Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2025 – 01:32 PM JST

PDB ID	:	8Z2B
Title	:	Crystal structure of apo Aspergillus terreus glutamate dehydrogenase (At-GDH) in the partially closed conformation (form II)
Authors	:	Godsora, B.K.J.; Bhaumik, P.
Deposited on	:	2024-04-12
Resolution	:	2.85 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:

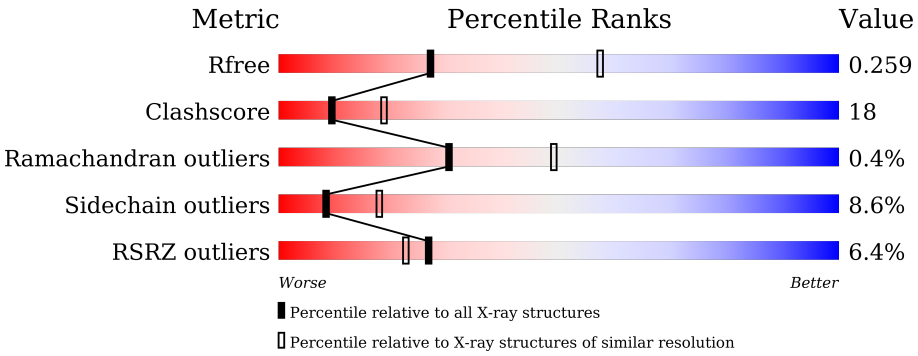
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 2.85 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}	164625	1268 (2.88-2.84)
Clashscore	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (2.88-2.84)
RSRZ outliers	164620	1269 (2.88-2.84)

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	460	5% 66% 30% 5%
1	B	460	4% 66% 31% ·
1	C	460	5% 60% 37% ·
1	D	460	8% 65% 31% ·
1	E	460	9% 61% 33% 5%
1	F	460	7% 68% 29% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 20860 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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	1	0
			3473	2193	604	663	13			
1	B	460	Total	C	N	O	S	0	1	0
			3469	2190	603	663	13			
1	C	460	Total	C	N	O	S	0	3	0
			3482	2198	605	666	13			
1	D	460	Total	C	N	O	S	0	2	0
			3473	2192	604	664	13			
1	E	460	Total	C	N	O	S	0	1	0
			3469	2190	603	663	13			
1	F	460	Total	C	N	O	S	0	1	0
			3471	2190	604	664	13			

- Molecule 2 is water.

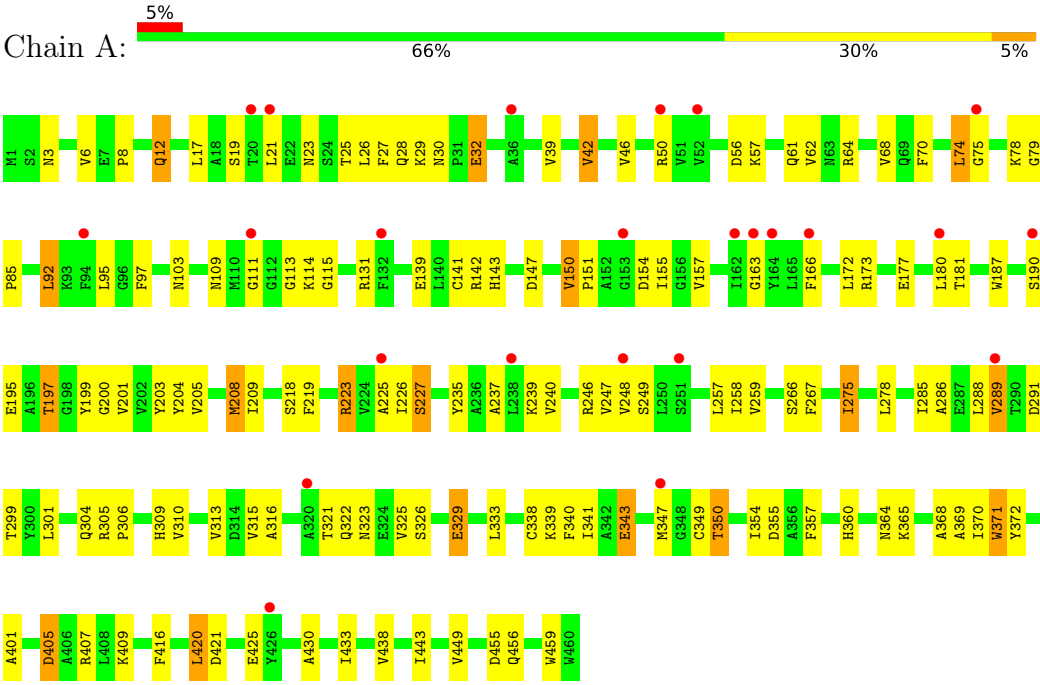
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	O	0	0
			6	6		
2	B	3	Total	O	0	0
			3	3		
2	C	3	Total	O	0	0
			3	3		
2	D	4	Total	O	0	0
			4	4		
2	E	2	Total	O	0	0
			2	2		
2	F	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

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

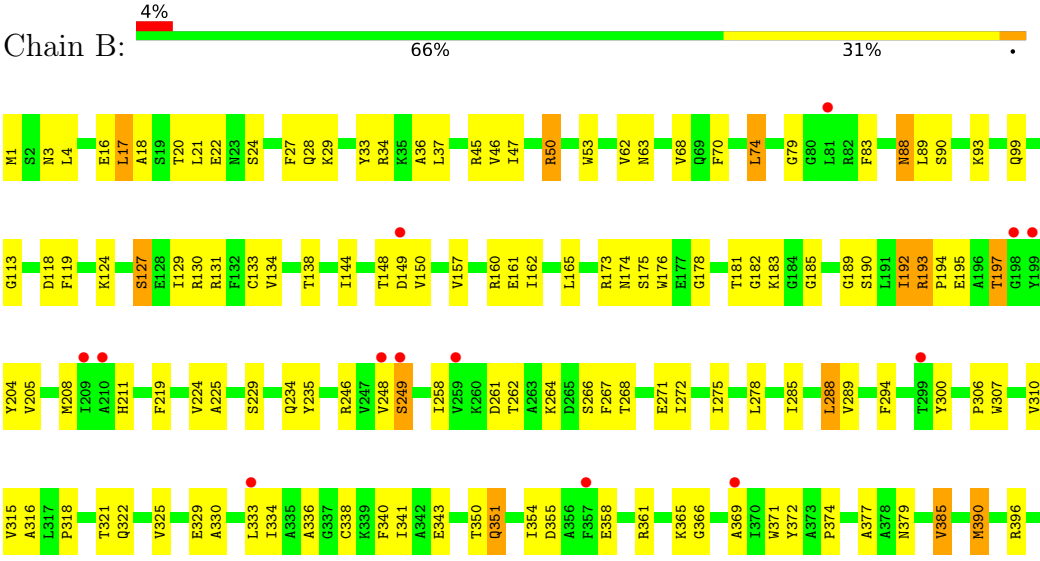
• Molecule 1: Glutamate dehydrogenase

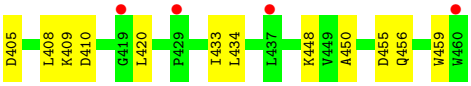
Chain A:



• Molecule 1: Glutamate dehydrogenase

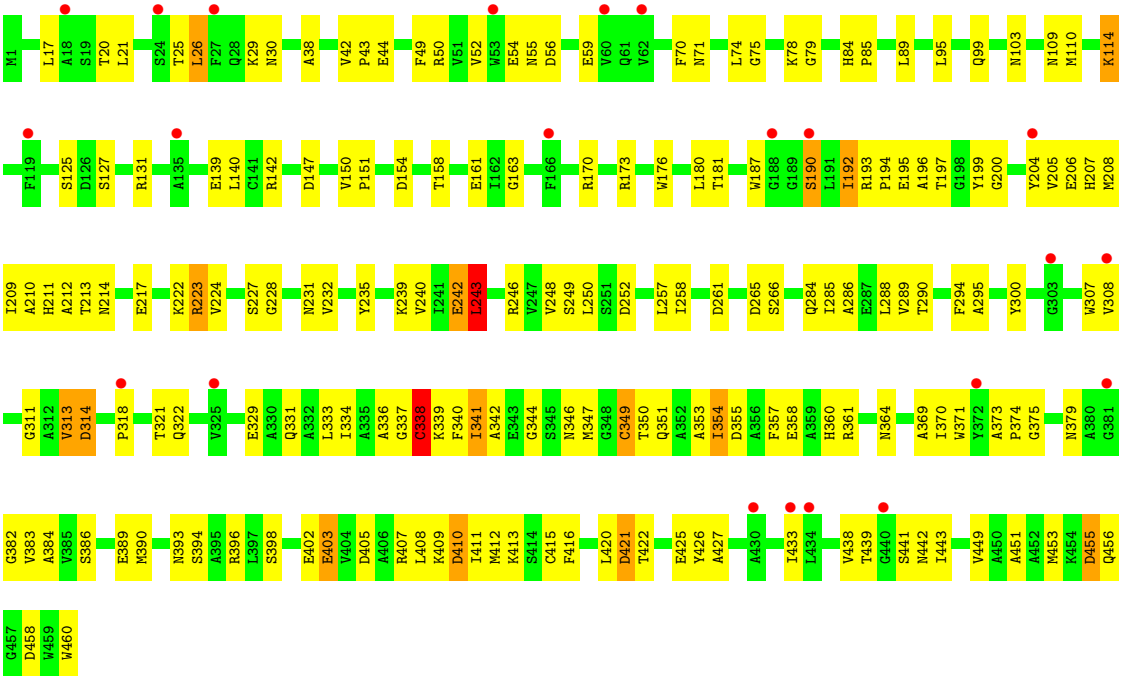
Chain B:





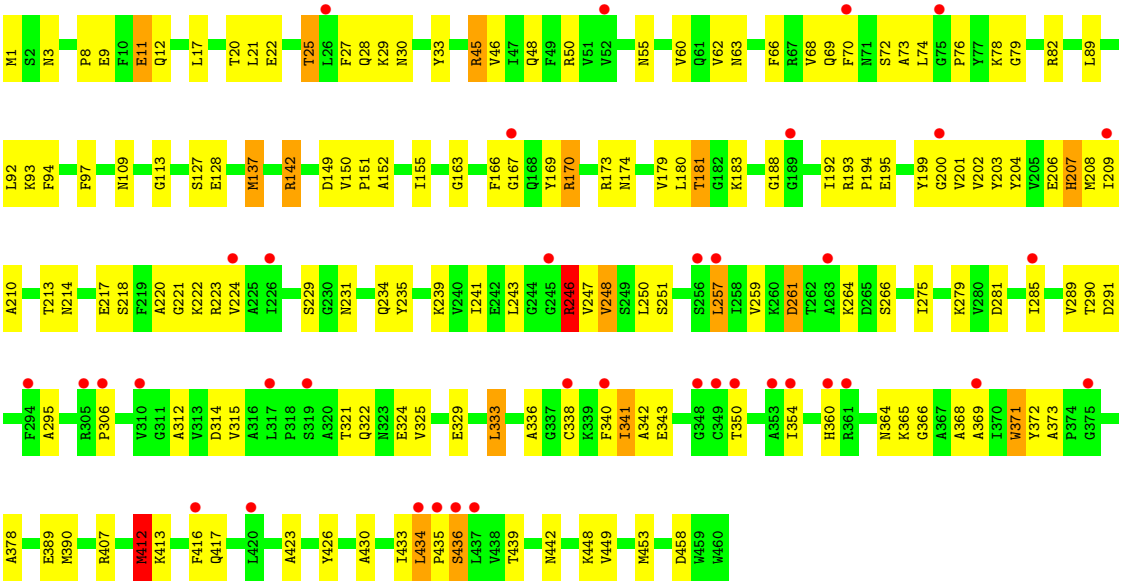
• Molecule 1: Glutamate dehydrogenase

Chain C:



