Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 01:26 PM EDT

PDB ID	:	7KQY
Title	:	Crystal Structure and Characterization of Human Heavy-Chain only Antibodies reveals a novel, stable dimeric structure similar to Monoclonal Antibodies
Authors	:	Bahmanjah, S.; Mieczkowski, C.; Yu, Y.; Baker, J.; Raghunathan, G.; Tomazela, D.; Hsieh, M.; Mccoy, M.; Strickland, C.; Fayadat-Dilman, L.
Deposited on	:	2020-11-18
Resolution	:	2.91 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:

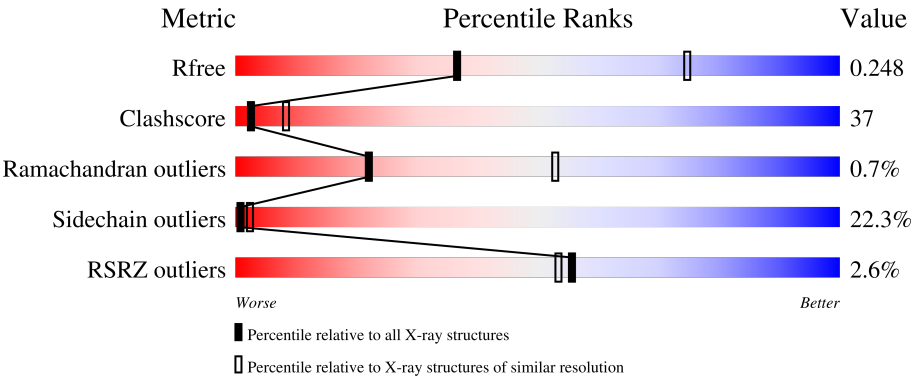
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	448	24% 18% 5% 52%
1	B	448	24% 18% 55%
1	C	448	17% 19% 9% 55%
1	D	448	19% 20% 6% 54%
1	E	448	23% 19% 6% 52%

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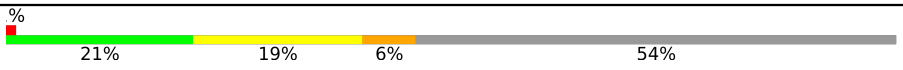
Mol	Chain	Length	Quality of chain
1	F	448	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9265 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 Heavy-Chain only Human Antibodies.

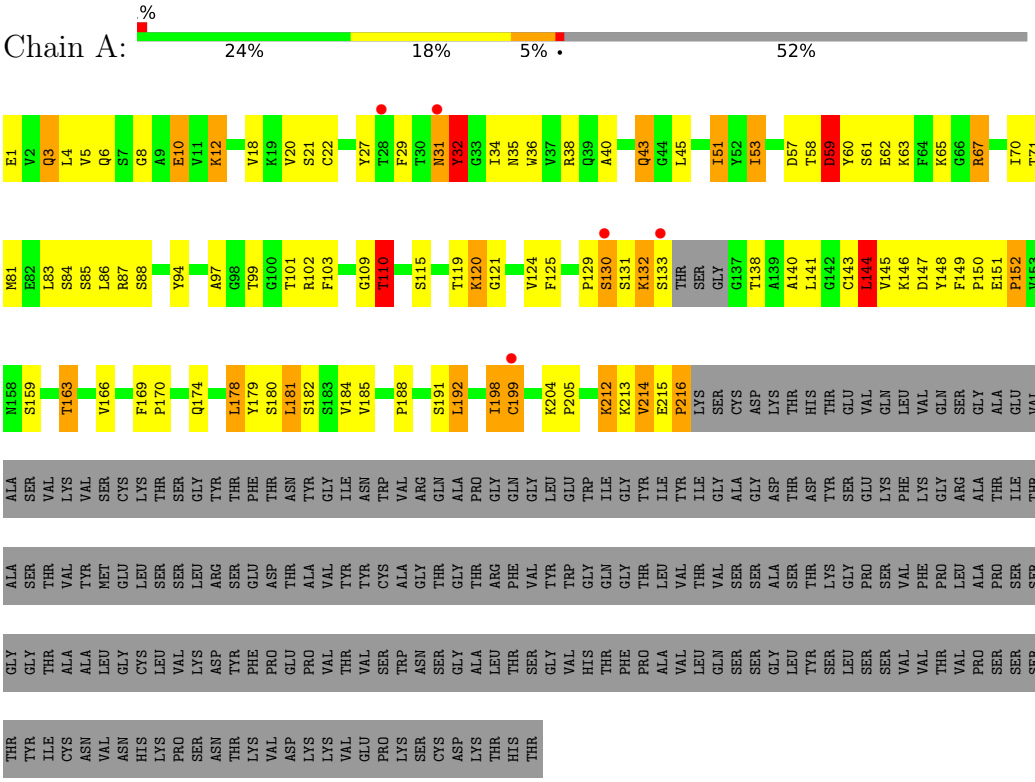
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1588	1006	259	318	5			
1	B	203	Total	C	N	O	S	0	0	0
			1504	953	244	302	5			
1	C	202	Total	C	N	O	S	0	0	0
			1508	959	246	298	5			
1	D	207	Total	C	N	O	S	0	0	0
			1542	981	249	307	5			
1	E	216	Total	C	N	O	S	0	0	0
			1605	1015	262	323	5			
1	F	204	Total	C	N	O	S	0	0	0
			1518	962	248	303	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.

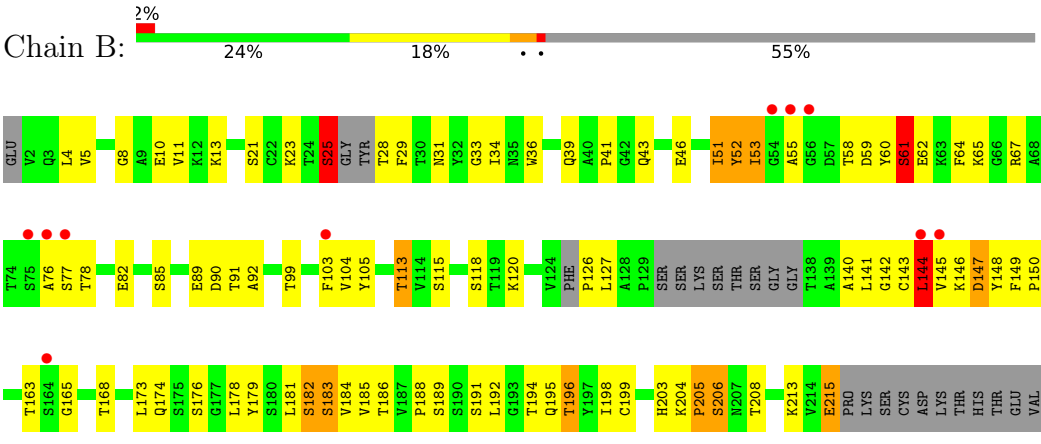
• Molecule 1: Heavy-Chain only Human Antibodies

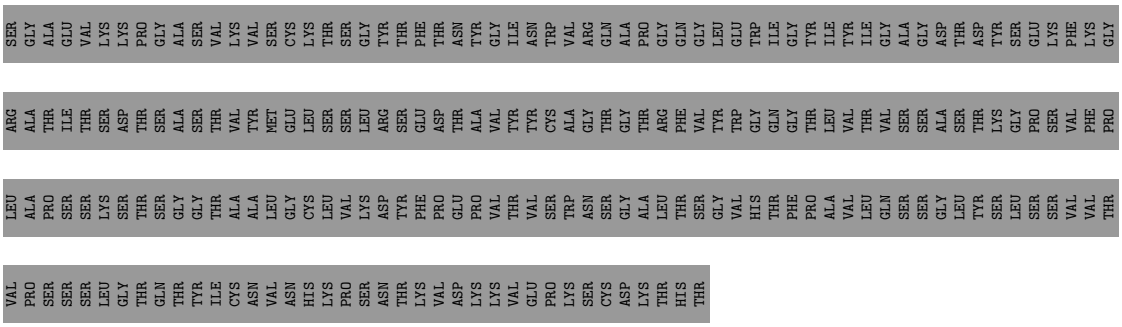
Chain A:



• Molecule 1: Heavy-Chain only Human Antibodies

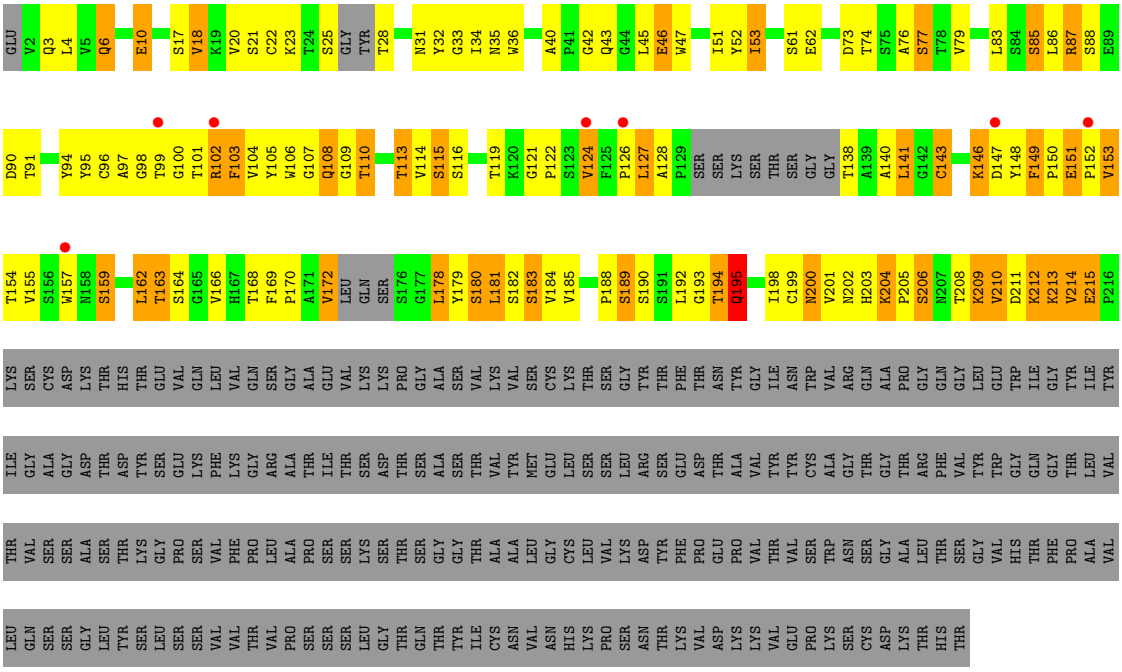
Chain B:





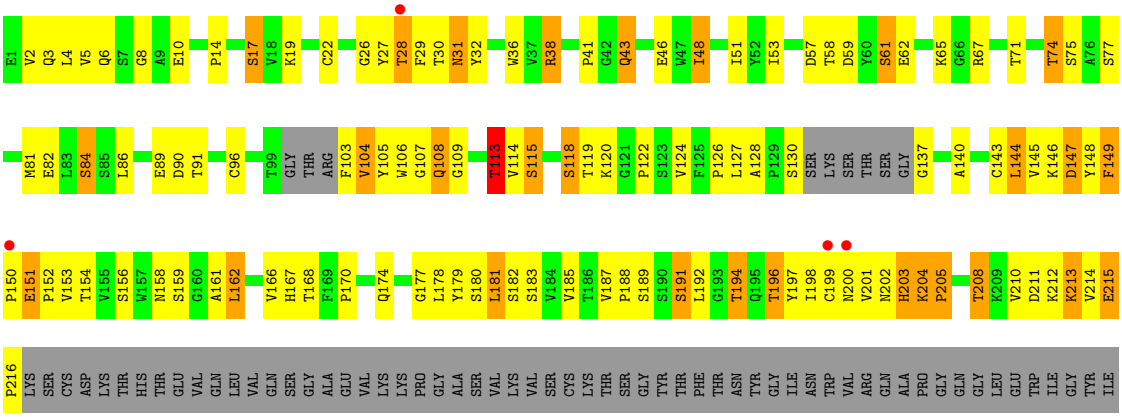
• Molecule 1: Heavy-Chain only Human Antibodies

