Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 03:33 AM EDT

PDB ID	:	7KGV
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:

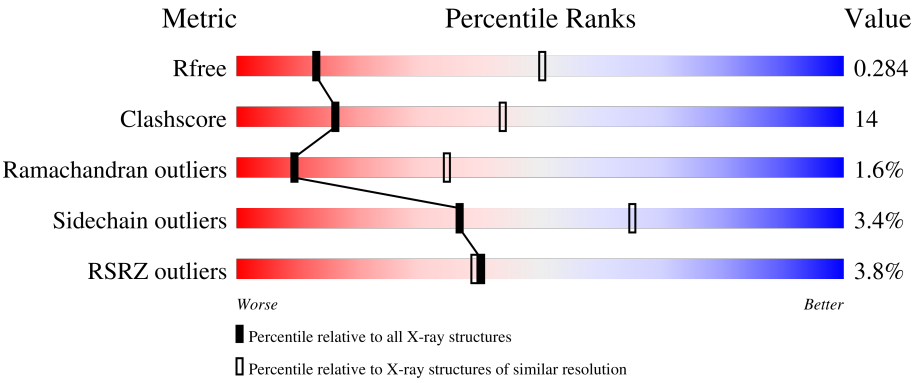
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	5% 46% 17% 34%
1	B	549	3% 47% 24% 26%
2	C	219	2% 72% 25%
2	D	219	4% 72% 26%
3	E	215	4% 66% 31%

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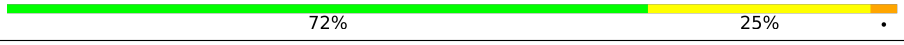
Mol	Chain	Length	Quality of chain
3	F	215	

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.

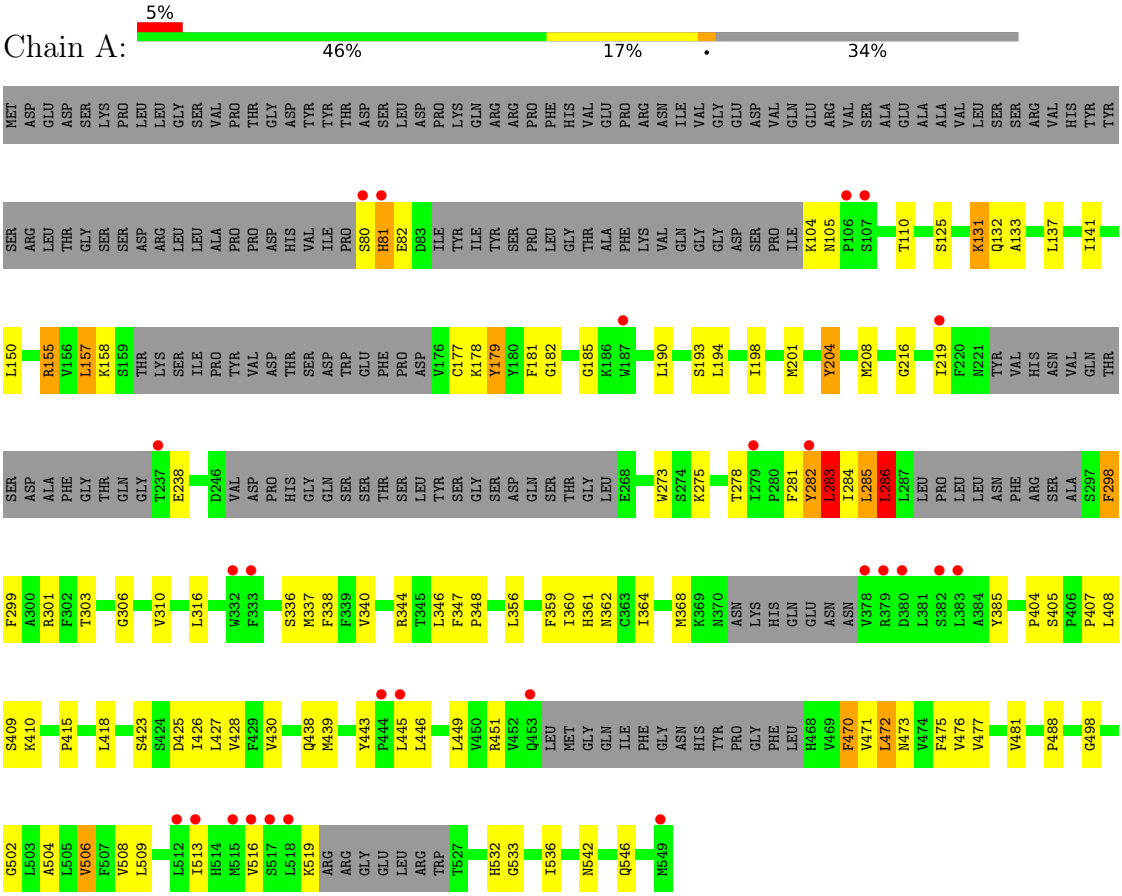
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	215	Total	C	N	O	S	0	0	0
			1648	1036	273	335	4			
3	F	215	Total	C	N	O	S	0	0	0
			1648	1036	273	335	4			