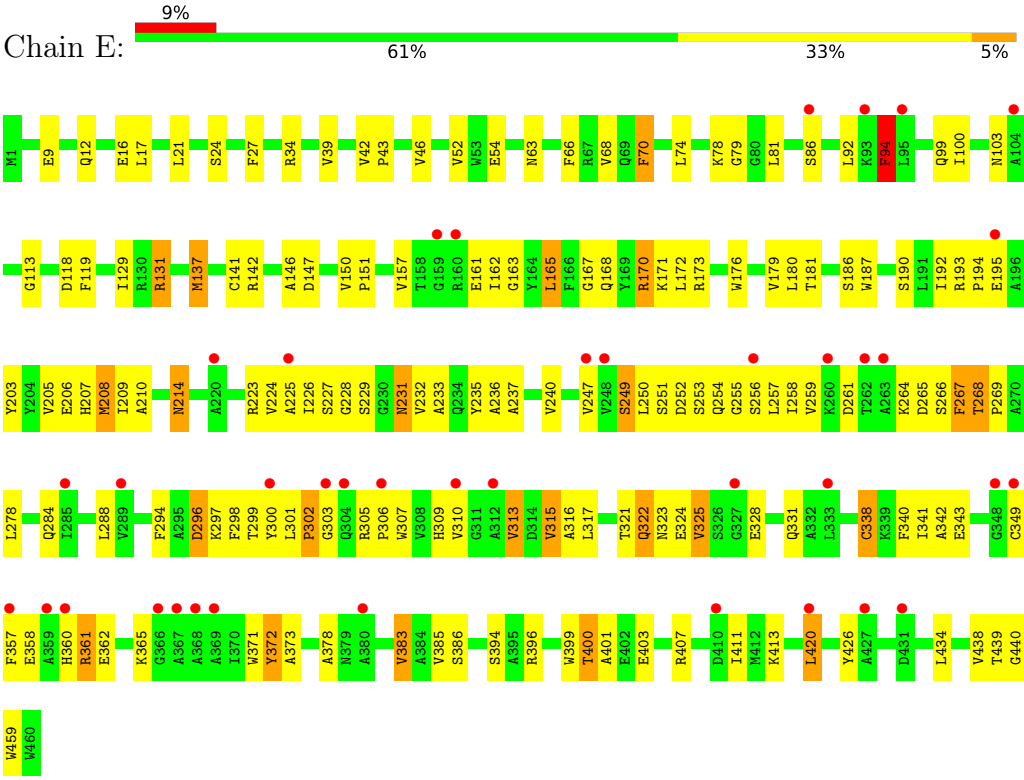
• Molecule 1: Glutamate dehydrogenase

Chain D:



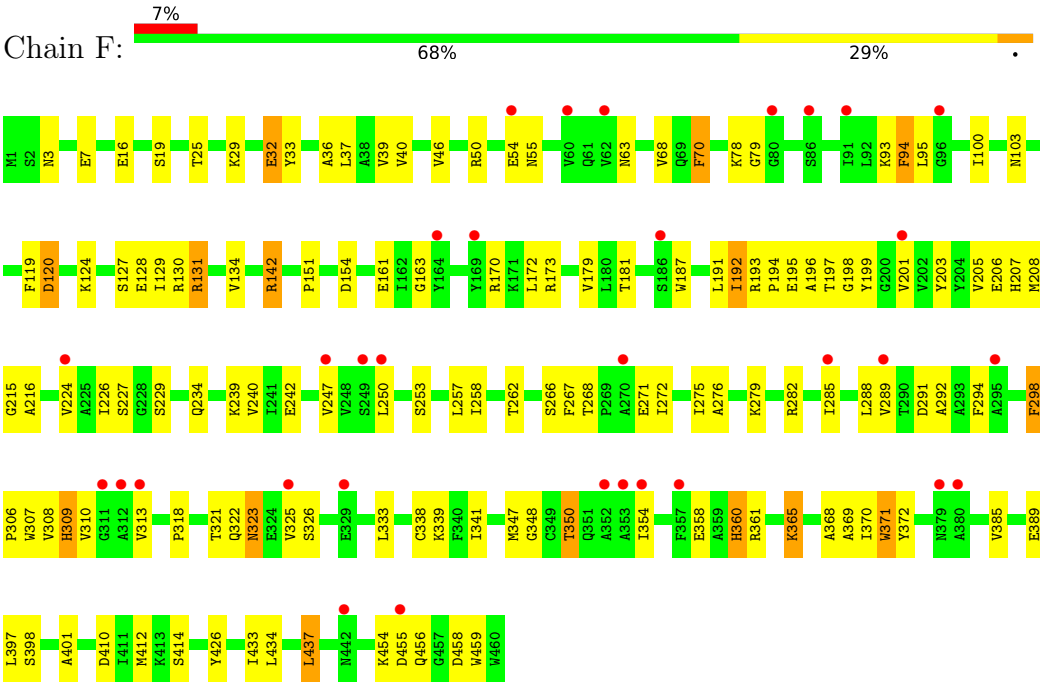
• Molecule 1: Glutamate dehydrogenase

Chain E:



• Molecule 1: Glutamate dehydrogenase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	101.69Å 101.69Å 271.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.89 – 2.85 29.89 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.89-2.85) 99.9 (29.89-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.85Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.192 , 0.268 0.197 , 0.259	Depositor DCC
R_{free} test set	3801 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.031 for -h,-k,l 0.053 for h,-h-k,-l 0.059 for -k,-h,-l	Xtriage
Reported twinning fraction	0.256 for H, K, L 0.248 for K, H, -L 0.246 for -h,-k,l 0.250 for -K, -H, -L	Depositor
Outliers	0 of 73338 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	20860	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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	0.44	0/3546	0.92	4/4795 (0.1%)
1	B	0.43	0/3542	0.90	4/4791 (0.1%)
1	C	0.43	0/3558	0.89	2/4811 (0.0%)
1	D	0.42	0/3546	0.91	6/4796 (0.1%)
1	E	0.44	0/3542	0.93	8/4791 (0.2%)
1	F	0.43	0/3541	0.90	5/4789 (0.1%)
All	All	0.43	0/21275	0.91	29/28773 (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	A	0	3
1	B	0	2
1	C	0	4
1	D	0	4
1	E	0	4
1	F	0	3
All	All	0	20

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	412	MET	CG-SD-CE	9.50	115.39	100.20
1	E	137	MET	CG-SD-CE	9.01	114.61	100.20
1	D	137	MET	CG-SD-CE	7.97	112.96	100.20
1	E	453	MET	CG-SD-CE	-7.81	87.70	100.20
1	E	94	PHE	N-CA-CB	7.75	124.56	110.60
1	F	120	ASP	CB-CG-OD1	-7.55	111.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	420	LEU	CB-CG-CD2	7.42	123.61	111.00
1	D	412	MET	CG-SD-CE	6.97	111.36	100.20
1	F	390	MET	CG-SD-CE	6.95	111.31	100.20
1	B	455	ASP	CB-CA-C	6.90	124.19	110.40
1	A	301	LEU	CB-CG-CD1	6.71	122.40	111.00
1	D	333	LEU	CB-CG-CD2	-6.64	99.72	111.00
1	E	74	LEU	CB-CG-CD2	6.57	122.18	111.00
1	A	405	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	D	1	MET	CG-SD-CE	5.97	109.75	100.20
1	E	118	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	E	131	ARG	CA-CB-CG	5.60	125.72	113.40
1	E	21	LEU	CB-CG-CD2	5.57	120.47	111.00
1	A	29	LYS	CB-CA-C	-5.55	99.30	110.40
1	A	92	LEU	CB-CG-CD2	5.45	120.26	111.00
1	C	453	MET	CG-SD-CE	5.41	108.86	100.20
1	C	243	LEU	CB-CG-CD1	-5.41	101.81	111.00
1	B	29	LYS	CB-CA-C	5.35	121.11	110.40
1	F	397	LEU	CB-CG-CD2	5.35	120.09	111.00
1	D	45	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	17	LEU	CB-CG-CD2	5.14	119.73	111.00
1	D	170	ARG	CA-CB-CG	5.12	124.67	113.40
1	B	390	MET	CG-SD-CE	-5.11	92.02	100.20
1	F	410	ASP	CB-CA-C	5.01	120.43	110.40

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	ARG	Sidechain
1	A	396	ARG	Sidechain
1	A	407	ARG	Sidechain
1	B	160	ARG	Sidechain
1	B	50	ARG	Sidechain
1	C	354	ILE	Peptide
1	C	396	ARG	Sidechain
1	C	407	ARG	Sidechain
1	C	451	ALA	Mainchain
1	D	142	ARG	Sidechain
1	D	246	ARG	Sidechain
1	D	368	ALA	Peptide
1	D	407	ARG	Sidechain
1	E	110	MET	Mainchain

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Mol	Chain	Res	Type	Group
1	E	170	ARG	Sidechain
1	E	296	ASP	Peptide
1	E	407	ARG	Sidechain
1	F	131	ARG	Mainchain,Peptide
1	F	282	ARG	Sidechain

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	3473	0	3425	122	0
1	B	3469	0	3417	123	0
1	C	3482	0	3431	145	0
1	D	3473	0	3419	135	8
1	E	3469	0	3417	143	8
1	F	3471	0	3414	122	0
2	A	6	0	0	1	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	4	0	0	0	0
2	E	2	0	0	0	0
2	F	5	0	0	0	0
All	All	20860	0	20523	728	8

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 18.