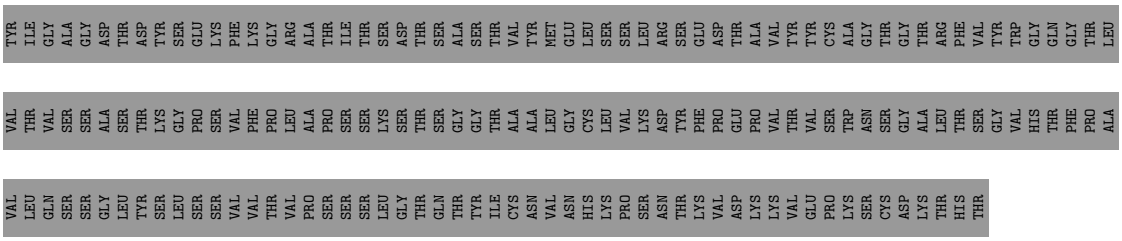
Chain C:



• Molecule 1: Heavy-Chain only Human Antibodies

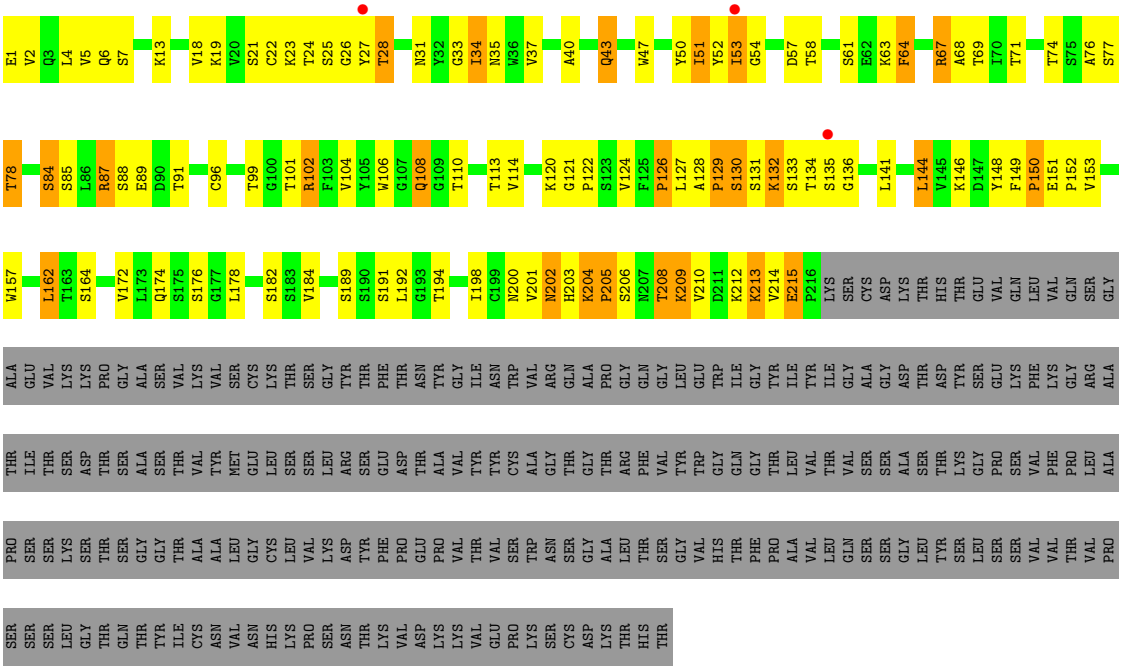
Chain D:





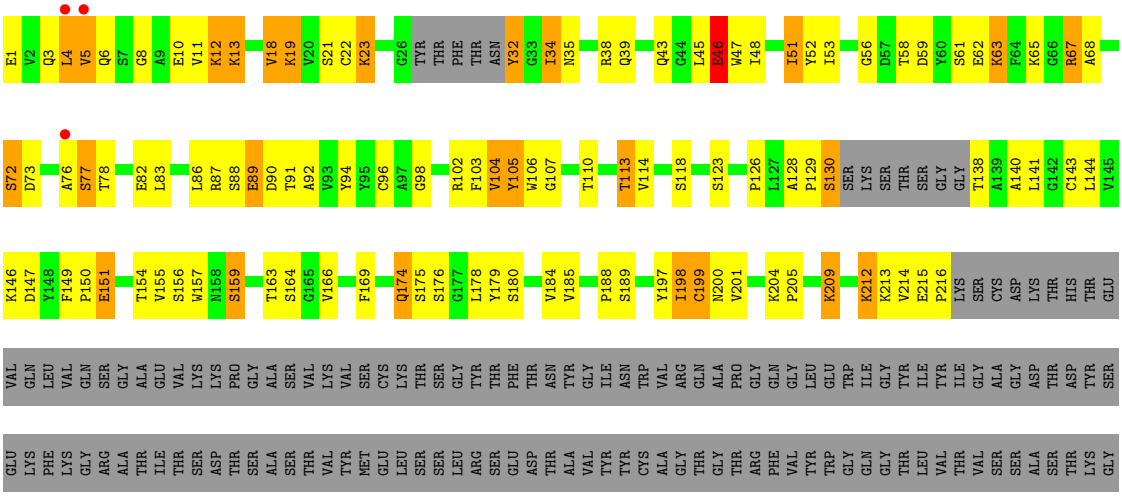
• Molecule 1: Heavy-Chain only Human Antibodies

Chain E:



• Molecule 1: Heavy-Chain only Human Antibodies

Chain F:



PRO SER VAL PHE PRO LEU ALA PRO SER SER LYS SER THR SER GLY GLY THR ALA ALA LEU GLY CYS LEU VAL LYS ASP TYR PHE PRO GLU PRO VAL THR VAL SER TRP ASN SER GLY ALA LEU THR SER GLY VAL HIS THR PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER LEU

SER SER VAL VAL THR VAL PRO SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	169.62Å 73.42Å 140.41Å 90.00° 125.71° 90.00°	Depositor
Resolution (Å)	114.01 – 2.91 114.01 – 2.91	Depositor EDS
% Data completeness (in resolution range)	73.4 (114.01-2.91) 73.5 (114.01-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.207 , 0.260 0.231 , 0.248	Depositor DCC
R_{free} test set	1082 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 55.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	9265	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.71% 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	1.51	7/1625 (0.4%)	1.11	6/2215 (0.3%)
1	B	1.63	19/1536 (1.2%)	1.15	5/2094 (0.2%)
1	C	1.44	9/1542 (0.6%)	1.12	2/2102 (0.1%)
1	D	1.65	19/1578 (1.2%)	1.23	5/2152 (0.2%)
1	E	1.46	12/1643 (0.7%)	1.16	4/2241 (0.2%)
1	F	1.38	5/1552 (0.3%)	1.07	3/2115 (0.1%)
All	All	1.52	71/9476 (0.7%)	1.14	25/12919 (0.2%)

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	151	GLU	CD-OE1	-10.22	1.14	1.25
1	B	62	GLU	CD-OE1	-8.80	1.16	1.25
1	D	151	GLU	CD-OE1	-8.22	1.16	1.25
1	F	151	GLU	CD-OE1	-7.71	1.17	1.25
1	B	62	GLU	CD-OE2	-7.48	1.17	1.25
1	D	89	GLU	CD-OE1	-7.47	1.17	1.25
1	C	21	SER	CA-CB	-7.11	1.42	1.52
1	D	82	GLU	CD-OE2	-7.09	1.17	1.25
1	B	152	PRO	N-CD	-6.92	1.38	1.47
1	C	10	GLU	CD-OE2	-6.62	1.18	1.25
1	D	82	GLU	CD-OE1	-6.58	1.18	1.25
1	D	10	GLU	CD-OE1	-6.32	1.18	1.25
1	B	61	SER	CA-CB	-6.20	1.43	1.52
1	B	182	SER	CA-CB	-6.18	1.43	1.52
1	E	182	SER	CA-CB	-6.05	1.43	1.52
1	D	113	THR	C-O	-5.95	1.12	1.23
1	C	10	GLU	CD-OE1	-5.95	1.19	1.25
1	A	94	TYR	C-O	-5.93	1.12	1.23
1	C	61	SER	CA-CB	-5.80	1.44	1.52
1	C	182	SER	CA-CB	-5.76	1.44	1.52
1	C	180	SER	CA-CB	-5.72	1.44	1.52
1	F	46	GLU	CD-OE2	-5.72	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	191	SER	CA-CB	-5.69	1.44	1.52
1	A	109	GLY	C-O	-5.65	1.14	1.23
1	D	75	SER	CA-CB	-5.64	1.44	1.52
1	C	77	SER	CA-CB	-5.60	1.44	1.52
1	B	10	GLU	CD-OE2	-5.59	1.19	1.25
1	D	203	HIS	C-O	-5.59	1.12	1.23
1	D	109	GLY	C-O	-5.54	1.14	1.23
1	B	21	SER	CA-CB	-5.54	1.44	1.52
1	B	151	GLU	CD-OE2	-5.53	1.19	1.25
1	F	176	SER	CA-CB	-5.53	1.44	1.52
1	B	208	THR	C-O	-5.51	1.12	1.23
1	D	36	TRP	C-O	-5.50	1.12	1.23
1	C	35	ASN	C-O	-5.48	1.12	1.23
1	E	176	SER	CA-CB	-5.48	1.44	1.52
1	A	78	THR	C-O	-5.46	1.12	1.23
1	E	205	PRO	C-O	-5.46	1.12	1.23
1	E	210	VAL	C-O	-5.46	1.12	1.23
1	D	61	SER	CA-CB	-5.44	1.44	1.52
1	D	89	GLU	CD-OE2	-5.42	1.19	1.25
1	A	159	SER	CA-CB	-5.41	1.44	1.52
1	E	61	SER	CA-CB	-5.35	1.45	1.52
1	E	206	SER	CA-CB	-5.31	1.45	1.52
1	F	159	SER	CA-CB	-5.30	1.45	1.52
1	B	82	GLU	CD-OE1	-5.29	1.19	1.25
1	B	113	THR	C-O	-5.29	1.13	1.23
1	E	209	LYS	C-O	-5.28	1.13	1.23
1	B	8	GLY	C-O	-5.27	1.15	1.23
1	F	151	GLU	CD-OE2	-5.26	1.19	1.25
1	D	48	ILE	C-O	-5.23	1.13	1.23
1	B	46	GLU	CD-OE1	-5.22	1.20	1.25
1	B	85	SER	CA-CB	-5.22	1.45	1.52
1	B	25	SER	CA-CB	-5.21	1.45	1.52
1	A	144	LEU	C-O	-5.20	1.13	1.23
1	A	156	SER	CA-CB	-5.20	1.45	1.52
1	D	38	ARG	C-O	-5.17	1.13	1.23
1	E	200	ASN	C-O	-5.16	1.13	1.23
1	D	208	THR	C-O	-5.15	1.13	1.23
1	B	36	TRP	C-O	-5.14	1.13	1.23
1	D	82	GLU	C-O	-5.14	1.13	1.23
1	E	84	SER	CA-CB	-5.13	1.45	1.52
1	C	45	LEU	C-O	-5.13	1.13	1.23
1	E	126	PRO	C-O	-5.11	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLU	CD-OE2	-5.10	1.20	1.25
1	E	151	GLU	CD-OE2	-5.08	1.20	1.25
1	A	181	LEU	C-O	-5.05	1.13	1.23
1	D	14	PRO	C-O	-5.05	1.13	1.23
1	D	90	ASP	CG-OD1	-5.05	1.13	1.25
1	B	33	GLY	C-O	-5.04	1.15	1.23
1	D	115	SER	C-O	-5.02	1.13	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	152	PRO	N-CD-CG	-8.41	90.59	103.20
1	A	3	GLN	CB-CA-C	-8.27	93.86	110.40
1	F	35	ASN	CB-CA-C	-8.10	94.20	110.40
1	B	52	TYR	CB-CA-C	-7.31	95.78	110.40
1	B	152	PRO	CA-N-CD	7.21	121.80	111.70
1	D	104	VAL	C-N-CA	7.10	139.44	121.70
1	D	46	GLU	CB-CA-C	-6.36	97.67	110.40
1	A	199	CYS	CA-CB-SG	6.14	125.06	114.00
1	D	194	THR	CB-CA-C	-6.08	95.20	111.60
1	F	105	TYR	C-N-CA	-6.01	106.66	121.70
1	C	195	GLN	CB-CG-CD	5.95	127.08	111.60
1	B	144	LEU	N-CA-CB	-5.95	98.51	110.40
1	A	32	TYR	CB-CA-C	5.92	122.25	110.40
1	E	67	ARG	CB-CA-C	-5.83	98.73	110.40
1	A	110	THR	CB-CA-C	5.76	127.15	111.60
1	D	105	TYR	CB-CA-C	-5.70	99.00	110.40
1	D	118	SER	N-CA-CB	5.68	119.02	110.50
1	F	43	GLN	CB-CA-C	5.55	121.51	110.40
1	C	46	GLU	CB-CA-C	5.46	121.32	110.40
1	A	59	ASP	CB-CA-C	-5.41	99.58	110.40
1	E	89	GLU	CB-CA-C	-5.36	99.69	110.40
1	B	41	PRO	N-CD-CG	-5.32	95.22	103.20
1	A	216	PRO	N-CD-CG	-5.15	95.47	103.20
1	B	58	THR	CB-CA-C	-5.13	97.76	111.60
1	E	67	ARG	CG-CD-NE	-5.05	101.20	111.80

