:283:LEU:HA	1:A:286:LEU:CD1	2.44	0.47
3:E:15:VAL:HG22	3:E:109:ILE:CG2	2.45	0.47
3:F:92:LEU:HD13	3:F:101:PHE:CZ	2.50	0.47
2:C:47:TRP:CE2	3:E:99:ARG:HD2	2.49	0.47
3:E:196:THR:HG22	3:E:211:SER:CB	2.45	0.47
1:B:85:TYR:HB3	1:B:449:LEU:HD11	1.97	0.46
1:B:87:TYR:HB3	1:B:88:SER:H	1.49	0.46
1:B:544:LEU:HA	1:B:544:LEU:HD23	1.73	0.46
2:D:143:THR:HA	2:D:188:THR:HA	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:36:ILE:HG13	3:E:92:LEU:O	2.15	0.46
1:B:79:PRO:O	1:B:438:GLN:NE2	2.48	0.46
1:B:114:ILE:HG22	1:B:118:MET:HE2	1.98	0.46
1:B:177:CYS:C	1:B:179:TYR:N	2.74	0.46
2:D:144:LEU:HD13	2:D:216:ILE:HG13	1.97	0.46
1:B:447:GLY:O	1:B:450:VAL:HG12	2.16	0.46
1:A:408:LEU:HB3	1:A:409:SER:H	1.59	0.46
1:B:183:GLY:C	1:B:185:GLY:H	2.23	0.46
3:E:32:TYR:CD1	3:E:32:TYR:N	2.83	0.46
1:B:418:LEU:HD22	1:B:428:VAL:HG13	1.98	0.46
2:C:172:PHE:CD1	3:E:167:THR:HG23	2.50	0.46
3:E:115:ALA:HB2	3:E:203:THR:HG21	1.98	0.46
3:E:64:ARG:HD2	3:E:80:PRO:O	2.16	0.46
1:A:82:GLU:HB3	1:A:359:PHE:HD1	1.81	0.46
1:A:340:VAL:HB	1:A:344:ARG:HD2	1.97	0.46
2:D:151:TYR:CE2	2:D:156:CYS:HB2	2.51	0.46
3:E:127:GLN:HE22	3:E:134:GLU:HG2	1.81	0.46
2:C:6:GLN:NE2	2:C:96:CYS:H	2.14	0.45
1:A:132:GLN:O	1:A:346:LEU:HB2	2.16	0.45
3:E:94:VAL:HG13	3:E:99:ARG:NH1	2.29	0.45
1:B:302:PHE:HD1	1:B:304:PHE:HE1	1.64	0.45
1:B:354:LEU:HD23	1:B:354:LEU:HA	1.81	0.45
2:C:2:ILE:CD1	2:C:98:ARG:NH1	2.79	0.45
1:B:272:TRP:O	1:B:273:TRP:CD2	2.70	0.45
1:B:316:LEU:HD22	1:B:431:ALA:HB2	1.99	0.45
2:C:194:TRP:CG	2:C:195:PRO:HA	2.52	0.45
3:F:181:THR:O	3:F:181:THR:OG1	2.30	0.45
1:A:133:ALA:C	1:A:344:ARG:HB2	2.41	0.45
2:C:1:GLN:CD	2:C:2:ILE:H	2.24	0.45
1:B:178:LYS:HE3	1:B:509:LEU:HB3	1.99	0.45
2:C:23:ALA:HA	2:C:78:THR:HG22	1.99	0.45
2:D:51:ILE:HD13	2:D:72:VAL:HG13	1.99	0.45
2:C:111:GLN:HG2	2:C:112:GLY:N	2.31	0.45
2:D:130:LEU:HD11	2:D:147:LEU:HB2	1.99	0.45
1:A:407:PRO:HG3	3:F:31:THR:HG21	1.99	0.44
1:B:545:GLY:O	1:B:549:MET:HG2	2.16	0.44
2:C:47:TRP:CG	3:E:99:ARG:HB2	2.52	0.44
1:A:150:LEU:HD13	1:A:385:TYR:HB2	1.99	0.44
1:B:183:GLY:C	1:B:185:GLY:N	2.75	0.44
2:D:51:ILE:HD12	2:D:58:THR:HG22	2.00	0.44
1:A:439:MET:HE3	1:A:439:MET:HB2	1.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:PHE:O	1:B:139:ILE:HG12	2.17	0.44