All (728) 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:C:213:THR:HG21	1:C:217:GLU:HB2	1.33	1.08
1:F:267:PHE:CZ	1:F:298:PHE:HZ	1.79	1.00
1:D:48:GLN:HE22	1:D:89:LEU:HD22	1.28	0.98
1:A:42:VAL:O	1:B:50:ARG:NH1	1.96	0.97
1:C:248:VAL:O	1:C:258:ILE:HG23	1.64	0.96
1:D:453:MET:HG3	1:D:458:ASP:HB2	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:322:GLN:O	1:F:323:ASN:ND2	2.02	0.93
1:F:267:PHE:CE2	1:F:298:PHE:CZ	2.59	0.90
1:A:42:VAL:HG13	1:B:50:ARG:HD3	1.53	0.90
1:B:33:TYR:CE1	1:B:459:TRP:HZ2	1.89	0.89
1:E:161:GLU:O	1:E:165:LEU:HD22	1.73	0.89
1:C:344:GLY:HA2	1:C:379:ASN:HB3	1.53	0.88
1:F:267:PHE:CE2	1:F:298:PHE:HZ	1.91	0.88
1:F:267:PHE:CZ	1:F:298:PHE:CZ	2.64	0.86
1:E:227:SER:HB2	1:E:306:PRO:HG3	1.57	0.86
1:B:33:TYR:CE1	1:B:459:TRP:CZ2	2.64	0.86
1:A:364:ASN:HD21	1:A:368:ALA:HB3	1.40	0.84
1:A:396:ARG:NE	1:E:394:SER:OG	2.11	0.84
1:D:221:GLY:HA2	1:D:246:ARG:HH12	1.44	0.83
1:B:396:ARG:NH1	1:D:109:ASN:O	2.11	0.83
1:D:207:HIS:HA	1:D:210:ALA:HB3	1.62	0.81
1:C:342:ALA:HA	1:C:373:ALA:HB3	1.61	0.80
1:C:20:THR:HG23	1:C:439:THR:HA	1.62	0.80
1:C:213:THR:HG21	1:C:217:GLU:CB	2.10	0.80
1:D:79:GLY:HA3	1:D:113:GLY:O	1.83	0.79
1:F:247:VAL:O	1:F:266:SER:CB	2.30	0.79
1:F:360:HIS:CD2	1:F:370:ILE:HG22	2.19	0.78
1:B:182:GLY:HA2	1:B:193:ARG:CD	2.14	0.77
1:A:42:VAL:HG13	1:B:50:ARG:CD	2.13	0.77
1:E:256:SER:O	1:E:301:LEU:HB3	1.84	0.77
1:E:341:ILE:CG2	1:E:372:TYR:HA	2.15	0.77
1:E:343:GLU:O	1:E:378:ALA:HB3	1.86	0.76
1:D:163:GLY:HA3	1:F:455:ASP:O	1.87	0.75
1:F:361:ARG:NH2	1:F:434:LEU:O	2.19	0.75
1:E:256:SER:HB3	1:E:301:LEU:HD23	1.69	0.74
1:D:246:ARG:CG	1:D:246:ARG:HH11	2.00	0.74
1:E:141:CYS:O	1:E:173:ARG:NH1	2.20	0.74
1:D:453:MET:CG	1:D:458:ASP:HB2	2.17	0.74
1:B:311:GLY:O	1:B:336:ALA:HB1	1.88	0.74
1:C:196:ALA:HB3	1:C:382:GLY:HA2	1.70	0.74
1:F:25:THR:HG22	1:F:426:TYR:HA	1.69	0.73
1:B:182:GLY:HA2	1:B:193:ARG:HD3	1.70	0.73
1:C:158:THR:OG1	1:C:161:GLU:OE1	2.04	0.73
1:D:170:ARG:NH2	1:F:458:ASP:OD2	2.21	0.73
1:C:394:SER:OG	1:E:396:ARG:NE	2.21	0.72
1:C:213:THR:CG2	1:C:217:GLU:HB2	2.15	0.72
1:C:307:TRP:HB2	1:C:329:GLU:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:247:VAL:O	1:F:266:SER:OG	2.07	0.72
1:A:396:ARG:NH2	1:E:146:ALA:O	2.22	0.72
1:A:172:LEU:O	1:F:142:ARG:NH1	2.16	0.71
1:E:168:GLN:OE1	1:E:171:LYS:NZ	2.22	0.71
1:E:193:ARG:HD2	1:E:385:VAL:HG23	1.71	0.71
1:A:343:GLU:OE1	1:A:347:MET:N	2.23	0.71
1:A:226:ILE:O	1:A:249:SER:OG	2.09	0.71
1:D:73:ALA:HB2	1:D:453:MET:HE1	1.72	0.70
1:B:178:GLY:HA2	1:B:183:LYS:NZ	2.06	0.70
1:C:20:THR:HG21	1:C:442:ASN:HB2	1.73	0.69
1:C:427:ALA:HB2	1:C:439:THR:HG21	1.74	0.69
1:C:142:ARG:HH21	1:D:45:ARG:HH21	1.40	0.69
1:E:205:VAL:HA	1:E:208:MET:HB2	1.74	0.69
1:F:325:VAL:O	1:F:350:THR:OG1	2.09	0.69
1:B:33:TYR:CZ	1:B:459:TRP:HZ2	2.09	0.69
1:B:316:ALA:O	1:B:341:ILE:HA	1.93	0.68
1:E:341:ILE:HG21	1:E:372:TYR:HA	1.74	0.68
1:B:399:TRP:HB3	1:B:403:GLU:OE1	1.92	0.68
1:D:142:ARG:NH2	1:E:171:LYS:O	2.25	0.68
1:F:94:PHE:CZ	1:F:347:MET:SD	2.87	0.68
1:D:48:GLN:NE2	1:D:89:LEU:HD22	2.06	0.68
1:E:16:GLU:OE2	1:E:351:GLN:HG2	1.94	0.68
1:C:193:ARG:NH2	1:C:386:SER:OG	2.27	0.67
1:D:325:VAL:O	1:D:350:THR:OG1	2.08	0.67
1:C:163:GLY:HA2	1:C:187:TRP:CH2	2.30	0.67
1:F:271:GLU:O	1:F:275:ILE:HG13	1.95	0.67
1:A:421:ASP:OD1	1:A:421:ASP:O	2.12	0.67
1:F:291:ASP:O	1:F:292:ALA:HB3	1.93	0.67
1:F:437:LEU:HD22	1:F:437:LEU:H	1.59	0.67
1:E:258:ILE:HG21	1:E:309:HIS:O	1.95	0.67
1:C:193:ARG:NH1	1:C:382:GLY:O	2.28	0.66
1:D:209:ILE:CD1	1:D:340:PHE:HD1	2.08	0.66
1:C:209:ILE:O	1:C:213:THR:HG23	1.95	0.66
1:C:349:CYS:SG	1:C:350:THR:N	2.68	0.66
1:E:331:GLN:HG2	1:E:360:HIS:CD2	2.31	0.66
1:F:247:VAL:O	1:F:266:SER:HB2	1.95	0.66
1:F:322:GLN:HA	1:F:348:GLY:HA2	1.76	0.66
1:A:203:TYR:CE1	1:A:239:LYS:HE3	2.31	0.66
1:E:197:THR:O	1:E:201:VAL:HG23	1.96	0.66
1:F:29:LYS:HD2	1:F:426:TYR:HE1	1.60	0.66
1:C:26:LEU:HA	1:C:426:TYR:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ALA:HB2	1:D:453:MET:CE	2.25	0.66
1:F:55:ASN:HA	1:F:128:GLU:HG2	1.78	0.65
1:A:131:ARG:NH2	1:F:54:GLU:OE2	2.29	0.65
1:A:150:VAL:HG21	1:A:390:MET:SD	2.36	0.65
1:E:227:SER:CB	1:E:306:PRO:HG3	2.25	0.65
1:E:224:VAL:HA	1:E:315:VAL:HG12	1.78	0.65
1:E:269:PRO:O	1:E:272:ILE:HG22	1.96	0.65
1:C:375:GLY:O	1:C:379:ASN:ND2	2.29	0.65
1:F:227:SER:OG	1:F:318:PRO:HA	1.96	0.65
1:A:12:GLN:O	1:A:12:GLN:NE2	2.30	0.65
1:A:396:ARG:HH12	1:E:147:ASP:HA	1.60	0.65
1:C:358:GLU:HG2	1:C:361:ARG:HH11	1.62	0.65
1:A:278:LEU:HD11	1:A:288:LEU:HD12	1.77	0.64
1:C:311:GLY:O	1:C:336:ALA:HB1	1.97	0.64
1:E:357:PHE:O	1:E:361:ARG:HG2	1.98	0.64
1:C:78:LYS:HD2	1:C:150:VAL:HG13	1.78	0.64
1:B:289:VAL:HG11	1:B:300:TYR:CD1	2.33	0.64
1:D:436:SER:HB2	1:D:439:THR:HB	1.78	0.64
1:E:9:GLU:HB3	1:E:94:PHE:CD2	2.32	0.64
1:D:209:ILE:HD12	1:D:340:PHE:CD1	2.33	0.64
1:C:54:GLU:O	1:C:131:ARG:NH1	2.30	0.64
1:C:204:TYR:CZ	1:C:208:MET:SD	2.91	0.64
1:E:193:ARG:HH11	1:E:385:VAL:HG23	1.62	0.64
1:C:344:GLY:CA	1:C:379:ASN:HB3	2.26	0.63
1:B:182:GLY:HA2	1:B:193:ARG:HD2	1.80	0.63
1:A:219:PHE:CE1	1:A:240:VAL:HG22	2.33	0.63
1:D:248:VAL:O	1:D:259:VAL:HG13	1.99	0.63
1:D:209:ILE:HD12	1:D:340:PHE:HD1	1.62	0.63
1:D:183:LYS:HB2	1:D:188:GLY:O	1.98	0.63
1:F:371:TRP:CD1	1:F:437:LEU:HD21	2.34	0.63
1:A:365:LYS:HB3	1:A:433:ILE:HD13	1.79	0.63
1:C:150:VAL:HG21	1:C:390:MET:SD	2.39	0.63
1:F:196:ALA:HB2	1:F:385:VAL:HG21	1.81	0.63
1:E:12:GLN:O	1:E:16:GLU:HG2	1.98	0.62
1:F:163:GLY:HA2	1:F:187:TRP:CH2	2.34	0.62
1:F:360:HIS:NE2	1:F:369:ALA:HA	2.13	0.62
1:C:364:ASN:O	1:C:369:ALA:HB2	1.99	0.62
1:A:74:LEU:H	1:A:74:LEU:HD22	1.63	0.62
1:E:237:ALA:HB1	1:E:247:VAL:HG21	1.82	0.62
1:B:288:LEU:O	1:B:288:LEU:HD22	2.00	0.62
1:F:240:VAL:HG11	1:F:247:VAL:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:229:SER:N	1:E:251:SER:O	2.32	0.62
1:C:261:ASP:HB3	1:C:265:ASP:HB2	1.82	0.61
1:D:25:THR:HG22	1:D:426:TYR:HA	1.80	0.61
1:A:205:VAL:O	1:A:209:ILE:HG12	2.00	0.61
1:F:333:LEU:HB3	1:F:338:CYS:HB3	1.82	0.61
1:C:331:GLN:HA	1:C:334:ILE:HD12	1.82	0.61
1:E:63:ASN:ND2	1:E:119:PHE:HB2	2.15	0.61
1:A:364:ASN:HD21	1:A:368:ALA:CB	2.11	0.61
1:A:223:ARG:HB3	1:A:248:VAL:CG2	2.30	0.61
1:C:20:THR:CG2	1:C:439:THR:HA	2.29	0.61
1:E:224:VAL:HG12	1:E:226:ILE:HG13	1.83	0.61
1:E:341:ILE:HG22	1:E:372:TYR:HA	1.83	0.61
1:D:21:LEU:HB3	1:D:27:PHE:HE2	1.65	0.60
1:A:341:ILE:HD13	1:A:357:PHE:CE2	2.36	0.60
1:D:218:SER:C	1:D:220:ALA:H	2.04	0.60
1:D:453:MET:HG3	1:D:458:ASP:CB	2.28	0.60
1:F:361:ARG:HG3	1:F:369:ALA:HB1	1.81	0.60
1:B:311:GLY:O	1:B:336:ALA:CB	2.49	0.60
1:B:195:GLU:HG3	1:B:235:TYR:CE2	2.36	0.60
1:E:197:THR:HB	1:E:232:VAL:HG13	1.83	0.60
1:C:193:ARG:CZ	1:C:386:SER:OG	2.49	0.60
1:C:360:HIS:HB3	1:C:370:ILE:HG22	1.83	0.60
1:D:30:ASN:HB3	1:D:33:TYR:CD1	2.35	0.60
1:A:248:VAL:HG11	1:A:313:VAL:HG11	1.83	0.60
1:B:21:LEU:HD12	1:B:37:LEU:HD13	1.84	0.60
1:D:201:VAL:HG13	1:D:378:ALA:HB1	1.82	0.60
1:D:369:ALA:HB3	1:D:434:LEU:HD21	1.84	0.60
1:C:142:ARG:NH2	1:D:45:ARG:HH21	2.00	0.60
1:F:224:VAL:HG11	1:F:240:VAL:HG21	1.84	0.60
1:D:78:LYS:HD3	1:D:390:MET:HE1	1.82	0.60
1:F:203:TYR:O	1:F:207:HIS:ND1	2.34	0.60
1:D:20:THR:CG2	1:D:439:THR:HA	2.32	0.59
1:C:85:PRO:O	1:D:3:ASN:HB3	2.02	0.59
1:D:200:GLY:O	1:D:412:MET:SD	2.60	0.59
1:E:63:ASN:HD21	1:E:119:PHE:HA	1.68	0.59
1:A:237:ALA:HB1	1:A:247:VAL:HG21	1.85	0.59
1:C:337:GLY:O	1:C:339:LYS:HG2	2.02	0.59
1:C:349:CYS:SG	1:C:350:THR:O	2.60	0.59
1:A:26:LEU:HD22	1:A:443:ILE:HG23	1.84	0.59
1:D:78:LYS:HD3	1:D:390:MET:CE	2.32	0.59
1:B:396:ARG:NH1	1:D:76:PRO:HD2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CE1	1:B:450:ALA:HB1	2.38	0.59
1:A:163:GLY:HA2	1:A:187:TRP:CH2	2.38	0.58
1:C:49:PHE:CZ	1:C:140:LEU:HG	2.37	0.58
1:D:11:GLU:HG2	1:D:12:GLN:N	2.18	0.58
1:C:206:GLU:CD	1:C:243:LEU:HD22	2.24	0.58
1:F:79:GLY:O	1:F:151:PRO:HA	2.04	0.58
1:B:46:VAL:HG13	1:B:68:VAL:HG22	1.86	0.58
1:B:74:LEU:HD13	1:B:111:GLY:HA2	1.84	0.58
1:B:211:HIS:NE2	1:B:420:LEU:HD11	2.19	0.58
1:F:267:PHE:CE2	1:F:298:PHE:CE2	2.92	0.58