3 Residue-property plots (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.

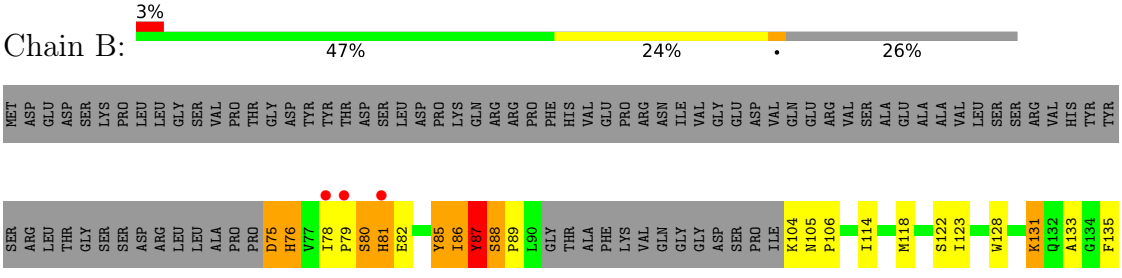
• Molecule 1: Sodium-coupled neutral amino acid transporter 9

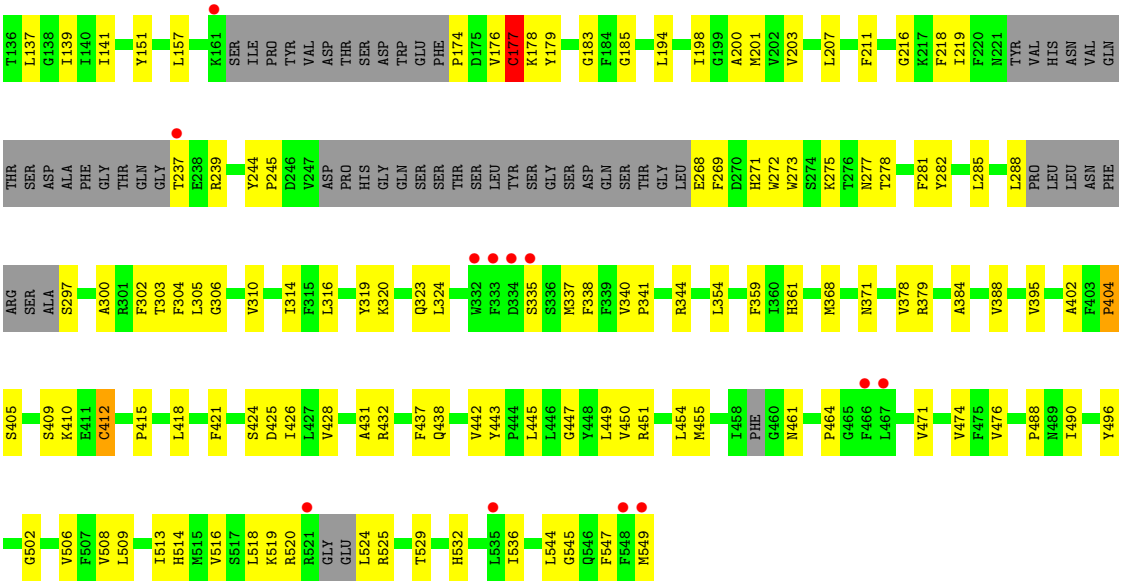
Chain A:



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

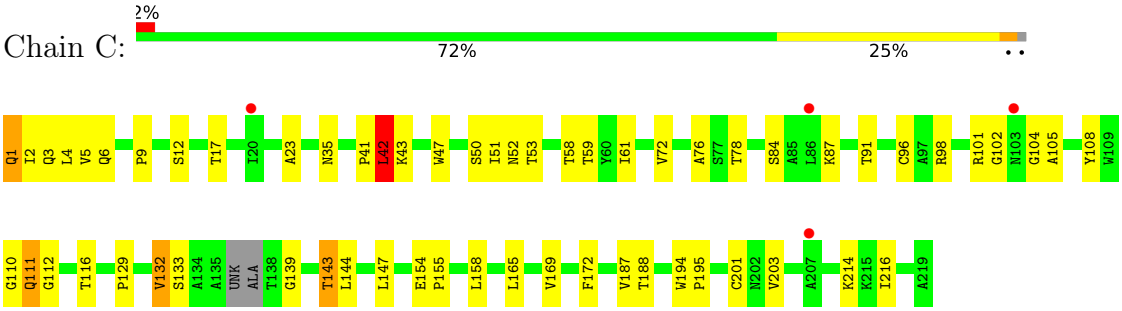
Chain B:





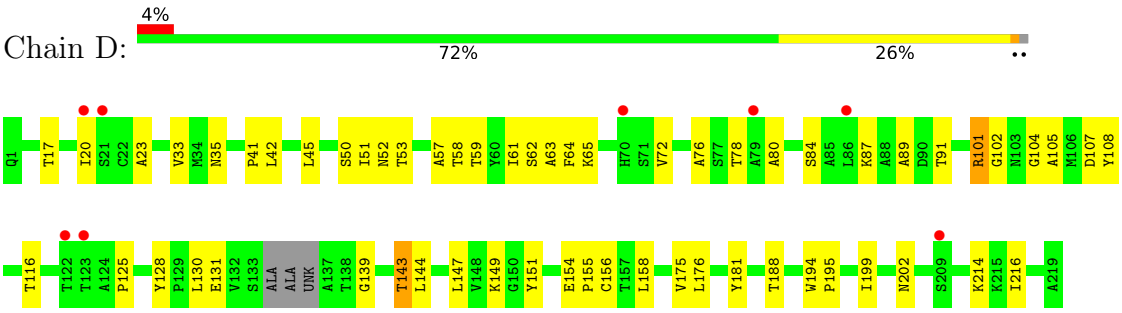
• Molecule 2: Monoclonal antibody Fab heavy chain

Chain C:



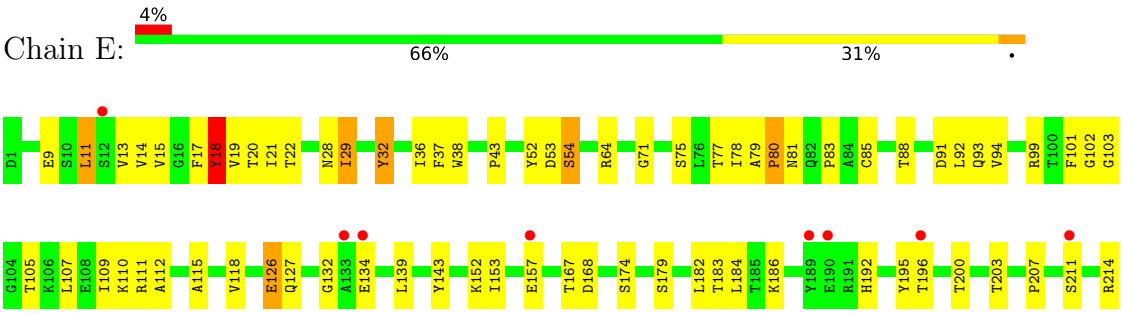
• Molecule 2: Monoclonal antibody Fab heavy chain