1:B:218:PHE:HD1	1:B:424:SER:HA	1.83	0.44
1:A:118:MET:HE2	1:A:388:VAL:HG11	1.99	0.44
2:D:130:LEU:HB2	2:D:145:GLY:C	2.43	0.44
3:E:28:ASN:OD1	3:E:71:GLY:HA2	2.18	0.44
1:A:193:SER:HA	1:A:362:ASN:HD21	1.82	0.44
1:A:336:SER:O	2:D:57:ALA:HB1	2.18	0.44
1:A:508:VAL:HG13	1:A:536:ILE:HG12	1.99	0.44
1:B:509:LEU:HD23	1:B:509:LEU:HA	1.87	0.44
2:D:61:ILE:CG2	2:D:64:PHE:HD2	2.30	0.44
3:F:9:GLU:CD	3:F:9:GLU:H	2.24	0.44
1:A:298:PHE:O	1:A:301:ARG:HG3	2.18	0.44
2:D:62:SER:HA	2:D:65:LYS:CE	2.48	0.44
3:E:43:PRO:HB3	3:E:168:ASP:OD2	2.18	0.44
1:A:306:GLY:O	1:A:310:VAL:HG23	2.17	0.44
1:B:85:TYR:HD2	1:B:85:TYR:O	2.00	0.44
1:B:86:ILE:HG13	1:B:87:TYR:N	2.33	0.44
1:B:105:ASN:HA	1:B:106:PRO:HD3	1.72	0.44
1:B:200:ALA:HA	1:B:203:VAL:HG22	1.99	0.44
1:B:359:PHE:HE1	1:B:361:HIS:HB2	1.83	0.44
3:F:95:LEU:HD23	3:F:96:ILE:HG13	1.99	0.44
3:E:94:VAL:HG22	3:E:99:ARG:NH1	2.33	0.44
2:C:52:ASN:HB2	2:C:101:ARG:HH22	1.83	0.43
3:F:192:HIS:C	3:F:214:ARG:HH21	2.26	0.43
1:A:504:ALA:O	1:A:509:LEU:HB2	2.18	0.43
1:B:114:ILE:HB	1:B:384:ALA:HB1	1.99	0.43
1:B:201:MET:SD	1:B:476:VAL:HG11	2.58	0.43
1:B:514:HIS:O	1:B:518:LEU:HG	2.17	0.43
2:C:9:PRO:HB2	2:C:155:PRO:HG3	1.99	0.43
3:E:88:THR:HA	3:E:105:THR:O	2.19	0.43
1:A:80:SER:C	1:A:81:HIS:HD1	2.22	0.43
1:B:128:TRP:CD1	1:B:415:PRO:HG3	2.54	0.43
1:B:524:LEU:HD12	1:B:529:THR:HG22	2.00	0.43
2:C:165:LEU:HD21	2:C:187:VAL:HG11	2.00	0.43
1:A:275:LYS:O	1:A:278:THR:HG22	2.18	0.43
2:C:6:GLN:HE21	2:C:110:GLY:HA3	1.83	0.43
2:D:149:LYS:NZ	3:F:183:THR:OG1	2.51	0.43
1:B:87:TYR:O	1:B:88:SER:HB3	2.18	0.43
1:B:305:LEU:HD13	1:B:437:PHE:HB3	2.01	0.43
2:D:107:ASP:OD1	2:D:108:TYR:N	2.52	0.43
1:A:337:MET:SD	2:D:50:SER:HB2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:MET:HE3	1:B:388:VAL:HA	2.00	0.43
3:E:29:ILE:HD12	3:E:71:GLY:O	2.19	0.43
3:F:29:ILE:HD12	3:F:36:ILE:HB	2.01	0.43
1:B:81:HIS:CB	1:B:122:SER:HB3	2.44	0.43
1:A:337:MET:HB2	2:D:59:THR:HG22	2.00	0.42
3:E:38:TRP:CE3	3:E:91:ASP:HB3	2.54	0.42
2:C:42:LEU:HA	2:C:42:LEU:HD22	1.79	0.42
3:F:11:LEU:CD2	3:F:19:VAL:HG23	2.48	0.42
1:A:347:PHE:CD1	1:A:348:PRO:HD3	2.53	0.42
2:D:20:ILE:O	2:D:80:ALA:HA	2.19	0.42