1:D:341:ILE:HG23	1:D:372:TYR:HA	1.85	0.58
1:B:162:ILE:HD13	1:B:165:LEU:HD12	1.86	0.57
1:E:190:SER:HB3	1:E:193:ARG:CB	2.34	0.57
1:B:229:SER:HB2	1:B:275:ILE:CG2	2.34	0.57
1:B:271:GLU:OE1	1:B:294:PHE:CD1	2.57	0.57
1:C:211:HIS:ND1	1:C:420:LEU:HD21	2.19	0.57
1:C:410:ASP:C	1:C:410:ASP:OD1	2.42	0.57
1:A:192:ILE:O	1:A:192:ILE:HG22	2.04	0.57
1:D:55:ASN:HB2	1:D:128:GLU:OE2	2.04	0.57
1:D:163:GLY:O	1:F:456:GLN:HA	2.04	0.57
1:D:365:LYS:O	1:D:434:LEU:HG	2.04	0.57
1:F:205:VAL:HA	1:F:208:MET:SD	2.44	0.57
1:F:365:LYS:O	1:F:368:ALA:HB3	2.05	0.57
1:E:79:GLY:HA3	1:E:113:GLY:O	2.04	0.57
1:E:237:ALA:HB3	1:E:272:ILE:CD1	2.35	0.57
1:E:372:TYR:CE2	1:E:438:VAL:HG11	2.40	0.57
1:B:350:THR:O	1:B:354:ILE:HG13	2.05	0.57
1:C:224:VAL:HG21	1:C:240:VAL:HG11	1.86	0.57
1:E:179:VAL:HG13	1:E:180:LEU:HD12	1.85	0.57
1:F:301:LEU:HD13	1:F:309:HIS:CD2	2.40	0.57
1:B:150:VAL:HG21	1:B:390:MET:HE3	1.87	0.57
1:A:421:ASP:OD1	1:A:421:ASP:C	2.43	0.57
1:C:42:VAL:HG21	1:D:62:VAL:HG11	1.86	0.57
1:F:325:VAL:C	1:F:350:THR:HG1	2.06	0.57
1:E:251:SER:HA	1:E:256:SER:HA	1.86	0.56
1:E:258:ILE:HG13	1:E:309:HIS:HB2	1.86	0.56
1:D:209:ILE:HG12	1:D:371:TRP:CE3	2.40	0.56
1:D:246:ARG:HH11	1:D:246:ARG:HG2	1.68	0.56
1:D:261:ASP:OD1	1:D:261:ASP:N	2.39	0.56
1:E:350:THR:O	1:E:354:ILE:HG13	2.05	0.56
1:F:131:ARG:HA	1:F:134:VAL:HB	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:LEU:HD13	1:F:309:HIS:HD2	1.69	0.56
1:B:173:ARG:O	1:B:175:SER:N	2.37	0.56
1:A:396:ARG:HE	1:E:394:SER:HG	1.47	0.56
1:C:358:GLU:CG	1:C:361:ARG:HH11	2.19	0.56
1:C:422:THR:HA	1:C:425:GLU:OE2	2.06	0.56
1:D:246:ARG:HG2	1:D:246:ARG:NH1	2.19	0.56
1:C:208:MET:HG2	1:C:416:PHE:CE1	2.41	0.56
1:C:223:ARG:NH1	1:C:314:ASP:OD2	2.38	0.56
1:E:193:ARG:HD2	1:E:385:VAL:CG2	2.35	0.56
1:A:325:VAL:HB	1:A:349:CYS:HA	1.86	0.56
1:C:246:ARG:HB3	1:C:266:SER:HB2	1.87	0.56
1:E:161:GLU:O	1:E:165:LEU:CD2	2.52	0.56
1:F:257:LEU:HD21	1:F:285:ILE:HG21	1.88	0.56
1:C:199:TYR:HD1	1:C:199:TYR:N	2.04	0.56
1:C:210:ALA:O	1:C:214:ASN:N	2.38	0.55
1:C:285:ILE:HD12	1:C:286:ALA:N	2.21	0.55
1:D:453:MET:SD	1:D:458:ASP:HB2	2.47	0.55
1:B:46:VAL:HG22	1:B:68:VAL:HG13	1.88	0.55
1:E:195:GLU:HG2	1:E:235:TYR:CE2	2.42	0.55
1:D:343:GLU:OE2	1:D:372:TYR:OH	2.08	0.55
1:E:190:SER:HB3	1:E:193:ARG:HB3	1.88	0.55
1:C:56:ASP:HA	1:C:131:ARG:HH22	1.71	0.55
1:B:127:SER:HB3	1:B:130:ARG:HH12	1.71	0.55
1:E:151:PRO:HD2	1:E:180:LEU:HG	1.88	0.55
1:F:46:VAL:HG22	1:F:68:VAL:HG13	1.89	0.55
1:A:141:CYS:O	1:A:173:ARG:NH2	2.39	0.55
1:B:354:ILE:HG23	1:B:372:TYR:CD2	2.42	0.55
1:C:313:VAL:HG12	1:C:333:LEU:HD22	1.89	0.55
1:E:325:VAL:HG13	1:E:349:CYS:HA	1.89	0.55
1:A:291:ASP:HB2	1:A:294:PHE:HB2	1.89	0.55
1:A:326:SER:OG	1:A:329:GLU:OE2	2.24	0.55
1:B:79:GLY:HA3	1:B:113:GLY:O	2.07	0.55
1:C:249:SER:O	1:C:250:LEU:HG	2.06	0.55
1:C:349:CYS:SG	1:C:354:ILE:N	2.80	0.55
1:E:210:ALA:O	1:E:214:ASN:N	2.40	0.55
1:F:7:GLU:OE1	1:F:93:LYS:NZ	2.27	0.55
1:C:285:ILE:HD12	1:C:286:ALA:H	1.72	0.55
1:C:289:VAL:O	1:C:295:ALA:HB2	2.06	0.55
1:C:350:THR:O	1:C:354:ILE:HG13	2.07	0.55
1:E:252:ASP:OD1	1:E:253:SER:N	2.40	0.55
1:D:218:SER:O	1:D:220:ALA:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TYR:CZ	1:B:459:TRP:CZ2	2.93	0.54
1:B:205:VAL:HA	1:B:208:MET:HG3	1.88	0.54
1:D:142:ARG:NH1	1:E:172:LEU:O	2.40	0.54
1:E:317:LEU:HG	1:E:342:ALA:HB3	1.89	0.54
1:A:46:VAL:HG22	1:A:68:VAL:HG13	1.90	0.54
1:C:311:GLY:O	1:C:336:ALA:CB	2.56	0.54
1:D:275:ILE:O	1:D:279:LYS:HG2	2.07	0.54
1:B:354:ILE:HG12	1:B:372:TYR:CE2	2.42	0.54
1:C:360:HIS:HB3	1:C:370:ILE:CG2	2.38	0.54
1:F:437:LEU:HD22	1:F:437:LEU:N	2.23	0.54
1:B:178:GLY:HA2	1:B:183:LYS:HZ1	1.73	0.54
1:A:84:HIS:ND1	1:A:85:PRO:HD2	2.22	0.54
1:B:74:LEU:HD12	1:B:74:LEU:H	1.73	0.54
1:C:95:LEU:HB3	1:C:114:LYS:HE2	1.90	0.54
1:D:46:VAL:HG22	1:D:68:VAL:HG13	1.89	0.54
1:C:204:TYR:CE1	1:C:208:MET:SD	3.00	0.54
1:E:231:ASN:C	1:E:231:ASN:HD22	2.11	0.54
1:A:248:VAL:HG11	1:A:313:VAL:CG1	2.37	0.53
1:E:78:LYS:NZ	1:E:150:VAL:O	2.35	0.53
1:E:236:ALA:O	1:E:240:VAL:HG23	2.08	0.53
1:A:150:VAL:HG21	1:A:390:MET:CE	2.38	0.53
1:B:99:GLN:NE2	1:B:103:ASN:OD1	2.41	0.53
1:A:338:CYS:SG	1:A:340:PHE:O	2.66	0.53
1:C:43:PRO:O	1:D:50:ARG:HB2	2.08	0.53
1:C:192:ILE:O	1:C:192:ILE:HG22	2.08	0.53
1:D:360:HIS:CE1	1:D:369:ALA:HA	2.44	0.53
1:D:25:THR:OG1	1:D:28:GLN:OE1	2.26	0.53
1:F:308:VAL:HG13	1:F:309:HIS:ND1	2.23	0.53
1:A:205:VAL:HA	1:A:208:MET:HB2	1.91	0.53
1:B:185:GLY:HA2	1:B:189:GLY:HA3	1.90	0.53
1:D:20:THR:HG21	1:D:442:ASN:HB2	1.91	0.53
1:E:266:SER:OG	1:E:267:PHE:N	2.42	0.53
1:F:257:LEU:HD23	1:F:294:PHE:HE1	1.74	0.53
1:B:33:TYR:HE1	1:B:450:ALA:HB1	1.72	0.53
1:C:199:TYR:N	1:C:199:TYR:CD1	2.75	0.53
1:B:18:ALA:O	1:B:22:GLU:HG2	2.09	0.53
1:B:53:TRP:HH2	1:B:124:LYS:HD2	1.74	0.53
1:B:288:LEU:HD21	1:B:294:PHE:CD1	2.44	0.53
1:C:349:CYS:SG	1:C:353:ALA:C	2.87	0.53
1:D:82:ARG:HG3	1:D:155:ILE:HB	1.91	0.53
1:B:62:VAL:O	1:B:63:ASN:ND2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:224:VAL:CG2	1:D:247:VAL:HA	2.39	0.52
1:D:314:ASP:HA	1:D:338:CYS:HA	1.90	0.52
1:B:197:THR:O	1:B:201:VAL:HG23	2.09	0.52
1:F:341:ILE:HG23	1:F:372:TYR:HA	1.92	0.52
1:D:167:GLY:HA3	1:F:456:GLN:O	2.09	0.52
1:D:350:THR:O	1:D:354:ILE:HG13	2.09	0.52
1:C:197:THR:HB	1:C:232:VAL:HG22	1.90	0.52
1:F:361:ARG:HG3	1:F:369:ALA:CB	2.39	0.52
1:A:258:ILE:HD13	1:A:310:VAL:HG13	1.92	0.52
1:A:208:MET:CE	1:A:371:TRP:HE3	2.23	0.52
1:A:350:THR:O	1:A:354:ILE:HG13	2.09	0.52
1:D:169:TYR:OH	1:D:173:ARG:NH1	2.43	0.52
1:E:301:LEU:HD12	1:E:302:PRO:HD2	1.91	0.52
1:F:361:ARG:HA	1:F:369:ALA:HB1	1.91	0.52
1:C:209:ILE:O	1:C:212:ALA:HB3	2.10	0.52
1:C:322:GLN:HG3	1:C:347:MET:O	2.09	0.52
1:D:166:PHE:CB	1:D:183:LYS:HZ1	2.23	0.52
1:A:42:VAL:CG1	1:B:50:ARG:HD3	2.35	0.52
1:C:252:ASP:OD2	1:C:285:ILE:HG13	2.10	0.52
1:D:74:LEU:HD21	1:D:448:LYS:HG2	1.92	0.52
1:E:203:TYR:O	1:E:206:GLU:HB2	2.10	0.52
1:F:46:VAL:HG13	1:F:68:VAL:HG22	1.92	0.51
1:F:103:ASN:HB3	1:F:110:MET:HB2	1.91	0.51
1:B:83:PHE:CD2	1:B:157:VAL:HG22	2.44	0.51
1:B:203:TYR:CE2	1:B:409:LYS:HG2	2.44	0.51
1:C:344:GLY:O	1:C:379:ASN:HB3	2.09	0.51
1:F:79:GLY:HA3	1:F:113:GLY:O	2.10	0.51
1:B:372:TYR:CZ	1:B:374:PRO:HA	2.46	0.51
1:C:460:TRP:OXT	1:D:60:VAL:HG21	2.10	0.51
1:F:16:GLU:O	1:F:19:SER:OG	2.26	0.51
1:A:288:LEU:O	1:A:288:LEU:HD23	2.10	0.51
1:C:208:MET:HE1	1:C:342:ALA:HB2	1.91	0.51
1:F:127:SER:O	1:F:130:ARG:O	2.28	0.51
1:B:365:LYS:CG	1:B:433:ILE:HD13	2.40	0.51
1:C:357:PHE:CD1	1:C:370:ILE:HG12	2.46	0.51
1:D:17:LEU:O	1:D:21:LEU:HG	2.10	0.51
1:A:74:LEU:HD22	1:A:74:LEU:N	2.26	0.51
1:E:252:ASP:N	1:E:255:GLY:O	2.44	0.51
1:F:224:VAL:O	1:F:247:VAL:HA	2.11	0.51
1:C:357:PHE:HD1	1:C:370:ILE:HG12	1.76	0.51
1:E:137:MET:HE3	1:E:165:LEU:HG	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:ILE:HA	1:E:165:LEU:CD2	2.40	0.51
1:B:365:LYS:HG2	1:B:433:ILE:HD13	1.92	0.51
1:C:341:ILE:HG22	1:C:370:ILE:HD11	1.93	0.51
1:D:247:VAL:O	1:D:266:SER:HA	2.11	0.51
1:A:275:ILE:HG12	1:A:288:LEU:HD13	1.93	0.51
1:A:360:HIS:CE1	1:A:369:ALA:HA	2.46	0.51
1:A:364:ASN:ND2	1:A:368:ALA:HB3	2.20	0.50
1:B:396:ARG:NH1	1:D:76:PRO:CD	2.74	0.50
1:B:288:LEU:HD21	1:B:294:PHE:CE1	2.46	0.50
1:C:408:LEU:HG	1:C:412:MET:HE2	1.92	0.50
1:D:312:ALA:HA	1:D:336:ALA:HB1	1.92	0.50
1:D:20:THR:HG21	1:D:439:THR:HA	1.92	0.50
1:F:289:VAL:HA	1:F:294:PHE:HB2	1.92	0.50
1:B:310:VAL:HG21	1:B:313:VAL:HB	1.93	0.50
1:C:458:ASP:OD2	1:E:170:ARG:NH1	2.43	0.50
1:F:291:ASP:O	1:F:292:ALA:CB	2.59	0.50
1:B:396:ARG:HH22	1:D:76:PRO:HD3	1.77	0.50
1:D:203:TYR:O	1:D:206:GLU:HB3	2.12	0.50
1:E:258:ILE:O	1:E:299:THR:HB	2.10	0.50
1:A:39:VAL:O	1:A:42:VAL:HG13	2.12	0.50
1:A:288:LEU:HD21	1:A:294:PHE:CG	2.47	0.50
1:E:226:ILE:HD12	1:E:247:VAL:HG13	1.93	0.50
1:B:195:GLU:HG3	1:B:235:TYR:CZ	2.47	0.50
1:D:166:PHE:HB2	1:D:183:LYS:HZ1	1.74	0.50
1:D:209:ILE:HG23	1:D:371:TRP:CE3	2.47	0.50
1:E:192:ILE:HD11	1:E:401:ALA:HB1	1.93	0.50
1:E:354:ILE:HG12	1:E:372:TYR:OH	2.12	0.50
1:C:139:GLU:OE1	1:C:142:ARG:NH2	2.45	0.49
1:F:339:LYS:HD2	1:F:368:ALA:HA	1.93	0.49