There are no chirality outliers.

There are no planarity outliers.

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	1588	0	1558	91	0
1	B	1504	0	1468	81	22
1	C	1508	0	1478	189	22
1	D	1542	0	1511	123	0
1	E	1605	0	1570	124	0
1	F	1518	0	1494	136	0
All	All	9265	0	9079	672	22

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 37.

All (672) 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:F:4:LEU:CD1	1:F:107:GLY:HA3	1.19	1.57
1:F:4:LEU:HD12	1:F:107:GLY:CA	1.10	1.56
1:F:5:VAL:CG1	1:F:23:LYS:CB	1.89	1.50
1:D:200:ASN:ND2	1:D:211:ASP:CB	1.72	1.50
1:F:5:VAL:CG1	1:F:23:LYS:HB2	1.43	1.47
1:C:22:CYS:SG	1:C:96:CYS:CB	2.08	1.40
1:C:22:CYS:SG	1:C:96:CYS:SG	1.45	1.40
1:D:188:PRO:HG2	1:D:191:SER:OG	1.20	1.38
1:F:5:VAL:HG11	1:F:23:LYS:CB	1.48	1.35
1:F:67:ARG:NH2	1:F:90:ASP:OD2	1.62	1.32
1:F:4:LEU:CD1	1:F:107:GLY:CA	1.79	1.31
1:C:151:GLU:OE2	1:C:179:TYR:CD2	1.83	1.30
1:C:146:LYS:HG3	1:C:180:SER:OG	1.35	1.26
1:E:122:PRO:HD3	1:E:203:HIS:ND1	1.49	1.25
1:C:150:PRO:C	1:C:152:PRO:HD2	1.57	1.24
1:A:151:GLU:CG	1:A:152:PRO:HA	1.66	1.23
1:E:6:GLN:H	1:E:108:GLN:NE2	1.36	1.23
1:D:150:PRO:HD2	1:D:205:PRO:CB	1.67	1.22
1:F:4:LEU:CG	1:F:107:GLY:HA2	1.70	1.22
1:F:5:VAL:HG12	1:F:23:LYS:O	1.37	1.22
1:A:61:SER:OG	1:B:103:PHE:CE2	1.91	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:PRO:HD2	1:D:205:PRO:CG	1.75	1.17
1:F:18:VAL:HG12	1:F:86:LEU:HD11	1.27	1.14
1:C:73:ASP:OD2	1:C:76:ALA:CB	1.94	1.13
1:E:6:GLN:N	1:E:108:GLN:HE21	1.46	1.13
1:C:152:PRO:HG2	1:C:205:PRO:HG2	1.19	1.13
1:C:76:ALA:O	1:C:77:SER:OG	1.65	1.12
1:E:6:GLN:N	1:E:108:GLN:NE2	1.96	1.12
1:E:51:ILE:HG13	1:E:58:THR:CG2	1.81	1.10
1:F:19:LYS:HD2	1:F:82:GLU:OE1	1.51	1.10
1:C:151:GLU:OE2	1:C:179:TYR:HD2	1.23	1.09
1:F:46:GLU:OE1	1:F:63:LYS:NZ	1.84	1.09
1:C:22:CYS:SG	1:C:96:CYS:HB3	1.90	1.09
1:F:68:ALA:HB2	1:F:83:LEU:HD12	1.32	1.08
1:A:151:GLU:HG2	1:A:152:PRO:HA	1.32	1.08
1:A:184:VAL:CG1	1:B:144:LEU:HD22	1.83	1.07
1:C:159:SER:HA	1:C:200:ASN:ND2	1.67	1.07
1:B:142:GLY:HA2	1:B:157:TRP:CZ2	1.89	1.07
1:F:174:GLN:HG3	1:F:178:LEU:O	1.55	1.06
1:C:28:THR:HG23	1:E:101:THR:O	1.54	1.06
1:D:150:PRO:CD	1:D:205:PRO:CB	2.33	1.05
1:D:150:PRO:CD	1:D:205:PRO:HB3	1.86	1.04
1:C:73:ASP:OD2	1:C:76:ALA:HB3	1.55	1.04
1:C:22:CYS:CB	1:C:96:CYS:SG	2.46	1.04
1:C:159:SER:HA	1:C:200:ASN:HD21	1.23	1.03
1:D:126:PRO:HB3	1:D:214:VAL:HG22	1.41	1.03
1:D:119:THR:HG23	1:D:149:PHE:O	1.59	1.02
1:F:4:LEU:HG	1:F:107:GLY:HA2	1.40	1.02
1:D:150:PRO:HD2	1:D:205:PRO:HG2	1.40	1.01
1:E:47:TRP:CE3	1:F:104:VAL:HG13	1.94	1.01
1:E:189:SER:HA	1:E:192:LEU:HD11	1.41	1.01
1:F:5:VAL:HG11	1:F:23:LYS:HB3	1.02	1.01
1:F:5:VAL:HG13	1:F:23:LYS:CB	1.69	1.01
1:C:212:LYS:HZ3	1:C:213:LYS:NZ	1.59	1.01
1:C:20:VAL:CG1	1:C:110:THR:HG21	1.88	1.01
1:F:51:ILE:HG13	1:F:58:THR:HG22	1.40	1.01
1:A:184:VAL:HG11	1:B:144:LEU:HD22	1.04	1.00
1:C:157:TRP:HB2	1:C:162:LEU:HD11	1.44	1.00
1:C:159:SER:CA	1:C:200:ASN:HD21	1.73	1.00
1:C:102:ARG:HD2	1:E:28:THR:HG22	1.44	0.99
1:E:192:LEU:H	1:E:192:LEU:HD12	1.26	0.99
1:C:102:ARG:HA	1:E:28:THR:HG23	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:TRP:CE3	1:F:198:ILE:O	2.15	0.99
1:C:28:THR:CG2	1:E:101:THR:O	2.11	0.98
1:C:157:TRP:CB	1:C:162:LEU:HD11	1.92	0.98
1:C:47:TRP:CD1	1:D:104:VAL:HG22	1.98	0.98
1:A:36:TRP:CD1	1:A:70:ILE:HD13	1.99	0.98
1:D:150:PRO:HD3	1:D:205:PRO:HB3	1.43	0.97
1:D:156:SER:O	1:D:199:CYS:O	1.82	0.97
1:E:189:SER:O	1:E:192:LEU:CD1	2.12	0.97
1:A:36:TRP:HD1	1:A:70:ILE:HD13	1.24	0.97
1:F:156:SER:O	1:F:199:CYS:O	1.81	0.97
1:D:188:PRO:CG	1:D:191:SER:OG	2.13	0.96
1:D:188:PRO:HG2	1:D:191:SER:HG	1.32	0.95
1:C:152:PRO:CG	1:C:205:PRO:HG2	1.96	0.95
1:F:51:ILE:CG1	1:F:58:THR:HG22	1.96	0.95
1:C:42:GLY:C	1:C:43:GLN:OE1	2.04	0.95
1:E:67:ARG:HD2	1:E:84:SER:O	1.67	0.95
1:F:5:VAL:HG13	1:F:23:LYS:HB2	0.96	0.94
1:E:51:ILE:HG13	1:E:58:THR:HG22	1.48	0.94
1:C:20:VAL:HG13	1:C:110:THR:HG21	1.48	0.94
1:F:4:LEU:CG	1:F:107:GLY:CA	2.35	0.93
1:C:150:PRO:C	1:C:152:PRO:CD	2.36	0.93
1:C:212:LYS:NZ	1:C:213:LYS:HZ3	1.65	0.93
1:C:146:LYS:CG	1:C:180:SER:OG	2.16	0.93
1:C:152:PRO:HG2	1:C:205:PRO:CG	1.97	0.92
1:F:5:VAL:CG1	1:F:23:LYS:CA	2.47	0.92
1:D:198:ILE:HG22	1:D:200:ASN:OD1	1.70	0.92
1:C:73:ASP:OD2	1:C:76:ALA:HB2	1.70	0.92
1:D:61:SER:O	1:D:65:LYS:HG3	1.67	0.92
1:B:99:THR:O	1:B:103:PHE:O	1.87	0.92
1:B:203:HIS:ND1	1:B:206:SER:OG	1.96	0.92
1:F:174:GLN:OE1	1:F:180:SER:OG	1.88	0.92
1:F:5:VAL:CG1	1:F:23:LYS:O	2.19	0.91
1:C:28:THR:HG21	1:E:102:ARG:HA	1.51	0.91
1:C:115:SER:HB3	1:C:149:PHE:HZ	1.35	0.91
1:E:120:LYS:O	1:E:203:HIS:HE1	1.55	0.90
1:D:150:PRO:CD	1:D:205:PRO:CG	2.48	0.90
1:C:151:GLU:N	1:C:152:PRO:HD2	1.87	0.90
1:C:168:THR:OG1	1:C:183:SER:OG	1.90	0.90
1:C:115:SER:HB3	1:C:149:PHE:CZ	2.07	0.89
1:A:151:GLU:HG3	1:A:152:PRO:HA	1.53	0.89
1:A:163:THR:O	1:A:166:VAL:HG12	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:GLN:OE1	1:C:43:GLN:N	2.06	0.88
1:C:157:TRP:HB2	1:C:162:LEU:CD1	2.02	0.88
1:A:184:VAL:HG11	1:B:144:LEU:CD2	1.99	0.88
1:A:61:SER:OG	1:B:103:PHE:CZ	2.22	0.87
1:E:189:SER:O	1:E:192:LEU:HD12	1.73	0.87
1:E:22:CYS:HG	1:E:96:CYS:HG	0.95	0.87
1:D:51:ILE:HG13	1:D:58:THR:HG22	1.57	0.86
1:D:126:PRO:CB	1:D:214:VAL:HG22	2.06	0.86
1:B:141:LEU:O	1:B:185:VAL:N	2.09	0.85
1:B:147:ASP:CB	1:B:178:LEU:HD13	2.06	0.85
1:E:198:ILE:HG23	1:E:212:LYS:O	1.77	0.84
1:F:51:ILE:HG13	1:F:58:THR:CG2	2.07	0.84
1:F:18:VAL:CG1	1:F:86:LEU:HD11	2.05	0.84
1:F:163:THR:O	1:F:166:VAL:HG12	1.77	0.84
1:E:202:ASN:O	1:E:208:THR:O	1.95	0.84
1:C:215:GLU:O	1:D:130:SER:OG	1.96	0.83
1:C:212:LYS:HZ3	1:C:213:LYS:HZ3	0.86	0.83
1:F:19:LYS:CD	1:F:82:GLU:OE1	2.26	0.83
1:A:151:GLU:HG2	1:A:152:PRO:CA	2.08	0.82
1:D:166:VAL:C	1:D:167:HIS:HD1	1.81	0.82
1:D:174:GLN:OE1	1:D:180:SER:OG	1.98	0.81
1:E:51:ILE:CG1	1:E:58:THR:CG2	2.58	0.81
1:F:5:VAL:HG13	1:F:23:LYS:N	1.95	0.81
1:C:102:ARG:HA	1:E:28:THR:CG2	2.10	0.81
1:B:142:GLY:HA2	1:B:157:TRP:HZ2	1.44	0.81
1:D:4:LEU:HD22	1:D:22:CYS:SG	2.21	0.81
1:F:4:LEU:HD13	1:F:96:CYS:SG	2.21	0.81
1:F:23:LYS:HE2	1:F:78:THR:HG21	1.62	0.81
1:C:159:SER:N	1:C:200:ASN:HD21	1.79	0.80
1:B:147:ASP:HB2	1:B:178:LEU:HD13	1.63	0.80
1:B:173:LEU:HD13	1:B:179:TYR:CZ	2.16	0.80
1:E:87:ARG:O	1:E:114:VAL:HG11	1.82	0.80
1:C:33:GLY:O	1:C:98:GLY:HA2	1.82	0.79
1:C:18:VAL:HG12	1:C:86:LEU:HD11	1.63	0.79
1:C:152:PRO:CG	1:C:205:PRO:CG	2.57	0.79
1:B:52:TYR:HD2	1:B:55:ALA:H	1.29	0.79
1:E:4:LEU:HD23	1:E:22:CYS:HG	1.48	0.79
1:E:189:SER:CA	1:E:192:LEU:HD11	2.13	0.79
1:B:142:GLY:HA2	1:B:157:TRP:CH2	2.17	0.79
1:E:91:THR:HG23	1:E:113:THR:HA	1.64	0.79
1:C:20:VAL:CG1	1:C:110:THR:CG2	2.60	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:HIS:ND1	1:C:206:SER:HB2	1.98	0.78
1:E:51:ILE:CG1	1:E:58:THR:HG22	2.13	0.78
1:D:119:THR:CG2	1:D:149:PHE:O	2.32	0.78
1:D:91:THR:HG23	1:D:113:THR:HA	1.64	0.78
1:E:124:VAL:HG21	1:E:201:VAL:HG21	1.64	0.78
1:C:146:LYS:HG3	1:C:180:SER:HG	1.45	0.78
1:E:22:CYS:CB	1:E:96:CYS:SG	2.71	0.77
1:D:200:ASN:HD21	1:D:211:ASP:CB	1.95	0.77
1:E:51:ILE:HG13	1:E:58:THR:HG23	1.67	0.77
1:C:212:LYS:NZ	1:C:213:LYS:NZ	2.26	0.77
1:E:4:LEU:HD23	1:E:22:CYS:SG	2.25	0.77
1:C:138:THR:OG1	1:C:189:SER:OG	2.00	0.77
1:D:113:THR:HG21	1:D:179:TYR:OH	1.85	0.76
1:F:73:ASP:OD1	1:F:76:ALA:HB3	1.86	0.76
1:F:4:LEU:HD11	1:F:107:GLY:CA	2.10	0.76
1:A:174:GLN:OE1	1:A:180:SER:OG	2.04	0.76
1:C:149:PHE:N	1:C:150:PRO:CD	2.49	0.76
1:E:126:PRO:HG3	1:E:212:LYS:HE2	1.66	0.76
1:A:61:SER:OG	1:B:103:PHE:HE2	1.60	0.76
1:D:119:THR:HA	1:D:149:PHE:HB3	1.68	0.76
1:D:122:PRO:HD2	1:D:208:THR:HG21	1.68	0.76
1:C:150:PRO:O	1:C:152:PRO:N	2.18	0.75
1:C:157:TRP:HB3	1:C:162:LEU:HD11	1.67	0.75
1:C:99:THR:OG1	1:E:31:ASN:ND2	2.19	0.75
1:D:166:VAL:O	1:D:167:HIS:ND1	2.12	0.75
1:D:17:SER:HB2	1:D:84:SER:HA	1.69	0.75
1:E:22:CYS:CB	1:E:96:CYS:HG	1.98	0.74
1:F:4:LEU:CD1	1:F:107:GLY:N	2.49	0.74
1:D:150:PRO:CD	1:D:205:PRO:HG2	2.14	0.74
1:C:103:PHE:HE2	1:D:62:GLU:HG2	1.53	0.74
1:C:184:VAL:HG21	1:D:144:LEU:HD13	1.70	0.74
1:F:39:GLN:O	1:F:92:ALA:HB1	1.88	0.74
1:D:198:ILE:CG2	1:D:200:ASN:OD1	2.36	0.73
1:A:36:TRP:CE2	1:A:81:MET:HB2	2.24	0.73
1:E:6:GLN:H	1:E:108:GLN:HE21	0.74	0.73
1:F:5:VAL:CG1	1:F:23:LYS:HB3	1.82	0.73
1:C:149:PHE:N	1:C:150:PRO:HD2	2.04	0.73
1:E:40:ALA:O	1:E:43:GLN:HB2	1.89	0.73
1:F:23:LYS:HG3	1:F:78:THR:HG22	1.69	0.72
1:C:22:CYS:CB	1:C:96:CYS:HG	1.96	0.72
1:D:126:PRO:HB3	1:D:214:VAL:CG2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:5:VAL:HG12	1:F:23:LYS:C	2.08	0.72
1:B:147:ASP:HB3	1:B:178:LEU:CB	2.20	0.72
1:C:102:ARG:CD	1:E:28:THR:HG22	2.19	0.72
1:C:163:THR:O	1:C:166:VAL:HG12	1.89	0.72
1:F:83:LEU:HD23	1:F:86:LEU:HD21	1.70	0.72
1:B:5:VAL:HB	1:B:23:LYS:HG2	1.71	0.72
1:C:53:ILE:HD13	1:C:53:ILE:N	2.04	0.71
1:F:213:LYS:HE3	1:F:215:GLU:HG2	1.72	0.71
1:B:168:THR:OG1	1:B:183:SER:OG	2.03	0.71
1:C:143:CYS:SG	1:C:199:CYS:CB	2.78	0.71
1:F:4:LEU:CB	1:F:107:GLY:HA2	2.21	0.71
1:E:120:LYS:O	1:E:203:HIS:CE1	2.42	0.71
1:C:126:PRO:HD3	1:C:212:LYS:HD3	1.73	0.70
1:C:87:ARG:O	1:C:114:VAL:HG11	1.90	0.70
1:F:5:VAL:HG13	1:F:23:LYS:CA	2.17	0.70
1:F:73:ASP:OD1	1:F:76:ALA:CB	2.40	0.70
1:A:5:VAL:HG21	1:D:5:VAL:CG2	2.22	0.70
1:C:121:GLY:O	1:C:147:ASP:O	2.09	0.70
1:F:213:LYS:HE3	1:F:215:GLU:CG	2.21	0.70
1:C:99:THR:HA	1:C:104:VAL:HG22	1.74	0.69
1:B:147:ASP:HB3	1:B:178:LEU:CD1	2.21	0.69
1:D:150:PRO:HD2	1:D:205:PRO:HB2	1.71	0.69
1:F:68:ALA:HB2	1:F:83:LEU:CD1	2.16	0.69
1:F:77:SER:O	1:F:77:SER:OG	2.09	0.69
1:A:58:THR:C	1:A:59:ASP:OD1	2.31	0.69
1:F:98:GLY:HA3	1:F:105:TYR:HB2	1.75	0.69
1:C:150:PRO:O	1:C:152:PRO:CD	2.41	0.69
1:F:5:VAL:HG13	1:F:23:LYS:H	1.57	0.69
1:C:201:VAL:HG22	1:C:210:VAL:HG12	1.74	0.68
1:B:147:ASP:HB3	1:B:178:LEU:HD13	1.73	0.68
1:E:37:VAL:HG11	1:F:106:TRP:CZ2	2.29	0.68
1:F:23:LYS:HG3	1:F:78:THR:CG2	2.23	0.68