1:B:341:PRO:HD2	1:B:344:ARG:HH11	1.83	0.42
2:D:175:VAL:O	2:D:181:TYR:HA	2.18	0.42
1:A:238:GLU:O	1:A:238:GLU:HG3	2.19	0.42
1:B:194:LEU:O	1:B:198:ILE:HG12	2.20	0.42
1:B:300:ALA:HB2	1:B:445:LEU:HD11	2.02	0.42
2:D:105:ALA:HB2	3:F:37:PHE:CE1	2.54	0.42
1:A:281:PHE:HZ	1:A:443:TYR:HB3	1.84	0.42
1:B:78:ILE:CG2	1:B:442:VAL:HG13	2.50	0.42
3:E:15:VAL:HG22	3:E:109:ILE:HG22	2.01	0.42
3:F:19:VAL:O	3:F:77:THR:HA	2.20	0.42
3:F:88:THR:HA	3:F:105:THR:O	2.19	0.42
1:A:155:ARG:HH22	1:A:158:LYS:HD3	1.84	0.42
1:A:157:LEU:HD11	1:A:368:MET:HB2	2.02	0.42
1:A:204:TYR:HD1	1:A:204:TYR:HA	1.68	0.42
1:B:340:VAL:HB	1:B:344:ARG:HD2	2.00	0.42
2:C:158:LEU:HD11	2:C:201:CYS:SG	2.60	0.42
1:B:496:TYR:HE1	1:B:547:PHE:CE1	2.38	0.42
2:D:102:GLY:C	2:D:104:GLY:N	2.77	0.42
3:E:92:LEU:HD13	3:E:101:PHE:CZ	2.54	0.42
1:A:131:LYS:C	1:A:131:LYS:HD2	2.45	0.42
1:A:446:LEU:HA	1:A:449:LEU:HD12	2.02	0.42
1:A:471:VAL:HG13	1:A:472:LEU:N	2.34	0.42
1:B:85:TYR:CE1	1:B:445:LEU:HD12	2.55	0.42
1:B:337:MET:HE2	1:B:338:PHE:CE1	2.54	0.42
2:C:50:SER:O	2:C:59:THR:N	2.48	0.42
1:A:359:PHE:HA	1:A:361:HIS:CE1	2.55	0.41
1:A:418:LEU:HD22	1:A:428:VAL:HG13	2.00	0.41
1:B:337:MET:SD	2:C:50:SER:HB2	2.60	0.41
2:C:61:ILE:HD13	2:C:61:ILE:HG21	1.80	0.41
2:D:194:TRP:CD1	2:D:195:PRO:HA	2.55	0.41
1:B:319:TYR:O	1:B:323:GLN:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:ALA:HB2	3:E:37:PHE:CD1	2.55	0.41
1:A:532:HIS:O	1:A:536:ILE:HD12	2.20	0.41
1:B:194:LEU:CD2	1:B:454:LEU:HG	2.47	0.41
1:B:244:TYR:CG	1:B:245:PRO:HD2	2.55	0.41
3:E:91:ASP:OD1	3:E:102:GLY:HA3	2.21	0.41
3:F:9:GLU:HG2	3:F:10:SER:N	2.33	0.41
1:A:80:SER:OG	1:A:204:TYR:OH	2.16	0.41
1:B:508:VAL:HG22	1:B:536:ILE:HG23	2.01	0.41
2:C:2:ILE:HD12	2:C:108:TYR:CE2	2.56	0.41
2:C:4:LEU:N	2:C:4:LEU:HD12	2.36	0.41
2:C:102:GLY:C	2:C:104:GLY:N	2.76	0.41
1:A:284:ILE:HD12	1:A:284:ILE:N	2.36	0.41
3:E:110:LYS:HA	3:E:143:TYR:OH	2.20	0.41
1:B:324:LEU:HD12	1:B:402:ALA:O	2.20	0.41
1:A:216:GLY:HA2	1:A:219:ILE:HG12	2.03	0.41
1:A:356:LEU:HB2	1:A:498:GLY:HA3	2.03	0.41
1:B:76:HIS:HB2	1:B:85:TYR:CE2	2.56	0.41
1:B:78:ILE:HG22	1:B:80:SER:HB3	2.03	0.41
1:B:496:TYR:CE1	1:B:547:PHE:CE1	3.09	0.41