1:A:151:PRO:HD2	1:A:180:LEU:HD23	1.94	0.49
1:D:246:ARG:HH11	1:D:246:ARG:HG3	1.75	0.49
1:E:341:ILE:CG2	1:E:373:ALA:H	2.25	0.49
1:E:399:TRP:HB3	1:E:403:GLU:OE1	2.12	0.49
1:F:275:ILE:HG12	1:F:288:LEU:CD2	2.42	0.49
1:E:141:CYS:SG	1:E:142:ARG:N	2.85	0.49
1:E:119:PHE:CE2	1:E:129:ILE:HG12	2.47	0.49
1:A:82:ARG:NH1	1:A:95:LEU:HD11	2.27	0.49
1:D:315:VAL:HG13	1:D:340:PHE:O	2.13	0.49
1:E:229:SER:HB3	1:E:275:ILE:HG21	1.95	0.49
1:F:275:ILE:HD11	1:F:294:PHE:HZ	1.77	0.49
1:A:75:GLY:HA2	1:C:176:TRP:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:TYR:CZ	1:B:377:ALA:HB1	2.48	0.49
1:B:261:ASP:OD2	1:B:264:LYS:NZ	2.45	0.49
1:D:246:ARG:CG	1:D:246:ARG:NH1	2.64	0.49
1:B:351:GLN:NE2	1:B:355:ASP:OD2	2.46	0.49
1:C:21:LEU:HD23	1:C:443:ILE:HG12	1.95	0.49
1:D:436:SER:HB2	1:D:439:THR:CB	2.42	0.49
1:C:402:GLU:HB2	1:C:403:GLU:OE1	2.13	0.49
1:D:208:MET:O	1:D:416:PHE:CZ	2.65	0.49
1:D:250:LEU:O	1:D:251:SER:OG	2.25	0.49
1:D:342:ALA:HA	1:D:373:ALA:HB3	1.95	0.49
1:E:278:LEU:HD13	1:E:288:LEU:HD13	1.93	0.49
1:B:88:ASN:HD21	1:B:90:SER:HB3	1.77	0.49
1:B:278:LEU:HD11	1:B:288:LEU:HB2	1.95	0.49
1:C:257:LEU:HD13	1:C:300:TYR:HB2	1.94	0.48
1:F:250:LEU:HB3	1:F:267:PHE:CZ	2.48	0.48
1:A:114:LYS:NZ	1:A:154:ASP:OD1	2.34	0.48
1:A:326:SER:HB2	2:A:504:HOH:O	2.13	0.48
1:B:289:VAL:HG11	1:B:300:TYR:HD1	1.78	0.48
1:C:227:SER:OG	1:C:318:PRO:HA	2.12	0.48
1:E:162:ILE:HA	1:E:165:LEU:HD21	1.95	0.48
1:B:268:THR:O	1:B:272:ILE:HG13	2.13	0.48
1:C:99:GLN:NE2	1:C:383:VAL:HG11	2.28	0.48
1:A:259:VAL:HG12	1:A:298:PHE:CE1	2.48	0.48
1:E:119:PHE:HE2	1:E:129:ILE:HG12	1.78	0.48
1:E:192:ILE:HG22	1:E:192:ILE:O	2.12	0.48
1:F:288:LEU:HD21	1:F:294:PHE:CE2	2.47	0.48
1:B:150:VAL:HG21	1:B:390:MET:CE	2.44	0.48
1:A:456:GLN:OE1	1:C:170:ARG:NH2	2.47	0.48
1:B:396:ARG:HH12	1:D:76:PRO:CD	2.26	0.48
1:C:55:ASN:OD1	1:C:59:GLU:N	2.47	0.48
1:E:205:VAL:HG12	1:E:209:ILE:HG13	1.95	0.48
1:A:288:LEU:HD21	1:A:294:PHE:CD2	2.48	0.48
1:C:455:ASP:OD1	1:E:187:TRP:HZ2	1.96	0.48
1:D:25:THR:HG22	1:D:426:TYR:O	2.13	0.48
1:D:248:VAL:HG23	1:D:259:VAL:HG22	1.96	0.48
1:A:42:VAL:HG13	1:B:50:ARG:HD2	1.95	0.48
1:A:56:ASP:O	1:A:57:LYS:HB2	2.12	0.48
1:A:341:ILE:HG23	1:A:372:TYR:HA	1.95	0.48
1:C:195:GLU:HG2	1:C:235:TYR:CZ	2.49	0.48
1:E:39:VAL:HG21	1:E:459:TRP:HB3	1.96	0.48
1:A:396:ARG:HH22	1:E:146:ALA:C	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:HZ	1:B:129:ILE:HG12	1.79	0.48
1:E:46:VAL:HG22	1:E:68:VAL:HG13	1.96	0.48
1:A:208:MET:HE3	1:A:371:TRP:HE3	1.79	0.47
1:D:25:THR:HG22	1:D:426:TYR:CA	2.43	0.47
1:A:420:LEU:HD13	1:A:420:LEU:O	2.14	0.47
1:B:127:SER:HB3	1:B:130:ARG:NH1	2.29	0.47
1:C:333:LEU:HB3	1:C:338:CYS:HB2	1.95	0.47
1:D:204:TYR:O	1:D:208:MET:N	2.47	0.47
1:E:24:SER:OG	1:E:426:TYR:HB3	2.13	0.47
1:E:297:LYS:O	1:E:297:LYS:HG2	2.14	0.47
1:E:372:TYR:CE2	1:E:438:VAL:CG1	2.98	0.47
1:E:63:ASN:HD22	1:E:119:PHE:HB2	1.80	0.47
1:A:74:LEU:HD21	1:A:449:VAL:HG22	1.97	0.47
1:C:74:LEU:HD11	1:C:449:VAL:HG22	1.97	0.47
1:C:205:VAL:O	1:C:209:ILE:HG13	2.14	0.47
1:A:50:ARG:HD2	1:A:62:VAL:HG11	1.96	0.47
1:A:425:GLU:OE2	1:A:425:GLU:HA	2.15	0.47
1:F:192:ILE:O	1:F:192:ILE:HG22	2.15	0.47
1:A:197:THR:O	1:A:201:VAL:HG23	2.14	0.47
1:D:69:GLN:HE21	1:D:149:ASP:HB2	1.79	0.47
1:E:66:PHE:HB2	1:E:92:LEU:CD1	2.45	0.47
1:E:323:ASN:HB3	1:E:350:THR:HG22	1.96	0.47
1:B:229:SER:O	1:B:234:GLN:NE2	2.47	0.47
1:C:125:SER:OG	1:C:127:SER:OG	2.31	0.47
1:A:79:GLY:HA3	1:A:113:GLY:O	2.15	0.47
1:B:278:LEU:HD11	1:B:288:LEU:CB	2.45	0.47
1:D:204:TYR:O	1:D:208:MET:HB2	2.15	0.46
1:E:302:PRO:HG2	1:E:303:GLY:H	1.79	0.46
1:C:351:GLN:O	1:C:355:ASP:OD1	2.33	0.46
1:E:201:VAL:CG1	1:E:342:ALA:HB1	2.45	0.46
1:F:78:LYS:HE2	1:F:390:MET:SD	2.54	0.46
1:A:3:ASN:OD1	1:A:3:ASN:N	2.48	0.46
1:B:396:ARG:NH2	1:D:76:PRO:CG	2.78	0.46
1:C:109:ASN:HB3	1:E:176:TRP:CZ2	2.50	0.46
1:E:207:HIS:CE1	1:E:413:LYS:HD2	2.50	0.46
1:F:37:LEU:O	1:F:40:VAL:HG12	2.14	0.46
1:E:190:SER:HB3	1:E:193:ARG:HB2	1.97	0.46
1:F:322:GLN:OE1	1:F:322:GLN:N	2.46	0.46
1:B:343:GLU:OE1	1:B:372:TYR:OH	2.24	0.46
1:B:456:GLN:OE1	1:F:170:ARG:NE	2.44	0.46
1:C:349:CYS:HG	1:C:350:THR:N	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:455:ASP:OD1	1:E:187:TRP:CZ2	2.68	0.46
1:D:208:MET:HA	1:D:416:PHE:CE1	2.50	0.46
1:D:453:MET:SD	1:D:458:ASP:OD2	2.74	0.46
1:F:36:ALA:O	1:F:39:VAL:CG1	2.64	0.46
1:F:275:ILE:HG12	1:F:288:LEU:HD22	1.98	0.46
1:A:209:ILE:HG21	1:A:218:SER:HA	1.97	0.46
1:C:207:HIS:CD2	1:C:413:LYS:HG3	2.51	0.46
1:C:421:ASP:O	1:C:425:GLU:HG3	2.16	0.46
1:D:289:VAL:O	1:D:295:ALA:HB2	2.14	0.46
1:E:210:ALA:HB1	1:E:214:ASN:O	2.16	0.46
1:C:25:THR:OG1	1:C:426:TYR:HA	2.15	0.46
1:C:196:ALA:CB	1:C:382:GLY:HA2	2.43	0.46
1:D:366:GLY:HA2	1:D:434:LEU:N	2.31	0.46
1:C:79:GLY:O	1:C:151:PRO:HA	2.16	0.46
1:C:337:GLY:O	1:C:339:LYS:N	2.49	0.46
1:E:208:MET:SD	1:E:341:ILE:O	2.74	0.46
1:F:214:ASN:O	1:F:216:ALA:N	2.49	0.46
1:F:338:CYS:SG	1:F:370:ILE:HD11	2.56	0.46
1:B:27:PHE:CE1	1:B:34:ARG:HG2	2.51	0.46
1:B:176:TRP:CD1	1:D:72:SER:O	2.69	0.46
1:D:430:ALA:O	1:D:433:ILE:HG22	2.15	0.46
1:F:203:TYR:O	1:F:206:GLU:HB3	2.16	0.46
1:F:389:GLU:O	1:F:393:ASN:OD1	2.34	0.46
1:A:42:VAL:CG1	1:B:50:ARG:CD	2.90	0.45
1:B:192:ILE:HG22	1:B:192:ILE:O	2.16	0.45
1:C:252:ASP:CG	1:C:285:ILE:HG13	2.36	0.45
1:C:360:HIS:HD2	1:C:360:HIS:O	1.98	0.45
1:E:16:GLU:CD	1:E:351:GLN:HG2	2.36	0.45
1:A:25:THR:HG22	1:A:28:GLN:HE22	1.81	0.45
1:B:144:ILE:HG22	1:B:149:ASP:HB2	1.98	0.45
1:C:384:ALA:HB1	1:C:411:ILE:HD13	1.98	0.45
1:C:200:GLY:HA2	1:C:412:MET:HE3	1.98	0.45
1:F:360:HIS:HD2	1:F:370:ILE:HG22	1.73	0.45
1:C:389:GLU:O	1:C:393:ASN:ND2	2.44	0.45
1:F:258:ILE:O	1:F:299:THR:HB	2.16	0.45
1:A:172:LEU:HD22	1:F:172:LEU:HD22	1.99	0.45
1:A:430:ALA:HB3	1:A:433:ILE:HG13	1.99	0.45
1:B:318:PRO:HG2	1:B:343:GLU:HA	1.98	0.45
1:D:209:ILE:HD11	1:D:371:TRP:HB3	1.99	0.45
1:A:17:LEU:HD22	1:A:97:PHE:CZ	2.52	0.45
1:A:204:TYR:O	1:A:208:MET:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:VAL:HB	1:F:50:ARG:HD3	1.98	0.45
1:F:95:LEU:HD13	1:F:114:LYS:HE2	1.98	0.45
1:F:268:THR:O	1:F:272:ILE:HD12	2.16	0.45
1:B:246:ARG:HB3	1:B:266:SER:HB2	1.99	0.45
1:B:330:ALA:O	1:B:334:ILE:HG13	2.17	0.45
1:C:75:GLY:HA2	1:E:176:TRP:CE2	2.52	0.45
1:C:408:LEU:HG	1:C:412:MET:CE	2.47	0.45
1:E:17:LEU:HA	1:E:442:ASN:HD22	1.81	0.45
1:E:224:VAL:HG13	1:E:317:LEU:HD13	1.99	0.45
1:F:321:THR:OG1	1:F:322:GLN:N	2.50	0.45
1:A:21:LEU:HD23	1:A:443:ILE:HG12	1.99	0.45
1:A:455:ASP:O	1:C:163:GLY:HA3	2.17	0.45
1:C:17:LEU:O	1:C:21:LEU:HG	2.17	0.45
1:E:205:VAL:O	1:E:209:ILE:HG13	2.16	0.45
1:F:16:GLU:OE1	1:F:16:GLU:HA	2.17	0.45
1:F:198:GLY:O	1:F:201:VAL:HG12	2.17	0.45
1:D:321:THR:OG1	1:D:322:GLN:N	2.50	0.44
1:B:33:TYR:HD1	1:B:36:ALA:CB	2.30	0.44
1:E:81:LEU:HB2	1:E:157:VAL:HG21	1.99	0.44
1:E:261:ASP:OD2	1:E:264:LYS:NZ	2.47	0.44
1:F:120:ASP:O	1:F:124:LYS:HG3	2.17	0.44
1:F:358:GLU:OE1	1:F:361:ARG:NH1	2.50	0.44
1:A:6:VAL:HG12	1:A:8:PRO:HD3	1.99	0.44
1:A:322:GLN:O	1:A:323:ASN:C	2.55	0.44
1:C:204:TYR:HE1	1:C:373:ALA:HB1	1.82	0.44
1:E:27:PHE:CE1	1:E:34:ARG:HG2	2.52	0.44
1:E:137:MET:HB2	1:E:165:LEU:HB2	1.98	0.44
1:E:195:GLU:HB3	1:E:235:TYR:CD2	2.51	0.44
1:A:321:THR:OG1	1:A:322:GLN:N	2.51	0.44
1:C:99:GLN:HG3	1:C:103:ASN:ND2	2.31	0.44
1:F:307:TRP:CH2	1:F:318:PRO:HB3	2.53	0.44
1:A:25:THR:HG22	1:A:28:GLN:NE2	2.33	0.44
1:D:195:GLU:HG3	1:D:235:TYR:CE1	2.53	0.44
1:E:321:THR:OG1	1:E:322:GLN:N	2.50	0.44
1:A:365:LYS:HB3	1:A:433:ILE:CD1	2.44	0.44
1:B:266:SER:OG	1:B:267:PHE:N	2.51	0.44
1:B:321:THR:OG1	1:B:322:GLN:N	2.51	0.44
1:B:329:GLU:O	1:B:333:LEU:HG	2.17	0.44
1:C:200:GLY:HA2	1:C:412:MET:CE	2.46	0.44
1:C:374:PRO:HG3	1:C:441:SER:OG	2.18	0.44
1:D:453:MET:SD	1:D:458:ASP:CG	2.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:119:PHE:HE2	1:F:129:ILE:HG12	1.81	0.44
1:A:42:VAL:HG22	1:B:50:ARG:HB2	1.98	0.44
1:B:366:GLY:O	1:B:434:LEU:HD11	2.17	0.44
1:D:180:LEU:HB2	1:D:183:LYS:HE2	1.99	0.44
1:E:163:GLY:HA2	1:E:187:TRP:CH2	2.53	0.44
1:F:360:HIS:CD2	1:F:370:ILE:H	2.35	0.44