1:D:147:ASP:HB3	1:D:178:LEU:HD22	1.74	0.68
1:C:150:PRO:HB2	1:C:152:PRO:HG2	1.73	0.68
1:C:97:ALA:HB2	1:C:106:TRP:CE3	2.28	0.68
1:A:8:GLY:HA3	1:D:19:LYS:HG2	1.75	0.67
1:C:159:SER:H	1:C:200:ASN:HD21	1.42	0.67
1:D:200:ASN:HA	1:D:211:ASP:HA	1.76	0.67
1:E:148:TYR:HB2	1:E:203:HIS:CE1	2.29	0.67
1:F:155:VAL:HG22	1:F:201:VAL:HG13	1.76	0.67
1:C:124:VAL:CG1	1:C:212:LYS:HD2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLU:N	1:C:152:PRO:CD	2.56	0.67
1:A:4:LEU:HD23	1:A:22:CYS:SG	2.35	0.67
1:C:143:CYS:CB	1:C:199:CYS:HG	2.07	0.67
1:E:47:TRP:CD2	1:F:104:VAL:HG13	2.29	0.67
1:A:132:LYS:HG3	1:B:126:PRO:HG3	1.75	0.67
1:A:31:ASN:O	1:A:31:ASN:ND2	2.28	0.66
1:B:115:SER:HB3	1:B:149:PHE:CZ	2.30	0.66
1:A:32:TYR:HE1	1:A:34:ILE:HD11	1.61	0.66
1:A:129:PRO:HG2	1:A:192:LEU:HD21	1.77	0.66
1:E:122:PRO:CD	1:E:203:HIS:ND1	2.43	0.66
1:A:32:TYR:CE1	1:A:34:ILE:HD11	2.30	0.66
1:B:196:THR:CG2	1:B:213:LYS:HE2	2.26	0.66
1:F:67:ARG:NH2	1:F:90:ASP:CG	2.48	0.66
1:C:204:LYS:N	1:C:205:PRO:CD	2.58	0.66
1:C:31:ASN:HB2	1:E:101:THR:HG22	1.77	0.65
1:C:149:PHE:H	1:C:150:PRO:CD	2.08	0.65
1:E:51:ILE:CG1	1:E:58:THR:HG23	2.26	0.65
1:F:5:VAL:CG1	1:F:23:LYS:N	2.58	0.65
1:C:200:ASN:OD1	1:C:200:ASN:N	2.30	0.65
1:C:127:LEU:HD11	1:D:140:ALA:O	1.97	0.65
1:D:29:PHE:HE2	1:D:74:THR:HA	1.61	0.65
1:F:174:GLN:CG	1:F:178:LEU:O	2.38	0.64
1:C:122:PRO:HA	1:C:146:LYS:O	1.98	0.64
1:E:124:VAL:CG2	1:E:201:VAL:HG21	2.27	0.64
1:C:6:GLN:HG2	1:C:110:THR:HG22	1.80	0.64
1:C:150:PRO:O	1:C:151:GLU:C	2.33	0.64
1:C:153:VAL:HG23	1:C:203:HIS:HD2	1.63	0.64
1:D:197:TYR:O	1:D:213:LYS:O	2.16	0.64
1:C:47:TRP:CG	1:D:104:VAL:HG22	2.32	0.64
1:D:199:CYS:SG	1:D:201:VAL:HG13	2.38	0.64
1:A:51:ILE:HG13	1:A:58:THR:HG22	1.79	0.64
1:F:4:LEU:HD11	1:F:107:GLY:HA3	1.61	0.63
1:C:126:PRO:HB3	1:C:212:LYS:HG2	1.80	0.63
1:B:144:LEU:O	1:B:144:LEU:HG	1.97	0.63
1:C:4:LEU:N	1:C:4:LEU:HD12	2.14	0.63
1:D:124:VAL:CG1	1:D:143:CYS:SG	2.86	0.63
1:F:4:LEU:HD11	1:F:96:CYS:O	1.98	0.63
1:D:199:CYS:SG	1:D:201:VAL:CG1	2.86	0.63
1:A:6:GLN:NE2	1:A:110:THR:HG22	2.14	0.63
1:B:34:ILE:HD12	1:B:34:ILE:N	2.13	0.63
1:C:127:LEU:O	1:C:214:VAL:HG12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LEU:HG	1:F:107:GLY:CA	2.14	0.63
1:A:67:ARG:O	1:A:83:LEU:HA	1.98	0.63
1:C:141:LEU:HD23	1:C:214:VAL:HB	1.80	0.63
1:C:151:GLU:OE2	1:C:179:TYR:CE2	2.50	0.63
1:F:126:PRO:CB	1:F:214:VAL:HG12	2.28	0.63
1:F:201:VAL:O	1:F:209:LYS:HG2	1.99	0.63
1:E:25:SER:O	1:E:25:SER:OG	2.14	0.62
1:F:163:THR:O	1:F:166:VAL:CG1	2.47	0.62
1:A:132:LYS:CG	1:B:126:PRO:HG3	2.30	0.62
1:F:5:VAL:CG1	1:F:23:LYS:H	2.12	0.62
1:C:152:PRO:O	1:C:203:HIS:CD2	2.52	0.62
1:C:20:VAL:HG13	1:C:110:THR:CG2	2.23	0.62
1:C:22:CYS:HB3	1:C:96:CYS:SG	2.37	0.62
1:E:34:ILE:HD13	1:E:96:CYS:SG	2.40	0.62
1:E:129:PRO:HD3	1:E:141:LEU:HD23	1.81	0.62
1:E:87:ARG:O	1:E:114:VAL:CG1	2.47	0.62
1:A:36:TRP:HD1	1:A:70:ILE:CD1	2.06	0.62
1:C:103:PHE:CE2	1:D:62:GLU:HG2	2.35	0.62
1:B:142:GLY:CA	1:B:157:TRP:CH2	2.83	0.61
1:F:51:ILE:CG1	1:F:58:THR:CG2	2.72	0.61
1:D:29:PHE:CE2	1:D:74:THR:HA	2.34	0.61
1:F:6:GLN:HA	1:F:21:SER:O	2.01	0.61
1:B:142:GLY:HA3	1:B:184:VAL:HA	1.82	0.61
1:F:198:ILE:HG22	1:F:212:LYS:O	2.00	0.61
1:E:47:TRP:CE3	1:F:104:VAL:CG1	2.78	0.61
1:E:192:LEU:HD12	1:E:192:LEU:N	2.07	0.61
1:A:188:PRO:O	1:A:191:SER:OG	2.18	0.60
1:B:142:GLY:HA3	1:B:183:SER:O	2.01	0.60
1:C:150:PRO:CA	1:C:152:PRO:HD2	2.31	0.60
1:B:91:THR:HG23	1:B:113:THR:HA	1.83	0.60
1:C:99:THR:O	1:C:103:PHE:O	2.19	0.60
1:F:5:VAL:HG13	1:F:5:VAL:O	2.01	0.60
1:F:67:ARG:HD3	1:F:83:LEU:CD1	2.31	0.60
1:D:120:LYS:O	1:D:148:TYR:HA	2.01	0.60
1:C:90:ASP:O	1:C:94:TYR:OH	2.17	0.60
1:C:47:TRP:CD1	1:D:104:VAL:CG2	2.82	0.60
1:D:150:PRO:CG	1:D:205:PRO:CG	2.79	0.60
1:A:20:VAL:HG11	1:A:110:THR:HG23	1.84	0.59
1:C:76:ALA:C	1:C:77:SER:HG	2.02	0.59
1:E:130:SER:HB2	1:F:126:PRO:HG2	1.84	0.59
1:F:12:LYS:O	1:F:114:VAL:HA	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ALA:CB	1:F:78:THR:HG23	2.33	0.59
1:F:138:THR:OG1	1:F:189:SER:N	2.33	0.59
1:B:203:HIS:CE1	1:B:206:SER:HG	2.20	0.59
1:C:103:PHE:N	1:C:103:PHE:CD1	2.71	0.59
1:C:6:GLN:NE2	1:C:107:GLY:HA3	2.18	0.59
1:E:127:LEU:HD21	1:F:140:ALA:O	2.03	0.59
1:E:6:GLN:CA	1:E:108:GLN:NE2	2.65	0.58
1:F:126:PRO:HB2	1:F:214:VAL:HG12	1.85	0.58
1:D:196:THR:O	1:D:196:THR:OG1	2.21	0.58
1:E:214:VAL:HG12	1:E:214:VAL:O	2.03	0.58
1:F:22:CYS:SG	1:F:96:CYS:SG	3.01	0.58
1:A:129:PRO:HD3	1:A:141:LEU:CD2	2.33	0.58
1:C:28:THR:CG2	1:E:102:ARG:HA	2.31	0.58
1:E:192:LEU:H	1:E:192:LEU:CD1	2.07	0.58
1:B:53:ILE:N	1:B:53:ILE:HD13	2.18	0.58
1:E:133:SER:HB2	1:F:126:PRO:HG2	1.84	0.58
1:C:172:VAL:HG23	1:C:172:VAL:O	2.02	0.58
1:B:173:LEU:CD1	1:B:179:TYR:CZ	2.86	0.58
1:C:166:VAL:HG13	1:C:166:VAL:O	2.04	0.58
1:E:174:GLN:HG3	1:E:178:LEU:O	2.03	0.58
1:F:39:GLN:C	1:F:92:ALA:HB1	2.24	0.58
1:C:124:VAL:HB	1:C:212:LYS:CD	2.33	0.58
1:F:4:LEU:HD11	1:F:107:GLY:N	2.17	0.58
1:B:28:THR:HG22	1:B:77:SER:HB2	1.85	0.57
1:C:124:VAL:HB	1:C:212:LYS:HD2	1.85	0.57
1:F:91:THR:HG23	1:F:113:THR:HA	1.87	0.57
1:F:159:SER:H	1:F:200:ASN:ND2	2.02	0.57
1:A:40:ALA:HB3	1:A:43:GLN:HB2	1.87	0.57
1:A:166:VAL:HB	1:A:185:VAL:HG23	1.85	0.57
1:F:5:VAL:CG1	1:F:23:LYS:C	2.68	0.57
1:A:129:PRO:HD3	1:A:141:LEU:HD23	1.87	0.57
1:B:115:SER:CB	1:B:149:PHE:CZ	2.87	0.57
1:D:214:VAL:HG12	1:D:214:VAL:O	2.03	0.57
1:E:23:LYS:HA	1:E:78:THR:HB	1.87	0.57
1:E:37:VAL:HG11	1:F:106:TRP:HZ2	1.67	0.57
1:A:5:VAL:HG21	1:D:5:VAL:HG22	1.86	0.57
1:F:23:LYS:CG	1:F:78:THR:HG22	2.34	0.57
1:F:102:ARG:HG2	1:F:102:ARG:HH11	1.70	0.57
1:C:31:ASN:O	1:E:101:THR:CG2	2.52	0.57
1:C:152:PRO:CG	1:C:205:PRO:HG3	2.34	0.57
1:C:28:THR:HG21	1:E:102:ARG:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLY:O	1:C:98:GLY:CA	2.52	0.57
1:E:124:VAL:HG12	1:E:212:LYS:HG3	1.87	0.57
1:F:67:ARG:HD3	1:F:83:LEU:HD11	1.87	0.57
1:D:137:GLY:O	1:D:189:SER:OG	2.13	0.57
1:F:19:LYS:HG3	1:F:82:GLU:HB2	1.85	0.57
1:C:114:VAL:HG12	1:C:114:VAL:O	2.04	0.56
1:A:148:TYR:CZ	1:A:179:TYR:HB3	2.40	0.56
1:C:115:SER:CB	1:C:149:PHE:HZ	2.11	0.56
1:F:94:TYR:CD1	1:F:94:TYR:N	2.73	0.56
1:B:142:GLY:CA	1:B:183:SER:O	2.54	0.56
1:C:31:ASN:CB	1:E:101:THR:HG22	2.34	0.56
1:B:147:ASP:HB3	1:B:178:LEU:HB3	1.87	0.55
1:F:51:ILE:HG12	1:F:58:THR:HG22	1.86	0.55
1:E:1:GLU:OE1	1:E:26:GLY:O	2.24	0.55
1:C:159:SER:HA	1:C:200:ASN:HD22	1.67	0.55
1:C:76:ALA:C	1:C:77:SER:OG	2.39	0.55
1:F:83:LEU:HD23	1:F:86:LEU:CD2	2.36	0.55
1:D:104:VAL:HG21	1:D:106:TRP:HE1	1.72	0.55
1:D:122:PRO:HB2	1:D:145:VAL:HG12	1.89	0.55
1:E:127:LEU:CD2	1:F:140:ALA:O	2.55	0.55
1:C:97:ALA:HB2	1:C:106:TRP:CD2	2.42	0.55
1:D:43:GLN:O	1:D:43:GLN:HG3	2.06	0.55
1:C:159:SER:CA	1:C:200:ASN:ND2	2.44	0.54
1:E:6:GLN:N	1:E:108:GLN:HE22	1.97	0.54
1:C:53:ILE:N	1:C:53:ILE:CD1	2.71	0.54
1:E:64:PHE:N	1:E:64:PHE:CD1	2.75	0.54
1:B:196:THR:CG2	1:B:213:LYS:CE	2.85	0.54
1:D:6:GLN:HG3	1:D:108:GLN:HG3	1.90	0.54
1:D:187:VAL:HG11	1:D:197:TYR:CE2	2.43	0.54
1:E:35:ASN:ND2	1:F:103:PHE:CD2	2.76	0.54
1:E:184:VAL:HG11	1:F:144:LEU:HD22	1.89	0.54
1:D:119:THR:HA	1:D:149:PHE:O	2.08	0.54
1:F:18:VAL:HG12	1:F:86:LEU:CD1	2.18	0.54
1:A:6:GLN:NE2	1:A:110:THR:CG2	2.71	0.54
1:A:198:ILE:HG12	1:A:198:ILE:O	2.08	0.54
1:E:63:LYS:HB3	1:E:64:PHE:CD1	2.43	0.53
1:C:126:PRO:HG3	1:C:212:LYS:HE3	1.90	0.53
1:B:145:VAL:CG2	1:B:181:LEU:HB3	2.39	0.53
1:D:2:VAL:HG22	1:D:26:GLY:HA3	1.91	0.53
1:D:126:PRO:HG3	1:D:212:LYS:HD2	1.91	0.53
1:D:204:LYS:CB	1:D:204:LYS:NZ	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HB2	1:A:185:VAL:HG12	1.90	0.53
1:C:32:TYR:CD2	1:C:34:ILE:HD11	2.43	0.53
1:D:200:ASN:HA	1:D:211:ASP:CA	2.37	0.53
1:D:197:TYR:N	1:D:197:TYR:CD1	2.76	0.53
1:E:76:ALA:O	1:E:77:SER:OG	2.24	0.53
1:E:104:VAL:HB	1:F:47:TRP:CG	2.43	0.53
1:C:153:VAL:HG23	1:C:203:HIS:CD2	2.42	0.53
1:E:106:TRP:CZ3	1:F:45:LEU:HD12	2.44	0.52
1:E:22:CYS:HB2	1:E:96:CYS:SG	2.50	0.52
1:C:103:PHE:N	1:C:103:PHE:HD1	2.07	0.52
1:C:146:LYS:HG3	1:C:180:SER:CB	2.33	0.52
1:F:67:ARG:CZ	1:F:90:ASP:OD2	2.49	0.52
1:B:151:GLU:N	1:B:152:PRO:CD	2.73	0.52
1:C:100:GLY:O	1:E:31:ASN:HB2	2.10	0.52
1:A:124:VAL:HG13	1:A:212:LYS:HG3	1.91	0.52
1:A:145:VAL:HB	1:A:181:LEU:HB3	1.91	0.52
1:A:6:GLN:HA	1:A:21:SER:O	2.09	0.52
1:B:34:ILE:HD12	1:B:34:ILE:H	1.74	0.52
1:D:166:VAL:C	1:D:167:HIS:ND1	2.57	0.52
1:F:157:TRP:HE3	1:F:198:ILE:O	1.85	0.52
1:A:20:VAL:CG1	1:A:110:THR:HG21	2.39	0.52
1:C:201:VAL:HG22	1:C:210:VAL:CG1	2.40	0.52
1:D:143:CYS:CB	1:D:199:CYS:HG	2.17	0.52
1:E:124:VAL:HG21	1:E:201:VAL:CG2	2.39	0.52
1:A:20:VAL:CG1	1:A:110:THR:CG2	2.88	0.52
1:C:157:TRP:O	1:C:200:ASN:OD1	2.28	0.52
1:E:213:LYS:HE2	1:E:215:GLU:HG2	1.93	0.51
1:A:148:TYR:O	1:A:179:TYR:HB2	2.10	0.51
1:C:32:TYR:CE2	1:C:34:ILE:HD11	2.46	0.51
1:E:189:SER:C	1:E:192:LEU:CD1	2.78	0.51
1:E:214:VAL:HA	1:F:130:SER:HB3	1.92	0.51
1:F:73:ASP:OD1	1:F:76:ALA:N	2.37	0.51
1:F:87:ARG:HD3	1:F:89:GLU:OE1	2.11	0.51
1:E:144:LEU:HD13	1:F:184:VAL:HG11	1.92	0.51
1:A:163:THR:O	1:A:166:VAL:CG1	2.51	0.51
1:A:120:LYS:HD2	1:A:147:ASP:O	2.10	0.51
1:E:189:SER:O	1:E:192:LEU:HD11	2.06	0.51
1:B:147:ASP:CB	1:B:178:LEU:CD1	2.80	0.50
1:C:28:THR:CG2	1:E:102:ARG:HG2	2.41	0.50
1:F:8:GLY:O	1:F:110:THR:HG23	2.11	0.50
1:B:115:SER:CB	1:B:149:PHE:HZ	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASP:HB3	1:B:178:LEU:HB2	1.93	0.50
1:A:204:LYS:N	1:A:205:PRO:CD	2.73	0.50
1:B:173:LEU:HD13	1:B:179:TYR:CE2	2.46	0.50
1:C:22:CYS:SG	1:C:36:TRP:CH2	3.04	0.50
1:B:147:ASP:OD1	1:B:174:GLN:NE2	2.44	0.50
1:C:33:GLY:HA2	1:C:51:ILE:O	2.12	0.50
1:E:128:ALA:N	1:F:128:ALA:O	2.41	0.50
1:A:12:LYS:HD3	1:A:18:VAL:HB	1.94	0.50
1:A:58:THR:O	1:A:59:ASP:OD1	2.29	0.50
1:B:192:LEU:CD1	1:B:192:LEU:N	2.75	0.50
1:D:29:PHE:O	1:D:32:TYR:HB2	2.11	0.50
1:D:124:VAL:HG13	1:D:143:CYS:SG	2.51	0.50
1:B:188:PRO:O	1:B:191:SER:OG	2.29	0.50