1:B:502:GLY:O	1:B:506:VAL:HB	2.21	0.41
3:E:19:VAL:O	3:E:77:THR:HA	2.21	0.41
3:E:37:PHE:HE1	3:E:53:ASP:H	1.58	0.41
1:A:509:LEU:O	1:A:513:ILE:HG12	2.21	0.41
2:D:214:LYS:HD3	2:D:214:LYS:HA	1.87	0.41
3:F:212:PHE:HD1	3:F:212:PHE:O	2.03	0.40
1:A:278:THR:HB	1:A:481:VAL:HG21	2.04	0.40
1:A:426:ILE:O	1:A:430:VAL:HG23	2.21	0.40
2:D:6:GLN:H	2:D:111:GLN:CD	2.27	0.40
2:D:131:GLU:H	2:D:131:GLU:HG3	1.39	0.40
1:B:324:LEU:HD13	1:B:404:PRO:HD3	2.02	0.40
3:F:14:VAL:HG22	3:F:110:LYS:HD3	2.04	0.40
3:F:18:TYR:HD1	3:F:19:VAL:N	2.19	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ASN:O	1:B:520:ARG:NH2[2_656]	2.18	0.02

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	343/549 (62%)	302 (88%)	37 (11%)	4 (1%)	10	35
1	B	388/549 (71%)	336 (87%)	43 (11%)	9 (2%)	5	23
2	C	213/219 (97%)	196 (92%)	13 (6%)	4 (2%)	6	26
2	D	212/219 (97%)	195 (92%)	13 (6%)	4 (2%)	6	26
3	E	213/215 (99%)	199 (93%)	12 (6%)	2 (1%)	14	42
3	F	213/215 (99%)	200 (94%)	11 (5%)	2 (1%)	14	42
All	All	1582/1966 (80%)	1428 (90%)	129 (8%)	25 (2%)	7	29

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	87	TYR
1	B	88	SER
1	B	89	PRO
1	B	177	CYS
1	B	488	PRO
2	C	42	LEU
2	D	42	LEU
1	A	488	PRO
1	B	81	HIS
1	B	464	PRO
2	C	132	VAL
3	F	157	GLU
1	A	81	HIS
1	B	80	SER
1	A	282	TYR
2	C	41	PRO
2	D	101	ARG
3	E	157	GLU
2	C	139	GLY
2	D	41	PRO

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Mol	Chain	Res	Type
1	B	404	PRO
2	D	139	GLY
3	F	80	PRO
1	A	182	GLY
3	E	80	PRO

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	322/487 (66%)	309 (96%)	13 (4%)	28	53
1	B	362/487 (74%)	351 (97%)	11 (3%)	36	59
2	C	174/174 (100%)	170 (98%)	4 (2%)	44	63
2	D	174/174 (100%)	171 (98%)	3 (2%)	53	67
3	E	186/186 (100%)	179 (96%)	7 (4%)	29	54
3	F	186/186 (100%)	176 (95%)	10 (5%)	20	47
All	All	1404/1694 (83%)	1356 (97%)	48 (3%)	32	57

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	155	ARG
1	A	157	LEU
1	A	179	TYR
1	A	190	LEU
1	A	283	LEU
1	A	285	LEU
1	A	286	LEU
1	A	303	THR
1	A	423	SER
1	A	451	ARG
1	A	472	LEU
1	A	506	VAL

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Mol	Chain	Res	Type
1	B	75	ASP
1	B	85	TYR
1	B	86	ILE
1	B	87	TYR
1	B	90	LEU
1	B	268	GLU
1	B	303	THR