1:A:343:GLU:OE1	1:A:347:MET:CA	2.66	0.44
1:C:394:SER:HG	1:E:396:ARG:NE	2.16	0.44
1:F:195:GLU:O	1:F:199:TYR:HB2	2.18	0.44
1:A:257:LEU:HD22	1:A:285:ILE:HG21	1.99	0.43
1:A:455:ASP:O	1:C:163:GLY:CA	2.65	0.43
1:B:311:GLY:C	1:B:336:ALA:HB1	2.39	0.43
1:B:354:ILE:HG12	1:B:372:TYR:CD2	2.53	0.43
1:E:63:ASN:ND2	1:E:119:PHE:CB	2.81	0.43
1:E:400:THR:HG23	1:E:403:GLU:H	1.83	0.43
1:A:226:ILE:HG22	1:A:227:SER:O	2.17	0.43
1:B:351:GLN:HA	1:B:354:ILE:HD12	2.00	0.43
1:B:396:ARG:NH2	1:D:76:PRO:CD	2.81	0.43
1:E:228:GLY:O	1:E:233[A]:ALA:HB3	2.17	0.43
1:F:191:LEU:O	1:F:192:ILE:HB	2.18	0.43
1:B:119:PHE:CZ	1:B:129:ILE:HG12	2.54	0.43
1:B:285:ILE:O	1:B:289:VAL:HG13	2.17	0.43
1:C:239:LYS:NZ	1:C:242:GLU:OE1	2.39	0.43
1:F:127:SER:OG	1:F:130:ARG:NH2	2.51	0.43
1:A:192:ILE:HD11	1:A:401:ALA:HB1	2.00	0.43
1:B:385:VAL:HG23	1:B:408:LEU:HD13	1.98	0.43
1:C:321:THR:OG1	1:C:322:GLN:N	2.50	0.43
1:F:325:VAL:C	1:F:350:THR:OG1	2.55	0.43
1:F:151:PRO:HD2	1:F:179:VAL:O	2.17	0.43
1:F:193:ARG:N	1:F:194:PRO:CD	2.82	0.43
1:D:257:LEU:HD22	1:D:285:ILE:HG21	1.99	0.43
1:E:70:PHE:HB3	1:E:100:ILE:HD11	2.01	0.43
1:B:315:VAL:HG22	1:B:340:PHE:HB2	2.00	0.43
1:C:344:GLY:O	1:C:379:ASN:CB	2.66	0.43
1:A:32:GLU:HB2	1:A:459:TRP:HZ3	1.84	0.43
1:B:310:VAL:CG2	1:B:313:VAL:HB	2.49	0.43
1:C:190:SER:OG	1:C:389:GLU:HB2	2.19	0.43
1:D:66:PHE:HB2	1:D:92:LEU:HD13	2.01	0.43
1:D:174:ASN:HB2	1:E:142:ARG:NH2	2.34	0.43
1:E:228:GLY:O	1:E:233[B]:ALA:HB3	2.18	0.43
1:E:258:ILE:HG22	1:E:259:VAL:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:36:ALA:O	1:F:39:VAL:HG12	2.18	0.43
1:C:50:ARG:HE	1:C:52:VAL:HG23	1.84	0.43
1:D:74:LEU:HD11	1:D:449:VAL:HG22	2.00	0.43
1:D:325:VAL:HA	1:D:329:GLU:OE1	2.19	0.43
1:E:305:ARG:HD3	1:E:324:GLU:O	2.18	0.43
1:A:225:ALA:HB2	1:A:313:VAL:HG21	2.01	0.43
1:F:119:PHE:CE2	1:F:129:ILE:HG12	2.54	0.43
1:A:226:ILE:HD12	1:A:247:VAL:HG13	2.00	0.42
1:B:314:ASP:HA	1:B:338:CYS:HA	2.02	0.42
1:C:290:THR:HG22	1:C:290:THR:O	2.19	0.42
1:D:220:ALA:HB2	1:D:243:LEU:O	2.19	0.42
1:A:195:GLU:O	1:A:199:TYR:HB2	2.20	0.42
1:B:193:ARG:O	1:B:193:ARG:NE	2.52	0.42
1:D:413:LYS:HE2	1:D:417:GLN:NE2	2.34	0.42
1:F:350:THR:O	1:F:354:ILE:HG13	2.19	0.42
1:B:354:ILE:O	1:B:358:GLU:N	2.46	0.42
1:B:361:ARG:O	1:B:433:ILE:HG23	2.20	0.42
1:D:163:GLY:C	1:F:456:GLN:HA	2.40	0.42
1:D:224:VAL:O	1:D:248:VAL:HG13	2.18	0.42
1:E:307:TRP:O	1:E:310:VAL:HG22	2.19	0.42
1:F:226:ILE:HG22	1:F:227:SER:O	2.19	0.42
1:A:304:GLN:OE1	1:A:309:HIS:NE2	2.35	0.42
1:B:193:ARG:N	1:B:194:PRO:CD	2.82	0.42
1:B:405:ASP:O	1:B:409:LYS:HG3	2.20	0.42
1:D:209:ILE:O	1:D:213:THR:HG23	2.20	0.42
1:B:103:ASN:ND2	1:B:111:GLY:O	2.52	0.42
1:C:193:ARG:N	1:C:194:PRO:CD	2.83	0.42
1:D:290:THR:O	1:D:290:THR:HG22	2.20	0.42
1:A:339:LYS:HA	1:A:370:ILE:HA	2.00	0.42
1:A:455:ASP:O	1:C:163:GLY:C	2.58	0.42
1:B:310:VAL:HG11	1:B:313:VAL:HG11	2.02	0.42
1:E:439:THR:OG1	1:E:440:GLY:N	2.52	0.42
1:A:142:ARG:HG3	1:A:143:HIS:CD2	2.55	0.42
1:C:103:ASN:HB3	1:C:110:MET:HB2	2.02	0.42
1:F:361:ARG:O	1:F:433:ILE:HD12	2.20	0.42
1:A:32:GLU:HB2	1:A:459:TRP:CZ3	2.55	0.42
1:B:229:SER:HB2	1:B:275:ILE:HG22	2.00	0.42
1:B:307:TRP:CE3	1:B:333:LEU:HD11	2.55	0.42
1:C:38:ALA:O	1:C:42:VAL:HG23	2.20	0.42
1:E:63:ASN:HD21	1:E:119:PHE:CA	2.31	0.42
1:A:157:VAL:HG23	1:A:157:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:CYS:SG	1:C:353:ALA:HB3	2.60	0.42
1:D:152:ALA:HB2	1:D:181:THR:HB	2.02	0.42
1:E:226:ILE:O	1:E:249:SER:OG	2.30	0.42
1:F:224:VAL:HB	1:F:247:VAL:HG22	2.01	0.42
1:A:139:GLU:CD	1:B:45:ARG:HH21	2.23	0.41
1:A:193:ARG:N	1:A:194:PRO:CD	2.83	0.41
1:A:203:TYR:CZ	1:A:239:LYS:HE3	2.54	0.41
1:A:204:TYR:CZ	1:A:416:PHE:HD1	2.37	0.41
1:B:325:VAL:O	1:B:350:THR:HG23	2.20	0.41
1:D:193:ARG:N	1:D:194:PRO:CD	2.83	0.41
1:B:16:GLU:O	1:B:20:THR:HG23	2.19	0.41
1:C:209:ILE:HG12	1:C:340:PHE:CE1	2.55	0.41
1:D:188:GLY:O	1:D:389:GLU:OE2	2.38	0.41
1:E:338:CYS:SG	1:E:340:PHE:O	2.78	0.41
1:F:229:SER:OG	1:F:285:ILE:HD11	2.20	0.41
1:F:234:GLN:HE22	1:F:276:ALA:HA	1.85	0.41
1:F:454:LYS:HB2	1:F:459:TRP:CZ2	2.55	0.41
1:C:308:VAL:CG1	1:C:329:GLU:HA	2.50	0.41
1:D:192:ILE:HG22	1:D:192:ILE:O	2.20	0.41
1:D:209:ILE:HD13	1:D:340:PHE:HD1	1.83	0.41
1:D:453:MET:SD	1:D:458:ASP:CB	3.09	0.41
1:F:192:ILE:HD11	1:F:401:ALA:HB1	2.01	0.41
1:F:239:LYS:NZ	1:F:242:GLU:OE1	2.35	0.41
1:A:19:SER:O	1:A:23:ASN:OD1	2.38	0.41
1:D:423:ALA:HB1	1:D:435:PRO:HB2	2.01	0.41
1:E:268:THR:OG1	1:E:271:GLU:OE1	2.38	0.41
1:A:266:SER:OG	1:A:267:PHE:N	2.53	0.41
1:D:163:GLY:CA	1:F:455:ASP:O	2.65	0.41
1:E:42:VAL:HB	1:F:50:ARG:CD	2.50	0.41
1:E:223:ARG:HB2	1:E:313:VAL:HA	2.01	0.41
1:E:316:ALA:HB3	1:E:341:ILE:HG13	2.01	0.41
1:F:70:PHE:CD1	1:F:100:ILE:HD11	2.55	0.41
1:F:262:THR:HG21	1:F:310:VAL:O	2.20	0.41
1:A:195:GLU:HG3	1:A:235:TYR:CD1	2.56	0.41
1:B:33:TYR:CD1	1:B:36:ALA:CB	3.04	0.41
1:B:354:ILE:HG23	1:B:372:TYR:HD2	1.83	0.41
1:D:218:SER:C	1:D:220:ALA:N	2.72	0.41
1:D:229:SER:O	1:D:234:GLN:NE2	2.54	0.41
1:E:99:GLN:HE22	1:E:383:VAL:HG21	1.86	0.41
1:E:106:THR:O	1:E:411:ILE:HG23	2.20	0.41
1:E:256:SER:O	1:E:301:LEU:CB	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:LYS:HB3	1:F:103:ASN:ND2	2.35	0.41
1:F:209:ILE:O	1:F:213:THR:HG22	2.21	0.41
1:A:150:VAL:HG21	1:A:390:MET:HE1	2.03	0.41
1:B:396:ARG:HG2	1:B:396:ARG:O	2.21	0.41
1:C:288:LEU:O	1:C:294:PHE:HB2	2.20	0.41
1:C:361:ARG:O	1:C:433:ILE:HG23	2.21	0.41
1:D:66:PHE:HB2	1:D:92:LEU:CD1	2.50	0.41
1:D:204:TYR:HE2	1:D:416:PHE:HA	1.86	0.41
1:F:257:LEU:CD2	1:F:294:PHE:HE1	2.33	0.41
1:F:258:ILE:HG21	1:F:310:VAL:HA	2.03	0.41
1:A:166:PHE:HE1	1:A:177:GLU:O	2.04	0.41
1:D:17:LEU:HD22	1:D:97:PHE:CZ	2.56	0.41
1:D:30:ASN:HB3	1:D:33:TYR:CG	2.56	0.41
1:D:199:TYR:CE2	1:D:239:LYS:HD3	2.56	0.41
1:E:86:SER:O	1:F:3:ASN:ND2	2.54	0.41
1:A:64:ARG:NH2	1:B:4:LEU:HD22	2.36	0.41
1:A:92:LEU:HD13	1:A:115:GLY:O	2.21	0.41
1:B:148:THR:HG22	1:B:149:ASP:N	2.36	0.41
1:C:44:GLU:OE2	1:E:170:ARG:NH2	2.54	0.41
1:C:109:ASN:ND2	1:E:176:TRP:CZ2	2.88	0.41
1:C:228:GLY:O	1:C:250:LEU:HD22	2.21	0.41
1:C:341:ILE:HG23	1:C:341:ILE:O	2.20	0.41
1:C:456:GLN:O	1:E:167:GLY:HA3	2.21	0.41
1:D:78:LYS:NZ	1:D:150:VAL:O	2.38	0.41
1:D:149:ASP:O	1:D:151:PRO:HD3	2.20	0.41
1:D:193:ARG:HB3	1:D:194:PRO:HD3	2.03	0.41
1:E:43:PRO:O	1:F:50:ARG:HB2	2.21	0.41
1:E:198:GLY:HA3	1:E:232:VAL:O	2.21	0.41
1:E:358:GLU:OE1	1:E:362:GLU:OE1	2.39	0.41
1:A:103:ASN:ND2	1:A:111:GLY:O	2.53	0.41
1:A:405:ASP:O	1:A:409:LYS:HG3	2.20	0.41
1:C:84:HIS:ND1	1:C:85:PRO:HD2	2.36	0.41
1:A:109:ASN:HD22	1:A:109:ASN:HA	1.76	0.40
1:A:200:GLY:HA2	1:A:203:TYR:CD2	2.56	0.40
1:B:89:LEU:O	1:B:93:LYS:HG3	2.21	0.40
1:B:219:PHE:HE1	1:B:224:VAL:HG21	1.86	0.40
1:D:89:LEU:O	1:D:93:LYS:HG3	2.22	0.40
1:E:54:GLU:O	1:E:131:ARG:HD2	2.21	0.40
1:A:315:VAL:HG22	1:A:340:PHE:HB2	2.03	0.40
1:B:134:VAL:O	1:B:138:THR:OG1	2.36	0.40
1:B:249:SER:OG	1:B:258:ILE:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:ASP:O	1:C:409:LYS:HG3	2.20	0.40
1:D:142:ARG:HH22	1:E:172:LEU:C	2.25	0.40
1:D:217:GLU:HG2	1:D:222:LYS:HE2	2.03	0.40
1:F:229:SER:HB3	1:F:250:LEU:HD21	2.02	0.40
1:A:286:ALA:HA	1:A:289:VAL:HG22	2.02	0.40
1:B:369:ALA:HB3	1:B:434:LEU:HD12	2.04	0.40
1:F:199:TYR:CE2	1:F:239:LYS:HD3	2.56	0.40
1:F:240:VAL:CG1	1:F:247:VAL:HG23	2.49	0.40
1:A:193:ARG:HG2	1:A:193:ARG:HH11	1.87	0.40
1:A:360:HIS:HE1	1:A:369:ALA:HA	1.85	0.40
1:C:95:LEU:HB3	1:C:114:LYS:CE	2.51	0.40
1:C:151:PRO:HD2	1:C:180:LEU:HD23	2.02	0.40
1:D:181:THR:HG23	1:D:193:ARG:HE	1.86	0.40
1:E:193:ARG:N	1:E:194:PRO:CD	2.84	0.40
1:E:225:ALA:HB3	1:E:316:ALA:HA	2.03	0.40
1:E:227:SER:CB	1:E:306:PRO:CG	2.98	0.40
1:E:278:LEU:CD2	1:E:288:LEU:HD22	2.52	0.40
1:E:343:GLU:OE1	1:E:372:TYR:HE1	2.04	0.40
1:F:32:GLU:OE1	1:F:33:TYR:N	2.55	0.40
1:A:78:LYS:HD2	1:A:150:VAL:HG23	2.03	0.40
1:A:316:ALA:HB2	1:A:333:LEU:HD13	2.03	0.40
1:B:225:ALA:HA	1:B:248:VAL:HB	2.03	0.40
1:B:396:ARG:HH12	1:D:76:PRO:HD3	1.86	0.40
1:C:21:LEU:HD22	1:C:26:LEU:CD1	2.51	0.40
1:C:403:GLU:OE1	1:C:403:GLU:N	2.55	0.40