Chain D:



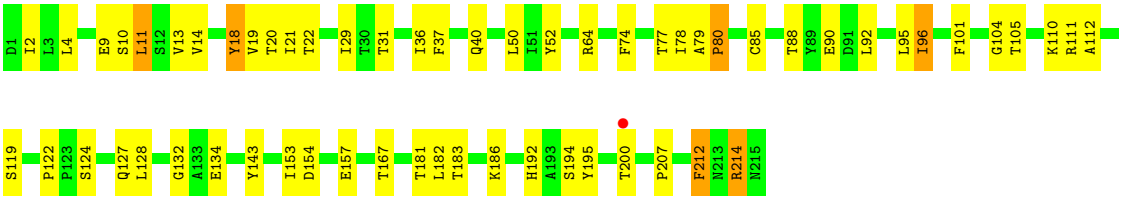
• Molecule 3: Monoclonal antibody Fab light chain

Chain E:



• Molecule 3: Monoclonal antibody Fab light chain

Chain F:



4 Data and refinement statistics (i)

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) 99.9 (49.37-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.36 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874+SVN	Depositor
R, R_{free}	0.251 , 0.284 0.251 , 0.284	Depositor DCC
R_{free} test set	1697 reflections (3.12%)	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)	0.23 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.43	0/2989	0.65	5/4059 (0.1%)
1	B	0.50	2/3367 (0.1%)	0.70	1/4575 (0.0%)
2	C	0.58	0/1610	0.76	0/2198
2	D	0.56	0/1605	0.75	1/2191 (0.0%)
3	E	0.60	0/1685	0.78	2/2296 (0.1%)
3	F	0.61	0/1685	0.74	1/2296 (0.0%)
All	All	0.53	2/12941 (0.0%)	0.72	10/17615 (0.1%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	CYS	CB-SG	-5.17	1.73	1.81
1	B	412	CYS	CB-SG	-5.09	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	286	LEU	CA-CB-CG	10.98	140.55	115.30
3	E	11	LEU	CB-CG-CD2	-8.63	96.33	111.00
1	A	286	LEU	CD1-CG-CD2	8.40	135.69	110.50
1	A	283	LEU	CA-CB-CG	7.27	132.03	115.30
3	F	11	LEU	CB-CG-CD2	-6.23	100.41	111.00
1	B	285	LEU	CA-CB-CG	5.71	128.42	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	283	LEU	CB-CG-CD2	5.68	120.66	111.00
1	A	470	PHE	CD1-CE1-CZ	5.62	126.84	120.10
2	D	45	LEU	CA-CB-CG	5.32	127.53	115.30
3	E	18	TYR	CA-CB-CG	5.03	122.96	113.40