1	B	324	LEU
1	B	378	VAL
1	B	525	ARG
1	B	536	ILE
2	C	12	SER
2	C	42	LEU
2	C	58	THR
2	C	143	THR
2	D	131	GLU
2	D	143	THR
2	D	144	LEU
3	E	9	GLU
3	E	29	ILE
3	E	32	TYR
3	E	54	SER
3	E	96	ILE
3	E	126	GLU
3	E	179	SER
3	F	15	VAL
3	F	22	THR
3	F	90	GLU
3	F	96	ILE
3	F	98	VAL
3	F	119	SER
3	F	167	THR
3	F	181	THR
3	F	212	PHE
3	F	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	349	GLN
1	A	453	GLN

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Mol	Chain	Res	Type
1	B	210	ASN
1	B	214	ASN
1	B	438	GLN
1	B	457	GLN
1	B	461	ASN
1	B	542	ASN
2	C	6	GLN
2	C	35	ASN
3	E	27	ASN
3	F	127	GLN
3	F	164	ASN
3	F	202	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 [i](#)

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	361/549 (65%)	1.74	126 (34%) 1 1	93, 149, 193, 261	0
1	B	404/549 (73%)	1.97	148 (36%) 1 1	70, 104, 160, 234	0
2	C	217/219 (99%)	1.35	48 (22%) 2 4	62, 89, 134, 162	0
2	D	216/219 (98%)	0.82	32 (14%) 5 7	61, 86, 124, 158	0
3	E	215/215 (100%)	1.17	45 (20%) 2 4	61, 85, 138, 160	0
3	F	215/215 (100%)	0.74	26 (12%) 8 9	61, 89, 134, 184	0
All	All	1628/1966 (82%)	1.42	425 (26%) 1 3	61, 103, 175, 261	0

All (425) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	ASP	24.0
1	B	335	SER	22.5
1	B	333	PHE	15.5
3	E	146	ASN	11.4
1	B	336	SER	11.3
1	B	174	PRO	11.3
2	C	55	ASN	11.3
1	B	86	ILE	10.5
1	B	160	THR	9.6
1	B	411	GLU	9.3
1	B	161	LYS	9.2
3	E	145	LYS	9.1
1	B	85	TYR	9.1
2	C	58	THR	9.0
3	F	45	GLN	9.0
1	B	549	MET	8.9
2	C	103	ASN	8.6
1	B	366	THR	8.6
3	E	125	SER	8.5

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Mol	Chain	Res	Type	RSRZ
1	B	331	HIS	8.4
3	E	44	GLY	8.3
3	F	148	ASN	8.2
3	F	146	ASN	8.0
1	B	417	PHE	7.9
1	A	81	HIS	7.9
1	A	395	VAL	7.8
2	C	50	SER	7.7
2	C	57	ALA	7.7
1	B	237	THR	7.7
1	A	240	VAL	7.6
3	E	126	GLU	7.5
1	A	399	ILE	7.3
1	B	414	GLU	7.2
2	C	56	GLY	7.1
2	C	59	THR	7.0
1	A	403	PHE	6.8
1	A	332	TRP	6.7
1	B	329	GLU	6.7
2	C	54	SER	6.5
1	B	84	ILE	6.5
1	B	416	ASN	6.5
1	B	81	HIS	6.5
1	B	419	ASP	6.4
1	B	369	LYS	6.4
3	E	130	SER	6.4
1	B	337	MET	6.4
1	A	394	TYR	6.3
3	F	31	THR	6.3
3	E	148	ASN	6.3
1	A	445	LEU	6.3
1	B	332	TRP	6.3
1	B	467	LEU	6.2
2	C	164	SER	6.1
3	F	164	ASN	6.0