1:E:215:GLU:N	1:F:130:SER:OG	2.44	0.50
1:C:47:TRP:HB2	1:D:104:VAL:HG23	1.94	0.49
1:D:204:LYS:HG3	1:D:204:LYS:O	2.11	0.49
1:B:73:ASP:HB2	1:B:78:THR:HB	1.93	0.49
1:C:103:PHE:HE2	1:D:62:GLU:CG	2.23	0.49
1:C:126:PRO:CD	1:C:212:LYS:HD3	2.41	0.49
1:D:200:ASN:CA	1:D:211:ASP:HA	2.41	0.49
1:D:149:PHE:H	1:D:203:HIS:CE1	2.31	0.49
1:B:31:ASN:H	1:B:53:ILE:HB	1.77	0.49
1:C:124:VAL:CB	1:C:212:LYS:HD2	2.42	0.49
1:D:150:PRO:CG	1:D:205:PRO:HG2	2.41	0.49
1:D:124:VAL:HG21	1:D:201:VAL:CG2	2.43	0.49
1:C:127:LEU:O	1:C:214:VAL:CG1	2.61	0.49
1:D:31:ASN:N	1:D:31:ASN:OD1	2.46	0.49
1:E:6:GLN:C	1:E:108:GLN:HE22	2.14	0.49
1:F:34:ILE:O	1:F:34:ILE:HG22	2.13	0.49
1:A:51:ILE:CG1	1:A:58:THR:HG22	2.42	0.49
1:A:78:THR:CG2	1:D:8:GLY:HA3	2.43	0.49
1:C:149:PHE:O	1:C:149:PHE:CD2	2.66	0.49
1:B:4:LEU:HD13	1:B:105:TYR:HB2	1.95	0.48
1:D:215:GLU:HG3	1:D:216:PRO:HD2	1.95	0.48
1:F:48:ILE:O	1:F:48:ILE:HG22	2.13	0.48
1:C:91:THR:HG23	1:C:113:THR:HA	1.94	0.48
1:C:148:TYR:HE2	1:C:153:VAL:HB	1.79	0.48
1:C:168:THR:HG23	1:C:181:LEU:HD21	1.95	0.48
1:E:108:GLN:H	1:E:108:GLN:HG3	1.36	0.48
1:E:120:LYS:HE3	1:E:178:LEU:HD21	1.95	0.48
1:F:32:TYR:N	1:F:32:TYR:CD1	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:GLN:HG3	1:A:178:LEU:O	2.12	0.48
1:E:189:SER:C	1:E:192:LEU:HD11	2.33	0.48
1:D:200:ASN:H	1:D:211:ASP:HA	1.78	0.48
1:A:59:ASP:OD1	1:A:59:ASP:N	2.43	0.48
1:B:127:LEU:HB2	1:B:142:GLY:O	2.13	0.48
1:E:128:ALA:O	1:F:128:ALA:O	2.32	0.48
1:A:125:PHE:O	1:A:143:CYS:HA	2.13	0.48
1:C:148:TYR:CE2	1:C:153:VAL:HB	2.48	0.48
1:D:162:LEU:HD21	1:D:185:VAL:HG21	1.95	0.48
1:E:63:LYS:HB3	1:E:64:PHE:CE1	2.49	0.48
1:F:141:LEU:HB2	1:F:185:VAL:HG12	1.95	0.48
1:D:53:ILE:N	1:D:53:ILE:HD13	2.29	0.48
1:F:76:ALA:C	1:F:78:THR:HG23	2.34	0.48
1:A:18:VAL:HG12	1:A:86:LEU:HD11	1.96	0.48
1:D:29:PHE:O	1:D:32:TYR:N	2.42	0.48
1:E:64:PHE:O	1:E:68:ALA:HB3	2.14	0.48
1:B:204:LYS:N	1:B:205:PRO:CD	2.77	0.47
1:A:151:GLU:CG	1:A:152:PRO:CA	2.61	0.47
1:B:60:TYR:CE2	1:B:70:ILE:HD12	2.49	0.47
1:B:29:PHE:O	1:B:53:ILE:HG12	2.14	0.47
1:F:147:ASP:HA	1:F:178:LEU:HB3	1.95	0.47
1:D:96:CYS:SG	1:D:107:GLY:HA3	2.55	0.47
1:B:143:CYS:HG	1:B:199:CYS:CB	2.21	0.47
1:C:6:GLN:HB2	1:C:108:GLN:HG3	1.96	0.47
1:C:148:TYR:CD1	1:C:179:TYR:O	2.67	0.47
1:E:121:GLY:HA2	1:E:203:HIS:CE1	2.50	0.47
1:C:203:HIS:CE1	1:C:205:PRO:HB2	2.49	0.47
1:D:67:ARG:HD2	1:D:84:SER:O	2.14	0.47
1:E:6:GLN:HA	1:E:21:SER:O	2.15	0.47
1:A:132:LYS:HG3	1:A:132:LYS:O	2.15	0.47
1:C:138:THR:CB	1:C:189:SER:HG	2.23	0.47
1:F:126:PRO:HB3	1:F:214:VAL:HG12	1.97	0.47
1:C:20:VAL:HG12	1:C:110:THR:HG21	1.88	0.47
1:C:127:LEU:CD1	1:D:140:ALA:O	2.62	0.47
1:C:152:PRO:HB2	1:C:205:PRO:CG	2.44	0.47
1:C:34:ILE:HG13	1:C:79:VAL:HG21	1.97	0.46
1:C:178:LEU:HD12	1:C:178:LEU:H	1.81	0.46
1:D:150:PRO:HG2	1:D:205:PRO:HG2	1.97	0.46
1:E:67:ARG:CD	1:E:84:SER:O	2.52	0.46
1:F:19:LYS:HD2	1:F:82:GLU:HB2	1.97	0.46
1:B:99:THR:HA	1:B:104:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:85:SER:O	1:E:85:SER:OG	2.22	0.46
1:E:128:ALA:HB1	1:E:129:PRO:HD2	1.97	0.46
1:E:2:VAL:HG11	1:E:27:TYR:CZ	2.51	0.46
1:F:68:ALA:HA	1:F:82:GLU:O	2.15	0.46
1:C:203:HIS:HB3	1:C:208:THR:HB	1.98	0.46
1:D:41:PRO:HD3	1:D:91:THR:O	2.15	0.46
1:A:115:SER:HB3	1:A:149:PHE:CE2	2.51	0.46
1:D:150:PRO:HG2	1:D:152:PRO:HD2	1.98	0.46
1:F:94:TYR:N	1:F:94:TYR:HD1	2.14	0.46
1:F:128:ALA:HB1	1:F:129:PRO:CD	2.46	0.46
1:C:162:LEU:O	1:C:162:LEU:HD12	2.15	0.46
1:D:200:ASN:CG	1:D:211:ASP:CB	2.70	0.46
1:F:53:ILE:HG22	1:F:72:SER:OG	2.15	0.46
1:A:35:ASN:HB2	1:A:97:ALA:HB3	1.97	0.46
1:A:120:LYS:HD3	1:A:121:GLY:O	2.16	0.46
1:B:165:GLY:O	1:B:185:VAL:HA	2.15	0.46
1:D:150:PRO:HG2	1:D:205:PRO:CG	2.46	0.46
1:D:198:ILE:HG22	1:D:200:ASN:CG	2.32	0.46
1:A:140:ALA:HB1	1:B:144:LEU:HD23	1.98	0.45
1:A:130:SER:OG	1:B:215:GLU:C	2.54	0.45
1:D:174:GLN:HE21	1:D:174:GLN:HB2	1.55	0.45
1:A:32:TYR:CD1	1:A:32:TYR:O	2.69	0.45
1:E:7:SER:O	1:E:110:THR:HG23	2.16	0.45
1:C:31:ASN:O	1:E:101:THR:HG22	2.16	0.45
1:F:141:LEU:HD11	1:F:197:TYR:CD2	2.51	0.45
1:A:60:TYR:HE1	1:A:70:ILE:HG13	1.81	0.45
1:C:102:ARG:HG3	1:C:102:ARG:HH21	1.81	0.45
1:D:38:ARG:HB3	1:D:48:ILE:HD11	1.97	0.45
1:D:143:CYS:CB	1:D:199:CYS:SG	3.03	0.45
1:F:102:ARG:HH11	1:F:102:ARG:CG	2.30	0.45
1:A:78:THR:HG21	1:D:8:GLY:HA3	1.97	0.45
1:A:146:LYS:HE3	1:A:147:ASP:OD2	2.16	0.45
1:E:69:THR:O	1:E:69:THR:HG22	2.17	0.45
1:C:52:TYR:CZ	1:E:52:TYR:CE1	3.05	0.45
1:C:62:GLU:OE2	1:C:62:GLU:HA	2.15	0.45
1:C:152:PRO:CB	1:C:205:PRO:CG	2.94	0.45
1:E:6:GLN:CA	1:E:108:GLN:HE22	2.27	0.45
1:F:155:VAL:HG13	1:F:201:VAL:HG22	1.98	0.45
1:D:86:LEU:HB3	1:D:114:VAL:HG11	1.97	0.45
1:D:122:PRO:CB	1:D:145:VAL:HG12	2.47	0.45
1:E:157:TRP:HB2	1:E:162:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:ALA:HB1	1:F:78:THR:HG23	1.99	0.45
1:C:169:PHE:CE1	1:D:182:SER:HB2	2.53	0.44
1:D:200:ASN:HA	1:D:211:ASP:CB	2.46	0.44
1:F:32:TYR:O	1:F:53:ILE:CG1	2.65	0.44
1:A:124:VAL:CG1	1:A:212:LYS:HG3	2.47	0.44
1:A:140:ALA:CB	1:B:144:LEU:HD23	2.48	0.44
1:C:83:LEU:HD12	1:C:83:LEU:HA	1.88	0.44
1:C:149:PHE:H	1:C:150:PRO:HD3	1.82	0.44
1:B:77:SER:O	1:B:78:THR:OG1	2.34	0.44
1:C:6:GLN:HG2	1:C:110:THR:CG2	2.46	0.44
1:F:215:GLU:HA	1:F:216:PRO:HD2	1.72	0.44
1:B:148:TYR:CD1	1:B:148:TYR:O	2.70	0.44
1:A:5:VAL:HG21	1:D:5:VAL:HG23	2.00	0.44
1:C:209:LYS:HB3	1:C:209:LYS:HE2	1.32	0.44
1:F:214:VAL:O	1:F:214:VAL:HG23	2.18	0.44
1:C:128:ALA:N	1:D:128:ALA:O	2.49	0.44
1:C:213:LYS:HD3	1:C:213:LYS:H	1.82	0.44
1:E:212:LYS:HA	1:E:212:LYS:HD2	1.55	0.44
1:E:149:PHE:CD1	1:E:150:PRO:HA	2.53	0.44
1:C:148:TYR:CE1	1:C:179:TYR:O	2.71	0.43
1:B:4:LEU:HD12	1:B:4:LEU:N	2.34	0.43
1:B:143:CYS:HG	1:B:199:CYS:HG	0.59	0.43
1:D:122:PRO:HB3	1:D:148:TYR:HB3	1.99	0.43
1:C:204:LYS:N	1:C:205:PRO:HD3	2.33	0.43
1:D:158:ASN:HB3	1:D:161:ALA:HB3	2.00	0.43
1:F:32:TYR:O	1:F:53:ILE:HG12	2.19	0.43
1:F:204:LYS:N	1:F:205:PRO:CD	2.82	0.43
1:A:53:ILE:HD13	1:A:53:ILE:HA	1.59	0.43
1:C:6:GLN:NE2	1:C:109:GLY:H	2.17	0.43
1:A:140:ALA:HB1	1:B:144:LEU:CD2	2.49	0.43
1:A:6:GLN:HE21	1:A:6:GLN:HB3	1.57	0.43
1:A:103:PHE:N	1:A:103:PHE:CD1	2.84	0.43
1:A:6:GLN:HB3	1:A:110:THR:CG2	2.48	0.43
1:C:122:PRO:CA	1:C:146:LYS:O	2.65	0.43
1:C:155:VAL:HG13	1:C:201:VAL:HG12	2.00	0.43
1:E:28:THR:O	1:E:28:THR:OG1	2.34	0.43
1:B:148:TYR:CD1	1:B:148:TYR:C	2.91	0.43
1:F:151:GLU:HB2	1:F:179:TYR:CE2	2.54	0.43
1:E:5:VAL:O	1:E:5:VAL:HG23	2.18	0.43
1:E:204:LYS:N	1:E:205:PRO:CD	2.81	0.43
1:A:155:VAL:CG1	1:A:199:CYS:SG	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TRP:HZ3	1:A:214:VAL:HG21	1.83	0.42
1:B:67:ARG:NH1	1:B:90:ASP:OD2	2.46	0.42
1:C:152:PRO:CB	1:C:205:PRO:HG2	2.48	0.42
1:F:13:LYS:HB3	1:F:13:LYS:HE2	1.55	0.42
1:C:102:ARG:CZ	1:C:102:ARG:HB3	2.48	0.42
1:D:124:VAL:CG2	1:D:201:VAL:HG21	2.49	0.42
1:E:172:VAL:HG23	1:F:169:PHE:CD1	2.55	0.42
1:C:76:ALA:O	1:C:77:SER:CB	2.63	0.42
1:A:169:PHE:HA	1:A:170:PRO:HD3	1.92	0.42
1:D:149:PHE:HE1	1:D:177:GLY:O	2.03	0.42
1:B:11:VAL:HG13	1:B:113:THR:HB	2.01	0.42
1:B:141:LEU:N	1:B:185:VAL:O	2.45	0.42
1:D:202:ASN:OD1	1:D:208:THR:O	2.37	0.42
1:A:144:LEU:HD22	1:B:184:VAL:HG11	2.02	0.42
1:A:215:GLU:HA	1:A:216:PRO:HD3	1.89	0.42
1:C:20:VAL:HG11	1:C:110:THR:CG2	2.46	0.42
1:D:27:TYR:HB3	1:D:28:THR:H	1.63	0.42
1:D:51:ILE:O	1:D:51:ILE:HG23	2.20	0.42
1:D:124:VAL:HG21	1:D:201:VAL:HG21	2.01	0.42
1:E:33:GLY:HA3	1:E:50:TYR:CZ	2.55	0.42
1:A:32:TYR:OH	1:A:77:SER:O	2.26	0.42
1:E:53:ILE:O	1:E:53:ILE:CG1	2.68	0.42
1:C:6:GLN:OE1	1:C:95:TYR:HA	2.20	0.42
1:A:10:GLU:HG2	1:A:12:LYS:CE	2.49	0.41
1:A:20:VAL:HG11	1:A:110:THR:CG2	2.47	0.41
1:C:162:LEU:CD1	1:C:162:LEU:O	2.68	0.41
1:E:64:PHE:HB3	1:E:68:ALA:HB2	2.02	0.41
1:E:148:TYR:CE2	1:E:153:VAL:HG23	2.55	0.41
1:B:195:GLN:OE1	1:B:196:THR:N	2.53	0.41
1:D:3:GLN:HE21	1:D:3:GLN:HB2	1.65	0.41
1:E:124:VAL:HG12	1:E:212:LYS:CG	2.50	0.41
1:E:208:THR:O	1:E:208:THR:CG2	2.69	0.41
1:E:6:GLN:HE21	1:E:6:GLN:HB3	1.53	0.41
1:E:132:LYS:HD3	1:E:132:LYS:HA	1.68	0.41
1:A:67:ARG:HB3	1:A:84:SER:O	2.21	0.41
1:A:27:TYR:CE2	1:A:29:PHE:HB2	2.55	0.41
1:C:47:TRP:CG	1:D:104:VAL:CG2	3.02	0.41
1:F:38:ARG:HB2	1:F:48:ILE:HD11	2.03	0.41
1:A:6:GLN:HB3	1:A:110:THR:HG22	2.02	0.41
1:B:151:GLU:N	1:B:152:PRO:HD2	2.36	0.41
1:C:140:ALA:O	1:D:127:LEU:HD21	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:PRO:HB2	1:C:205:PRO:HG2	2.02	0.41
1:C:151:GLU:CD	1:C:179:TYR:CD2	2.81	0.41
1:C:166:VAL:HA	1:C:185:VAL:HG22	2.03	0.41
1:D:200:ASN:N	1:D:211:ASP:HA	2.35	0.41
1:B:173:LEU:CD1	1:B:179:TYR:CE1	3.04	0.41
1:C:170:PRO:HD2	1:D:170:PRO:HD2	2.03	0.41
1:F:149:PHE:HB2	1:F:178:LEU:HD23	2.03	0.41
1:A:119:THR:HA	1:A:149:PHE:O	2.20	0.41
1:A:130:SER:HG	1:B:215:GLU:C	2.23	0.41
1:A:149:PHE:HA	1:A:150:PRO:HA	1.83	0.41
1:B:61:SER:HB3	1:B:64:PHE:HD2	1.86	0.41
1:C:126:PRO:HG3	1:C:212:LYS:CE	2.50	0.41
1:C:178:LEU:HD12	1:C:178:LEU:N	2.36	0.41
1:D:103:PHE:O	1:D:104:VAL:HG12	2.21	0.41
1:D:103:PHE:C	1:D:104:VAL:CG1	2.89	0.41
1:E:18:VAL:O	1:E:18:VAL:HG13	2.21	0.41
1:E:102:ARG:HE	1:E:102:ARG:HB3	1.62	0.41
1:E:5:VAL:O	1:E:5:VAL:CG2	2.69	0.41
1:F:52:TYR:O	1:F:56:GLY:N	2.50	0.41
1:B:140:ALA:HA	1:B:186:THR:HA	2.02	0.40
1:C:40:ALA:HB3	1:C:43:GLN:HB2	2.04	0.40
1:C:166:VAL:O	1:C:166:VAL:CG1	2.69	0.40
1:D:168:THR:HG23	1:D:181:LEU:HD21	2.04	0.40
1:D:204:LYS:N	1:D:205:PRO:CD	2.84	0.40
1:F:76:ALA:HB1	1:F:78:THR:CG2	2.51	0.40
1:B:142:GLY:CA	1:B:157:TRP:HH2	2.32	0.40
1:B:51:ILE:O	1:B:51:ILE:HG23	2.21	0.40
1:C:73:ASP:OD2	1:C:76:ALA:N	2.53	0.40
1:C:122:PRO:HA	1:C:147:ASP:O	2.21	0.40
1:A:51:ILE:HG13	1:A:58:THR:CG2	2.49	0.40
1:B:39:GLN:C	1:B:92:ALA:HB1	2.41	0.40
1:C:201:VAL:HG23	1:C:201:VAL:O	2.20	0.40
1:D:151:GLU:O	1:D:151:GLU:CG	2.69	0.40
1:E:53:ILE:O	1:E:53:ILE:HG13	2.21	0.40
1:C:97:ALA:HA	1:C:105:TYR:O	2.21	0.40
1:C:201:VAL:O	1:C:201:VAL:CG2	2.69	0.40