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	84	0
1	B	3269	0	3333	97	1
2	C	1574	0	1533	46	0
2	D	1569	0	1528	44	0
3	E	1648	0	1590	61	0
3	F	1648	0	1590	52	0
All	All	12613	0	12544	363	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 (363) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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: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
3:F:127:GLN:HE22	3:F:134:GLU:CD	1.97	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
1:A:81:HIS:CG	1:A:82:GLU:N	2.65	0.65
3:E:118:VAL:HG22	3:E:139:LEU:HG	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:208:MET:HE1	1:A:439:MET:O	1.98	0.63
1:B:471:VAL:HA	1:B:474:VAL:HG12	1.80	0.63
1:A:80:SER:OG	1:A:204:TYR:OH	2.16	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: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
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: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
3:E:14:VAL:HG22	3:E:110:LYS:HG2	1.82	0.60
3:F:212:PHE:C	3:F:212:PHE:HD1	2.04	0.60
1:A:201:MET:SD	1:A:476:VAL:HG11	2.42	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
1:A:80:SER:HG	1:A:204:TYR:HH	1.50	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
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
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
3:F:212:PHE:C	3:F:212:PHE:CD1	2.78	0.57
1:B:131:LYS:HD2	1:B:410:LYS:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:THR:HB	2:C:188:THR:HG22	1.87	0.57
1:B:275:LYS:C	1:B:277:ASN:H	2.09	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
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
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
1:B:80:SER:C	1:B:82:GLU:H	2.10	0.54
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
1:B:85:TYR:C	1:B:85:TYR:HD2	2.11	0.54
2:D:52:ASN:HB2	2:D:101:ARG:NH2	2.23	0.54
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
1:B:118:MET:HE3	1:B:388:VAL:HG21	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:177:CYS:C	1:B:179:TYR:H	2.13	0.52
1:B:85:TYR:C	1:B:85:TYR:CD2	2.83	0.52
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
2:C:17:THR:HG22	2:C:84:SER:HA	1.92	0.51
1:B:118:MET:CE	1:B:388:VAL:HG21	2.40	0.50
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
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:174:PRO:C	1:B:176:VAL:H	2.16	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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
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:29:ILE:C	3:F:95:LEU:HD13	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:144:LEU:HD13	2:D:216:ILE:HG13	1.97	0.46
1:B:133:ALA:C	1:B:344:ARG:HB2	2.35	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
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:275:LYS:C	1:B:277:ASN:N	2.70	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: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
1:B:80:SER:C	1:B:82:GLU:N	2.71	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:85:TYR:HD2	1:B:85:TYR:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ILE:HD12	2:D:58:THR:HG22	2.00	0.44
1:A:439:MET:HE3	1:A:439:MET:HB2	1.71	0.44
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
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
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: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
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: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:179:TYR:C	1:A:179:TYR:CD2	2.91	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:C:102:GLY:C	2:C:104:GLY:H	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:GLY:C	2:D:104:GLY:H	2.22	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:151:TYR:HH	1:B:532:HIS:CE1	2.37	0.42
1:B:496:TYR:HE1	1:B:547:PHE:CE1	2.38	0.42
3:E:92:LEU:HD13	3:E:101:PHE:CZ	2.54	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
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
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:177:CYS:C	1:B:179:TYR:N	2.74	0.41
1:B:194:LEU:CD2	1:B:454:LEU:HG	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:183:GLY:C	1:B:185:GLY:H	2.23	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:131:GLU:H	2:D:131:GLU:HG3	1.39	0.40
1:A:133:ALA:C	1:A:344:ARG:HB2	2.41	0.40
1:B:183:GLY:C	1:B:185:GLY:N	2.75	0.40
1:B:324:LEU:HD13	1:B:404:PRO:HD3	2.02	0.40
2:C:1:GLN:CD	2:C:2:ILE:H	2.24	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 (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	343/549 (62%)	302 (88%)	37 (11%)	4 (1%)	13	41
1	B	388/549 (71%)	336 (87%)	43 (11%)	9 (2%)	6	28
2	C	213/219 (97%)	196 (92%)	13 (6%)	4 (2%)	8	31
2	D	212/219 (97%)	195 (92%)	13 (6%)	4 (2%)	8	31
3	E	213/215 (99%)	199 (93%)	12 (6%)	2 (1%)	17	49
3	F	213/215 (99%)	200 (94%)	11 (5%)	2 (1%)	17	49
All	All	1582/1966 (80%)	1428 (90%)	129 (8%)	25 (2%)	9	34

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 (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	322/487 (66%)	306 (95%)	16 (5%)	24	54
1	B	362/487 (74%)	351 (97%)	11 (3%)	41	68
2	C	174/174 (100%)	168 (97%)	6 (3%)	37	65
2	D	174/174 (100%)	173 (99%)	1 (1%)	86	94
3	E	186/186 (100%)	179 (96%)	7 (4%)	33	61
3	F	186/186 (100%)	179 (96%)	7 (4%)	33	61
All	All	1404/1694 (83%)	1356 (97%)	48 (3%)	37	65