1	B	548	PHE	5.9
1	B	339	PHE	5.8
2	D	42	LEU	5.7
3	F	43	PRO	5.7
2	D	1	GLN	5.6
1	A	405	SER	5.6
1	A	191	VAL	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	316	LEU	5.6
1	A	239	ARG	5.6
1	B	78	ILE	5.6
3	E	134	GLU	5.5
2	C	198	SER	5.4
1	B	75	ASP	5.4
1	A	419	ASP	5.4
1	B	421	PHE	5.4
1	B	341	PRO	5.4
2	D	70	HIS	5.3
1	A	396	GLY	5.3
1	A	80	SER	5.3
2	D	21	SER	5.2
1	A	219	ILE	5.2
3	E	205	THR	5.2
1	B	274	SER	5.2
1	B	420	ASN	5.1
1	A	484	ALA	5.1
2	D	41	PRO	5.0
1	A	548	PHE	5.0
2	C	70	HIS	5.0
3	F	32	TYR	5.0
1	B	154	TYR	5.0
2	C	204	ALA	4.9
1	B	268	GLU	4.9
1	A	417	PHE	4.9
2	D	165	LEU	4.9
1	B	484	ALA	4.9
3	E	129	THR	4.9
1	A	272	TRP	4.9
3	E	12	SER	4.8
1	A	406	PRO	4.8
1	A	190	LEU	4.8
1	A	287	LEU	4.8
1	B	159	SER	4.8
1	B	418	LEU	4.8
3	F	202	GLN	4.7
1	B	338	PHE	4.7
1	A	404	PRO	4.7
2	D	164	SER	4.7
3	E	131	GLY	4.7
1	A	326	PHE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	277	ASN	4.7
1	A	333	PHE	4.6
2	C	154	GLU	4.6
1	A	367	LEU	4.6
1	B	468	HIS	4.6
1	B	394	TYR	4.6
1	B	458	ILE	4.6
3	F	44	GLY	4.5
3	F	42	LYS	4.5
1	B	517	SER	4.5
2	C	166	SER	4.5
2	C	1	GLN	4.4
3	F	200	THR	4.4
3	E	202	GLN	4.3
1	A	206	VAL	4.3
1	B	90	LEU	4.3
1	B	365	ILE	4.3
1	B	239	ARG	4.3
2	C	52	ASN	4.3
2	C	167	SER	4.3
1	B	443	TYR	4.3
1	A	453	GLN	4.3
1	A	482	LEU	4.3
1	B	317	VAL	4.3
1	A	117	THR	4.2
1	A	107	SER	4.2
1	B	272	TRP	4.2
1	A	274	SER	4.2
1	A	408	LEU	4.2
1	A	123	ILE	4.2
2	D	207	ALA	4.2
2	C	65	LYS	4.2
1	B	76	HIS	4.1
3	E	108	GLU	4.1
3	E	96	ILE	4.1
3	E	133	ALA	4.1
2	C	102	GLY	4.1
1	B	476	VAL	4.0
1	A	297	SER	4.0
1	B	340	VAL	4.0
1	B	205	TRP	4.0
1	B	363	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	98	VAL	4.0
3	E	1	ASP	4.0
1	A	187	TRP	3.9
2	C	163	GLY	3.9
1	B	175	ASP	3.9
1	B	280	PRO	3.9
3	E	147	ILE	3.9
2	D	219	ALA	3.9
1	A	378	VAL	3.8
1	B	278	THR	3.8
1	B	104	LYS	3.8
3	E	10	SER	3.8
2	D	103	ASN	3.7
1	B	199	GLY	3.7
1	B	412	CYS	3.7
1	A	362	ASN	3.7
1	B	79	PRO	3.7
1	B	281	PHE	3.7
2	C	138	THR	3.7
2	C	24	ALA	3.7
1	B	242	CYS	3.7
1	B	108	ILE	3.7
1	B	106	PRO	3.7
1	B	238	GLU	3.6
2	D	167	SER	3.6
1	B	201	MET	3.6
1	B	158	LYS	3.6
1	A	424	SER	3.6
3	F	147	ILE	3.6
1	A	449	LEU	3.6
1	A	241	ILE	3.6
3	E	124	SER	3.6
1	A	471	VAL	3.6