All (22) 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:23:LYS:CE	1:C:194:THR:CB[2_546]	0.36	1.84
1:B:25:SER:C	1:C:195:GLN:OE1[2_546]	0.50	1.70
1:B:23:LYS:NZ	1:C:194:THR:CA[2_546]	0.62	1.58
1:B:23:LYS:CD	1:C:194:THR:CG2[2_546]	0.73	1.47
1:B:23:LYS:NZ	1:C:194:THR:N[2_546]	0.99	1.21
1:B:25:SER:O	1:C:195:GLN:OE1[2_546]	1.00	1.20
1:B:23:LYS:CE	1:C:194:THR:OG1[2_546]	1.16	1.04
1:B:23:LYS:CE	1:C:194:THR:CA[2_546]	1.47	0.73
1:B:23:LYS:NZ	1:C:194:THR:CB[2_546]	1.55	0.65
1:B:23:LYS:CE	1:C:194:THR:CG2[2_546]	1.55	0.65
1:B:23:LYS:CD	1:C:194:THR:CB[2_546]	1.55	0.65
1:B:25:SER:CA	1:C:195:GLN:OE1[2_546]	1.62	0.58
1:B:25:SER:C	1:C:195:GLN:CD[2_546]	1.65	0.55
1:B:89:GLU:OE2	1:C:85:SER:OG[4_546]	1.74	0.46
1:B:25:SER:O	1:C:195:GLN:CD[2_546]	1.87	0.33
1:B:76:ALA:CB	1:C:188:PRO:CG[2_546]	1.90	0.30
1:B:23:LYS:CD	1:C:194:THR:OG1[2_546]	1.96	0.24
1:B:89:GLU:CD	1:C:85:SER:OG[4_546]	1.99	0.21
1:B:23:LYS:NZ	1:C:193:GLY:C[2_546]	2.01	0.19
1:B:23:LYS:NZ	1:C:194:THR:C[2_546]	2.05	0.15
1:B:89:GLU:OE1	1:C:85:SER:OG[4_546]	2.13	0.07
1:B:23:LYS:NZ	1:C:194:THR:CG2[2_546]	2.15	0.05