All (8) 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:D:246:ARG:NH2	1:E:328:GLU:O[3_465]	1.34	0.86
1:D:214:ASN:ND2	1:E:299:THR:OG1[3_465]	1.74	0.46
1:D:364:ASN:OD1	1:E:302:PRO:CG[3_465]	1.89	0.31
1:D:246:ARG:CZ	1:E:328:GLU:O[3_465]	1.90	0.30
1:D:223:ARG:N	1:E:328:GLU:OE1[3_465]	2.01	0.19
1:D:222:LYS:O	1:E:328:GLU:OE2[3_465]	2.04	0.16
1:D:222:LYS:C	1:E:328:GLU:OE2[3_465]	2.10	0.10
1:D:223:ARG:N	1:E:328:GLU:OE2[3_465]	2.14	0.06

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	459/460 (100%)	436 (95%)	22 (5%)	1 (0%)	44	63
1	B	459/460 (100%)	437 (95%)	20 (4%)	2 (0%)	30	49
1	C	461/460 (100%)	435 (94%)	23 (5%)	3 (1%)	19	36
1	D	460/460 (100%)	428 (93%)	31 (7%)	1 (0%)	44	63
1	E	459/460 (100%)	429 (94%)	28 (6%)	2 (0%)	30	49
1	F	459/460 (100%)	441 (96%)	15 (3%)	3 (1%)	19	36
All	All	2757/2760 (100%)	2606 (94%)	139 (5%)	12 (0%)	30	49