1	A	479	ALA	3.6
3	F	73	ASP	3.6
3	F	193	ALA	3.5
1	B	105	ASN	3.5
3	F	96	ILE	3.5
2	C	156	CYS	3.5
1	A	345	THR	3.5
2	C	49	GLY	3.5
1	A	316	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	480	GLY	3.5
1	A	421	PHE	3.5
1	A	379	ARG	3.5
1	A	202	VAL	3.5
1	B	195	VAL	3.5
3	E	128	LEU	3.5
1	B	282	TYR	3.4
1	A	285	LEU	3.4
3	E	127	GLN	3.4
1	A	365	ILE	3.4
2	C	196	SER	3.4
1	B	131	LYS	3.4
1	A	334	ASP	3.4
1	A	338	PHE	3.4
1	A	383	LEU	3.4
1	A	418	LEU	3.4
1	A	369	LYS	3.4
1	B	209	SER	3.4
1	B	409	SER	3.3
2	D	122	THR	3.3
1	A	346	LEU	3.3
3	E	97	VAL	3.3
1	A	238	GLU	3.3
1	A	108	ILE	3.3
1	B	425	ASP	3.3
1	A	485	ARG	3.3
1	B	279	ILE	3.3
1	A	281	PHE	3.3
1	B	403	PHE	3.2
1	A	440	THR	3.2
1	B	240	VAL	3.2
3	F	97	VAL	3.2
1	B	473	ASN	3.2
1	A	199	GLY	3.2
1	B	319	TYR	3.2
1	A	330	PHE	3.2
1	B	399	ILE	3.2
3	E	55	SER	3.2
3	E	45	GLN	3.2
2	C	122	THR	3.2
3	E	200	THR	3.2
1	A	486	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	107	SER	3.2
1	A	329	GLU	3.2
1	A	105	ASN	3.2
2	C	60	TYR	3.2
1	B	477	VAL	3.2
1	A	481	VAL	3.1
1	B	346	LEU	3.1
1	B	481	VAL	3.1
1	B	273	TRP	3.1
1	B	198	ILE	3.1
2	C	42	LEU	3.1
2	C	197	GLN	3.1
1	A	363	CYS	3.1
2	C	124	ALA	3.0
2	C	25	GLY	3.0
1	B	378	VAL	3.0
1	B	315	PHE	3.0
2	D	192	SER	3.0
3	F	12	SER	3.0
1	B	111	ILE	3.0
1	B	208	MET	3.0
1	A	400	PHE	3.0
3	E	80	PRO	2.9
3	E	193	ALA	2.9
1	B	480	GLY	2.9
1	A	366	THR	2.9
2	C	157	THR	2.9
3	E	43	PRO	2.9
2	D	198	SER	2.9
3	F	26	SER	2.9
1	B	298	PHE	2.9
1	A	283	LEU	2.9
1	B	206	VAL	2.9
1	B	184	PHE	2.9
2	C	101	ARG	2.9
1	A	246	ASP	2.9
1	A	549	MET	2.9
1	A	237	THR	2.9
1	A	402	ALA	2.9
1	A	275	LYS	2.9
1	A	516	VAL	2.8
3	E	123	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	81	ASN	2.8
1	B	328	LEU	2.8
3	F	18	TYR	2.8
1	A	113	ALA	2.8
2	C	41	PRO	2.8
1	B	109	VAL	2.8
1	B	318	THR	2.8
2	D	179	ASP	2.8
2	D	163	GLY	2.8
1	B	322	ILE	2.8
1	A	392	TYR	2.8
1	A	488	PRO	2.8
1	B	304	PHE	2.7
1	B	499	ALA	2.7
1	B	422	PRO	2.7
2	D	123	THR	2.7
1	A	420	ASN	2.7
2	C	174	ALA	2.7
1	B	203	VAL	2.7
1	B	436	LEU	2.7
1	B	521	ARG	2.7
1	B	413	ILE	2.7
1	B	463	TYR	2.7
2	C	128	TYR	2.7
3	E	84	ALA	2.7
3	E	3	LEU	2.7
2	C	126	SER	2.7
1	B	202	VAL	2.7
3	E	189	TYR	2.7
3	E	166	TRP	2.6
1	B	326	PHE	2.6
1	B	396	GLY	2.6