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	209/448 (47%)	198 (95%)	10 (5%)	1 (0%)	29 60
1	B	195/448 (44%)	187 (96%)	8 (4%)	0	100 100
1	C	194/448 (43%)	180 (93%)	12 (6%)	2 (1%)	15 43
1	D	201/448 (45%)	183 (91%)	16 (8%)	2 (1%)	15 43
1	E	214/448 (48%)	198 (92%)	13 (6%)	3 (1%)	11 34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	F	198/448 (44%)	182 (92%)	15 (8%)	1 (0%)	29 60
All	All	1211/2688 (45%)	1128 (93%)	74 (6%)	9 (1%)	22 53

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	147	ASP
1	D	30	THR
1	E	135	SER
1	A	131	SER
1	E	136	GLY
1	C	151	GLU
1	E	54	GLY
1	C	149	PHE
1	F	5	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	178/376 (47%)	136 (76%)	42 (24%)	1 2
1	B	168/376 (45%)	142 (84%)	26 (16%)	2 8
1	C	168/376 (45%)	114 (68%)	54 (32%)	0 0
1	D	172/376 (46%)	139 (81%)	33 (19%)	1 4
1	E	180/376 (48%)	145 (81%)	35 (19%)	1 4
1	F	170/376 (45%)	129 (76%)	41 (24%)	0 2
All	All	1036/2256 (46%)	805 (78%)	231 (22%)	1 2