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	192	ILE
1	C	192	ILE
1	F	192	ILE
1	A	192	ILE
1	B	174	ASN
1	F	215	GLY
1	C	338	CYS
1	D	8	PRO
1	E	214	ASN
1	E	302	PRO
1	F	214	ASN
1	C	341	ILE

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	352/351 (100%)	322 (92%)	30 (8%)	8 18
1	B	351/351 (100%)	322 (92%)	29 (8%)	9 19
1	C	353/351 (101%)	322 (91%)	31 (9%)	8 17
1	D	351/351 (100%)	320 (91%)	31 (9%)	8 17
1	E	351/351 (100%)	315 (90%)	36 (10%)	6 11
1	F	351/351 (100%)	326 (93%)	25 (7%)	12 26
All	All	2109/2106 (100%)	1927 (91%)	182 (9%)	8 18

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

Mol	Chain	Res	Type
1	A	12	GLN
1	A	27	PHE
1	A	30	ASN
1	A	32	GLU
1	A	42	VAL
1	A	61	GLN
1	A	70	PHE
1	A	74	LEU
1	A	84	HIS
1	A	147	ASP
1	A	150	VAL
1	A	155	ILE
1	A	181	THR
1	A	190	SER
1	A	197	THR
1	A	208	MET
1	A	223	ARG
1	A	227	SER
1	A	275	ILE
1	A	289	VAL
1	A	299	THR
1	A	305	ARG
1	A	306	PRO
1	A	329	GLU
1	A	343	GLU
1	A	350	THR
1	A	355	ASP
1	A	371	TRP

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Mol	Chain	Res	Type
1	A	420	LEU
1	A	438	VAL
1	B	1	MET
1	B	3	ASN
1	B	17	LEU
1	B	24	SER
1	B	28	GLN
1	B	47	ILE
1	B	70	PHE
1	B	74	LEU
1	B	88	ASN
1	B	118	ASP
1	B	127	SER
1	B	131	ARG
1	B	133	CYS
1	B	161	GLU
1	B	181	THR
1	B	190	SER
1	B	193	ARG
1	B	197	THR
1	B	249	SER
1	B	262	THR
1	B	288	LEU
1	B	306	PRO
1	B	314	ASP
1	B	351	GLN
1	B	371	TRP
1	B	379	ASN
1	B	385	VAL
1	B	410	ASP
1	B	448	LYS
1	C	26	LEU
1	C	29	LYS
1	C	30	ASN
1	C	70	PHE
1	C	71	ASN
1	C	89	LEU
1	C	114	LYS
1	C	147	ASP
1	C	154	ASP
1	C	173	ARG
1	C	181	THR

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Mol	Chain	Res	Type
1	C	190	SER
1	C	222	LYS
1	C	223	ARG
1	C	231	ASN
1	C	242	GLU
1	C	243	LEU
1	C	284	GLN
1	C	313	VAL
1	C	314	ASP
1	C	338	CYS
1	C	346	ASN
1	C	349	CYS
1	C	371	TRP
1	C	398	SER
1	C	403	GLU
1	C	410	ASP
1	C	415	CYS
1	C	421	ASP
1	C	438	VAL
1	C	455	ASP
1	D	9	GLU
1	D	11	GLU
1	D	22	GLU
1	D	25	THR
1	D	29	LYS
1	D	63	ASN
1	D	70	PHE
1	D	94	PHE
1	D	127	SER
1	D	137	MET
1	D	179	VAL
1	D	181	THR
1	D	202	VAL
1	D	207	HIS
1	D	231	ASN
1	D	241	ILE
1	D	246	ARG
1	D	248	VAL
1	D	257	LEU
1	D	261	ASP
1	D	264	LYS
1	D	281	ASP

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Mol	Chain	Res	Type
1	D	291	ASP
1	D	306	PRO
1	D	324	GLU
1	D	333	LEU
1	D	341	ILE
1	D	371	TRP
1	D	412	MET
1	D	434	LEU
1	D	436	SER
1	E	52	VAL
1	E	70	PHE
1	E	94	PHE
1	E	103	ASN
1	E	165	LEU
1	E	181	THR
1	E	186	SER
1	E	197	THR
1	E	208	MET
1	E	231	ASN
1	E	249	SER
1	E	250	LEU
1	E	254	GLN
1	E	257	LEU
1	E	265	ASP
1	E	267	PHE
1	E	268	THR
1	E	284	GLN
1	E	294	PHE
1	E	296	ASP
1	E	298	PHE
1	E	300	TYR
1	E	313	VAL
1	E	315	VAL
1	E	322	GLN
1	E	325	VAL
1	E	338	CYS
1	E	361	ARG
1	E	365	LYS
1	E	371	TRP
1	E	372	TYR
1	E	383	VAL
1	E	386	SER

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Mol	Chain	Res	Type
1	E	400	THR
1	E	420	LEU
1	E	434	LEU
1	F	32	GLU
1	F	63	ASN
1	F	70	PHE
1	F	94	PHE
1	F	142	ARG
1	F	154	ASP
1	F	161	GLU
1	F	173	ARG
1	F	181	THR
1	F	197	THR
1	F	253	SER
1	F	279	LYS
1	F	298	PHE
1	F	306	PRO
1	F	309	HIS
1	F	313	VAL
1	F	323	ASN
1	F	326	SER
1	F	350	THR
1	F	360	HIS
1	F	365	LYS
1	F	371	TRP
1	F	398	SER
1	F	414	SER
1	F	437	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	30	ASN
1	A	174	ASN
1	A	211	HIS
1	A	254	GLN
1	A	346	ASN
1	A	351	GLN
1	A	364	ASN
1	A	379	ASN
1	A	417	GLN

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Mol	Chain	Res	Type
1	B	28	GLN
1	B	99	GLN
1	B	168	GLN
1	B	351	GLN
1	B	393	ASN
1	C	109	ASN
1	C	231	ASN
1	C	284	GLN
1	C	360	HIS
1	C	364	ASN
1	C	417	GLN
1	D	48	GLN
1	D	143	HIS
1	D	309	HIS
1	E	63	ASN
1	E	99	GLN
1	E	231	ASN
1	E	323	ASN
1	F	323	ASN
1	F	393	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

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	460/460 (100%)	0.29	24 (5%)	34	29	16, 42, 66, 89	2 (0%)
1	B	460/460 (100%)	0.28	18 (3%)	44	38	18, 43, 70, 102	1 (0%)
1	C	460/460 (100%)	0.34	22 (4%)	36	32	12, 44, 69, 92	4 (0%)
1	D	460/460 (100%)	0.53	38 (8%)	19	16	14, 49, 89, 133	2 (0%)
1	E	460/460 (100%)	0.52	42 (9%)	16	14	12, 52, 90, 144	1 (0%)
1	F	460/460 (100%)	0.39	32 (6%)	24	20	17, 46, 75, 102	2 (0%)
All	All	2760/2760 (100%)	0.39	176 (6%)	27	23	12, 46, 79, 144	12 (0%)

All (176) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	107	GLY	8.7
1	D	256	SER	6.4
1	D	349	CYS	6.0
1	F	380	ALA	5.6
1	C	372	TYR	5.1
1	E	368	ALA	4.9
1	E	367	ALA	4.8
1	F	289	VAL	4.7
1	D	75	GLY	4.6
1	E	300	TYR	4.5
1	B	249	SER	4.5
1	A	36	ALA	4.4
1	F	311	GLY	4.3
1	D	257	LEU	4.3
1	C	119	PHE	4.2
1	E	220	ALA	4.2
1	E	248	VAL	4.2
1	E	285	ILE	4.1
1	F	285	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	303	GLY	4.1
1	E	289	VAL	4.0
1	E	360	HIS	4.0
1	F	442	ASN	3.9
1	D	338	CYS	3.9
1	F	169	TYR	3.9
1	E	427	ALA	3.8
1	F	80	GLY	3.8
1	C	18	ALA	3.7
1	B	369	ALA	3.6
1	A	164	TYR	3.5
1	E	327	GLY	3.5
1	C	430	ALA	3.4
1	C	53	TRP	3.4
1	C	308	VAL	3.3
1	B	199	TYR	3.3
1	D	263	ALA	3.3
1	A	20	THR	3.3
1	D	436	SER	3.2
1	E	359	ALA	3.2
1	D	348	GLY	3.2
1	E	366	GLY	3.2
1	A	94	PHE	3.1
1	B	404	VAL	3.1
1	F	250	LEU	3.1
1	B	437	LEU	3.1
1	B	248	VAL	3.0
1	D	209	ILE	3.0
1	F	270	ALA	3.0
1	B	299	THR	3.0
1	C	188	GLY	2.9
1	D	437	LEU	2.9
1	A	180	LEU	2.8
1	E	310	VAL	2.8
1	A	111	GLY	2.8
1	C	318	PRO	2.8
1	E	260	LYS	2.8
1	A	289	VAL	2.7
1	D	26	LEU	2.7
1	F	86	SER	2.7
1	D	375	GLY	2.7
1	D	305	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	247	VAL	2.6
1	E	225	ALA	2.6
1	C	190	SER	2.6
1	D	435	PRO	2.6
1	C	60	VAL	2.6
1	A	225	ALA	2.6
1	F	352	ALA	2.6
1	D	340	PHE	2.6
1	A	320	ALA	2.6
1	F	164	TYR	2.6
1	F	353	ALA	2.6
1	D	189	GLY	2.6
1	C	62	VAL	2.6
1	E	256	SER	2.6
1	A	75	GLY	2.5
1	D	310	VAL	2.5
1	B	81	LEU	2.5
1	F	312	ALA	2.5
1	A	163	GLY	2.5
1	F	60	VAL	2.5
1	A	248	VAL	2.5
1	E	333	LEU	2.5
1	D	416	PHE	2.5
1	D	360	HIS	2.5
1	B	333	LEU	2.5
1	B	259	VAL	2.5
1	C	433	ILE	2.5
1	F	354	ILE	2.5
1	E	410	ASP	2.4
1	F	249	SER	2.4
1	D	420	LEU	2.4
1	F	295	ALA	2.4
1	A	426	TYR	2.4
1	E	160	ARG	2.4
1	D	285	ILE	2.4
1	E	86	SER	2.4
1	F	91	ILE	2.4
1	C	381	GLY	2.3
1	F	455	ASP	2.3
1	A	162	ILE	2.3
1	B	357	PHE	2.3
1	E	263	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	306	PRO	2.3
1	F	54	GLU	2.3
1	C	135	ALA	2.3
1	E	104	ALA	2.3
1	B	419	GLY	2.3
1	F	201	VAL	2.3
1	A	132	PHE	2.3
1	C	166	PHE	2.3
1	D	294	PHE	2.3
1	D	361	ARG	2.3
1	E	105	LEU	2.3
1	E	304	GLN	2.3
1	F	247	VAL	2.3
1	A	50	ARG	2.3
1	D	319	SER	2.3
1	F	313	VAL	2.2
1	A	166	PHE	2.2
1	C	27	PHE	2.2
1	D	70	PHE	2.2
1	D	353	ALA	2.2
1	C	434	LEU	2.2
1	A	52	VAL	2.2
1	E	349	CYS	2.2
1	B	209	ILE	2.2
1	D	52	VAL	2.2
1	E	159	GLY	2.2
1	F	325	VAL	2.2
1	D	369	ALA	2.2
1	E	431	ASP	2.2
1	D	224	VAL	2.2
1	E	357	PHE	2.2
1	F	379	ASN	2.2
1	A	347	MET	2.2
1	B	210	ALA	2.2
1	C	24	SER	2.2
1	D	354	ILE	2.2
1	D	350	THR	2.1
1	F	329	GLU	2.1
1	D	200	GLY	2.1
1	F	186	SER	2.1
1	D	434	LEU	2.1
1	E	369	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	190	SER	2.1
1	E	93	LYS	2.1
1	A	238	LEU	2.1
1	E	195	GLU	2.1
1	B	429	PRO	2.1
1	E	306	PRO	2.1
1	B	460	TRP	2.1
1	F	224	VAL	2.1
1	E	348	GLY	2.1
1	F	96	GLY	2.1
1	B	149	ASP	2.1
1	E	420	LEU	2.1
1	E	312	ALA	2.1
1	D	226	ILE	2.1
1	A	153	GLY	2.1
1	D	167	GLY	2.1
1	E	303	GLY	2.1
1	A	21	LEU	2.0
1	E	262	THR	2.0
1	E	380	ALA	2.0
1	C	204	TYR	2.0
1	F	62	VAL	2.0
1	B	198	GLY	2.0
1	C	440	GLY	2.0
1	D	317	LEU	2.0
1	E	95	LEU	2.0
1	F	357	PHE	2.0
1	A	251	SER	2.0
1	E	442	ASN	2.0
1	C	325	VAL	2.0
1	D	245	GLY	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.