1	B	283	LEU	2.6
2	D	178	SER	2.6
2	D	196	SER	2.6
1	A	284	ILE	2.6
1	A	176	VAL	2.6
1	B	77	VAL	2.6
1	B	276	THR	2.6
3	F	46	ALA	2.6
2	C	162	SER	2.6
2	D	2	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	313	LEU	2.6
1	B	275	LYS	2.6
1	B	320	LYS	2.6
2	C	47	TRP	2.6
1	A	299	PHE	2.6
3	E	52	TYR	2.6
1	B	285	LEU	2.5
1	A	505	LEU	2.5
2	D	209	SER	2.5
2	D	19	LYS	2.5
2	C	219	ALA	2.5
1	A	242	CYS	2.5
1	B	405	SER	2.5
1	A	452	VAL	2.5
2	C	125	PRO	2.5
1	A	397	VAL	2.5
1	B	177	CYS	2.5
2	D	137	ALA	2.5
1	A	315	PHE	2.5
1	A	472	LEU	2.5
1	B	286	LEU	2.5
1	A	203	VAL	2.5
1	A	382	SER	2.4
1	B	330	PHE	2.4
1	B	520	ARG	2.4
1	B	344	ARG	2.4
1	A	244	TYR	2.4
1	B	479	ALA	2.4
1	B	410	LYS	2.4
2	D	166	SER	2.4
1	B	89	PRO	2.4
3	F	28	ASN	2.4
3	E	53	ASP	2.4
1	B	179	TYR	2.4
2	D	20	ILE	2.4
1	B	132	GLN	2.4
1	A	398	LEU	2.4
1	B	356	LEU	2.4
3	E	211	SER	2.4
1	A	83	ASP	2.4
1	B	345	THR	2.3
1	B	204	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	450	VAL	2.3
1	A	335	SER	2.3
1	A	407	PRO	2.3
1	B	485	ARG	2.3
1	B	439	MET	2.3
1	B	395	VAL	2.3
2	C	104	GLY	2.3
3	E	132	GLY	2.3
1	A	370	ASN	2.3
3	E	81	ASN	2.3
3	F	95	LEU	2.3
3	F	72	ARG	2.3
1	A	121	THR	2.3
2	D	138	THR	2.3
1	A	414	GLU	2.3
1	A	245	PRO	2.3
1	A	493	ILE	2.3
1	A	503	LEU	2.3
2	C	188	THR	2.3
1	B	220	PHE	2.3
1	B	297	SER	2.3
1	A	540	VAL	2.2
1	A	194	LEU	2.2
2	D	56	GLY	2.2
1	A	273	TRP	2.2
1	B	408	LEU	2.2
2	D	25	GLY	2.2
1	A	269	PHE	2.2
1	A	159	SER	2.2
1	A	137	LEU	2.2
3	E	190	GLU	2.2
3	F	173	ASP	2.2
1	A	195	VAL	2.2
3	E	15	VAL	2.2
1	A	492	SER	2.2
1	B	141	ILE	2.2
2	D	30	THR	2.1
2	C	27	TYR	2.1
1	A	343	PHE	2.1
1	A	527	THR	2.1
2	C	151	TYR	2.1
3	E	106	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	424	SER	2.1
1	B	466	PHE	2.1
1	A	506	VAL	2.1
1	B	287	LEU	2.1
2	D	58	THR	2.1
1	B	374	GLN	2.1
2	C	218	PRO	2.1
1	A	500	LEU	2.1
1	B	462	HIS	2.1
1	A	337	MET	2.1
1	B	127	PRO	2.1
1	A	423	SER	2.1
2	C	215	LYS	2.1
1	A	380	ASP	2.1
1	A	357	ALA	2.1
2	D	79	ALA	2.1
1	B	415	PRO	2.1
1	A	119	MET	2.0
1	A	276	THR	2.0
1	A	347	PHE	2.0
2	C	121	LYS	2.0
1	A	512	LEU	2.0
3	E	11	LEU	2.0
3	F	163	LEU	2.0
3	E	2	ILE	2.0
2	D	24	ALA	2.0
1	A	179	TYR	2.0
1	A	487	TYR	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.