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	3	GLN

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Mol	Chain	Res	Type
1	A	10	GLU
1	A	12	LYS
1	A	31	ASN
1	A	32	TYR
1	A	38	ARG
1	A	43	GLN
1	A	45	LEU
1	A	51	ILE
1	A	53	ILE
1	A	57	ASP
1	A	59	ASP
1	A	62	GLU
1	A	63	LYS
1	A	65	LYS
1	A	67	ARG
1	A	71	THR
1	A	77	SER
1	A	85	SER
1	A	87	ARG
1	A	88	SER
1	A	99	THR
1	A	101	THR
1	A	102	ARG
1	A	110	THR
1	A	120	LYS
1	A	130	SER
1	A	132	LYS
1	A	133	SER
1	A	138	THR
1	A	144	LEU
1	A	152	PRO
1	A	154	THR
1	A	163	THR
1	A	178	LEU
1	A	182	SER
1	A	192	LEU
1	A	198	ILE
1	A	212	LYS
1	A	213	LYS
1	A	214	VAL
1	B	13	LYS
1	B	25	SER

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Mol	Chain	Res	Type
1	B	43	GLN
1	B	51	ILE
1	B	53	ILE
1	B	59	ASP
1	B	61	SER
1	B	65	LYS
1	B	69	THR
1	B	118	SER
1	B	120	LYS
1	B	144	LEU
1	B	146	LYS
1	B	147	ASP
1	B	150	PRO
1	B	163	THR
1	B	176	SER
1	B	182	SER
1	B	183	SER
1	B	189	SER
1	B	194	THR
1	B	196	THR
1	B	198	ILE
1	B	205	PRO
1	B	206	SER
1	B	215	GLU
1	C	3	GLN
1	C	6	GLN
1	C	10	GLU
1	C	17	SER
1	C	18	VAL
1	C	23	LYS
1	C	25	SER
1	C	46	GLU
1	C	53	ILE
1	C	74	THR
1	C	85	SER
1	C	87	ARG
1	C	88	SER
1	C	101	THR
1	C	102	ARG
1	C	103	PHE
1	C	108	GLN
1	C	110	THR

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Mol	Chain	Res	Type
1	C	113	THR
1	C	115	SER
1	C	116	SER
1	C	119	THR
1	C	124	VAL
1	C	127	LEU
1	C	141	LEU
1	C	143	CYS
1	C	146	LYS
1	C	153	VAL
1	C	154	THR
1	C	159	SER
1	C	162	LEU
1	C	163	THR
1	C	164	SER
1	C	172	VAL
1	C	178	LEU
1	C	181	LEU
1	C	183	SER
1	C	189	SER
1	C	190	SER
1	C	192	LEU
1	C	194	THR
1	C	195	GLN
1	C	198	ILE
1	C	200	ASN
1	C	202	ASN
1	C	204	LYS
1	C	206	SER
1	C	209	LYS
1	C	210	VAL
1	C	211	ASP
1	C	212	LYS
1	C	213	LYS
1	C	214	VAL
1	C	215	GLU
1	D	17	SER
1	D	28	THR
1	D	31	ASN
1	D	43	GLN
1	D	57	ASP
1	D	59	ASP

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Mol	Chain	Res	Type
1	D	71	THR
1	D	74	THR
1	D	77	SER
1	D	81	MET
1	D	84	SER
1	D	108	GLN
1	D	113	THR
1	D	115	SER
1	D	118	SER
1	D	144	LEU
1	D	146	LYS
1	D	149	PHE
1	D	153	VAL
1	D	154	THR
1	D	159	SER
1	D	162	LEU
1	D	181	LEU
1	D	183	SER
1	D	191	SER
1	D	192	LEU
1	D	194	THR
1	D	196	THR
1	D	204	LYS
1	D	205	PRO
1	D	210	VAL
1	D	213	LYS
1	D	215	GLU
1	E	13	LYS
1	E	19	LYS
1	E	24	THR
1	E	28	THR
1	E	34	ILE
1	E	43	GLN
1	E	51	ILE
1	E	53	ILE
1	E	57	ASP
1	E	64	PHE
1	E	71	THR
1	E	74	THR
1	E	78	THR
1	E	87	ARG
1	E	88	SER

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Mol	Chain	Res	Type
1	E	99	THR
1	E	102	ARG
1	E	108	GLN
1	E	129	PRO
1	E	130	SER
1	E	131	SER
1	E	132	LYS
1	E	134	THR
1	E	144	LEU
1	E	146	LYS
1	E	150	PRO
1	E	162	LEU
1	E	164	SER
1	E	194	THR
1	E	202	ASN
1	E	204	LYS
1	E	208	THR
1	E	209	LYS
1	E	213	LYS
1	E	215	GLU
1	F	1	GLU
1	F	3	GLN
1	F	4	LEU
1	F	10	GLU
1	F	11	VAL
1	F	12	LYS
1	F	13	LYS
1	F	18	VAL
1	F	19	LYS
1	F	23	LYS
1	F	32	TYR
1	F	34	ILE
1	F	46	GLU
1	F	51	ILE
1	F	59	ASP
1	F	61	SER
1	F	62	GLU
1	F	63	LYS
1	F	65	LYS
1	F	67	ARG
1	F	72	SER
1	F	77	SER

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Mol	Chain	Res	Type
1	F	88	SER
1	F	89	GLU
1	F	104	VAL
1	F	113	THR
1	F	118	SER
1	F	123	SER
1	F	130	SER
1	F	143	CYS
1	F	146	LYS
1	F	150	PRO
1	F	154	THR
1	F	164	SER
1	F	174	GLN
1	F	175	SER
1	F	188	PRO
1	F	198	ILE
1	F	199	CYS
1	F	209	LYS
1	F	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	31	ASN
1	B	43	GLN
1	C	108	GLN
1	C	195	GLN
1	C	200	ASN
1	D	3	GLN
1	D	195	GLN
1	D	202	ASN
1	E	31	ASN
1	E	108	GLN
1	E	203	HIS
1	F	200	ASN

5.3.3 RNA

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 monosaccharides 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, 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	213/448 (47%)	0.05	5 (2%)	60	59	10, 32, 61, 76	0
1	B	203/448 (45%)	0.08	10 (4%)	29	26	14, 31, 57, 72	0
1	C	202/448 (45%)	0.24	7 (3%)	44	40	18, 45, 71, 100	0
1	D	207/448 (46%)	0.06	4 (1%)	66	65	14, 35, 79, 110	0
1	E	216/448 (48%)	0.15	3 (1%)	75	76	26, 43, 71, 90	0
1	F	204/448 (45%)	0.15	3 (1%)	73	73	25, 47, 75, 86	0
All	All	1245/2688 (46%)	0.12	32 (2%)	56	53	10, 39, 71, 110	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	THR	5.1
1	E	27	TYR	4.5
1	C	124	VAL	4.3
1	E	135	SER	4.3
1	F	5	VAL	4.2
1	B	76	ALA	4.1
1	C	152	PRO	3.9
1	B	56	GLY	3.5
1	A	31	ASN	3.4
1	D	150	PRO	3.4
1	B	75	SER	3.2
1	C	126	PRO	3.2
1	D	200	ASN	3.2
1	B	54	GLY	3.1
1	E	53	ILE	3.1
1	B	77	SER	2.9
1	F	76	ALA	2.7
1	C	99	THR	2.7
1	A	199	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	147	ASP	2.6
1	F	4	LEU	2.5
1	C	102	ARG	2.5
1	B	55	ALA	2.5
1	D	28	THR	2.3
1	A	133	SER	2.3
1	D	199	CYS	2.2
1	C	157	TRP	2.2
1	B	144	LEU	2.2
1	B	145	VAL	2.2
1	B	103	PHE	2.1
1	A	130	SER	2.1
1	B	164	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 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.