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

Mol	Chain	Res	Type
1	A	104	LYS
1	A	131	LYS
1	A	155	ARG
1	A	157	LEU
1	A	179	TYR
1	A	190	LEU
1	A	204	TYR
1	A	283	LEU
1	A	285	LEU
1	A	286	LEU
1	A	298	PHE
1	A	303	THR
1	A	423	SER

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Mol	Chain	Res	Type
1	A	451	ARG
1	A	472	LEU
1	A	506	VAL
1	B	75	ASP
1	B	76	HIS
1	B	85	TYR
1	B	86	ILE
1	B	87	TYR
1	B	131	LYS
1	B	268	GLU
1	B	303	THR
1	B	378	VAL
1	B	379	ARG
1	B	525	ARG
2	C	12	SER
2	C	42	LEU
2	C	58	THR
2	C	111	GLN
2	C	143	THR
2	C	147	LEU
2	D	143	THR
3	E	9	GLU
3	E	18	TYR
3	E	29	ILE
3	E	32	TYR
3	E	54	SER
3	E	126	GLU
3	E	179	SER
3	F	18	TYR
3	F	22	THR
3	F	96	ILE
3	F	119	SER
3	F	167	THR
3	F	212	PHE
3	F	214	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	349	GLN
1	B	438	GLN
2	C	6	GLN

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Mol	Chain	Res	Type
2	C	35	ASN
3	F	127	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides 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, 95^{th} 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%)	0.19	26 (7%)	15	17	93, 149, 193, 261	0
1	B	404/549 (73%)	-0.00	15 (3%)	41	40	70, 104, 160, 234	0
2	C	217/219 (99%)	-0.02	4 (1%)	68	67	62, 89, 134, 162	0
2	D	216/219 (98%)	0.02	8 (3%)	41	40	61, 86, 124, 158	0
3	E	215/215 (100%)	-0.01	8 (3%)	41	40	61, 85, 138, 160	0
3	F	215/215 (100%)	-0.20	1 (0%)	91	90	62, 89, 134, 184	0
All	All	1628/1966 (82%)	0.01	62 (3%)	40	39	61, 103, 175, 261	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	549	MET	6.3
1	A	81	HIS	5.0
1	A	516	VAL	4.6
1	B	334	ASP	4.6
1	A	80	SER	4.5
1	A	515	MET	4.4
1	B	333	PHE	4.2
1	B	79	PRO	3.6
2	D	21	SER	3.4
3	E	189	TYR	3.4
1	A	380	ASP	3.3
1	A	332	TRP	3.3
1	A	107	SER	3.1
2	D	209	SER	3.1
1	A	237	THR	3.1
1	B	335	SER	3.1
1	B	548	PHE	3.1
3	E	157	GLU	3.0
1	A	513	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	134	GLU	3.0
1	A	444	PRO	3.0
2	C	86	LEU	3.0
1	B	237	THR	2.9
1	A	518	LEU	2.9
1	A	219	ILE	2.9
1	B	332	TRP	2.8
1	A	445	LEU	2.7
1	B	78	ILE	2.7
3	E	196	THR	2.7
1	A	512	LEU	2.7
1	A	378	VAL	2.6
1	A	282	TYR	2.5
2	D	86	LEU	2.5
1	B	521	ARG	2.5
2	D	122	THR	2.5
2	D	123	THR	2.5
1	B	467	LEU	2.4
1	A	549	MET	2.4
2	D	20	ILE	2.4
1	B	466	PHE	2.4
1	A	379	ARG	2.4
1	A	453	GLN	2.3
1	A	382	SER	2.3
1	A	106	PRO	2.3
2	D	70	HIS	2.3
1	A	333	PHE	2.3
1	A	279	ILE	2.3
1	B	535	LEU	2.3
2	C	207	ALA	2.3
1	A	517	SER	2.2
2	D	79	ALA	2.2
1	A	383	LEU	2.2
1	B	81	HIS	2.2
2	C	103	ASN	2.2
1	A	187	TRP	2.2
3	E	190	GLU	2.2
2	C	20	ILE	2.1
3	E	133	ALA	2.1
3	E	211	SER	2.1
3	E	12	SER	2.1
1	B	161	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	200	THR	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 monosaccharides 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.