



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:04 PM UTC

PDB ID : 9GYB / pdb_00009gyb
Title : Crystal structure of the recombinant CODH from Rhodospirillum rubrum produced in Escherichia coli
Authors : Cavazza, C.; Contaldo, U.
Deposited on : 2024-10-01
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

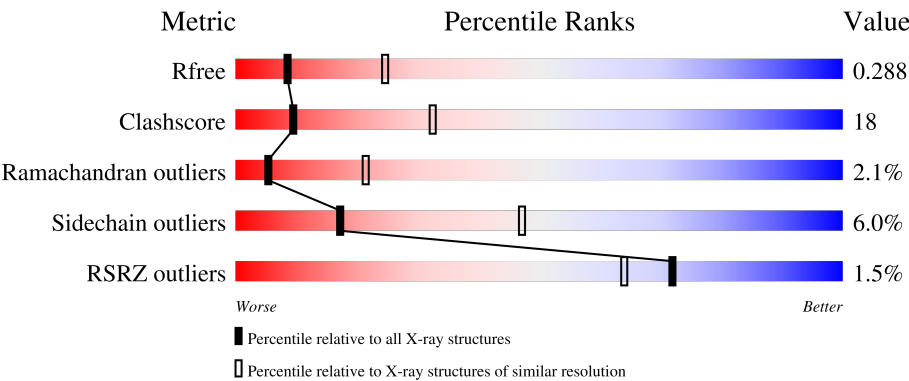
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



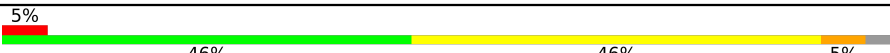
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	639	65%30%.
1	B	639	65%30%.
1	C	639	2% 68%27%.
1	D	639	64%30%.
1	E	639	2% 51%41%.

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Mol	Chain	Length	Quality of chain
1	F	639	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	RQM	A	702	-	-	X	-
3	RQM	B	703	-	-	X	-
3	RQM	E	703	-	-	X	-
3	RQM	F	702	-	-	X	-

2 Entry composition [i](#)

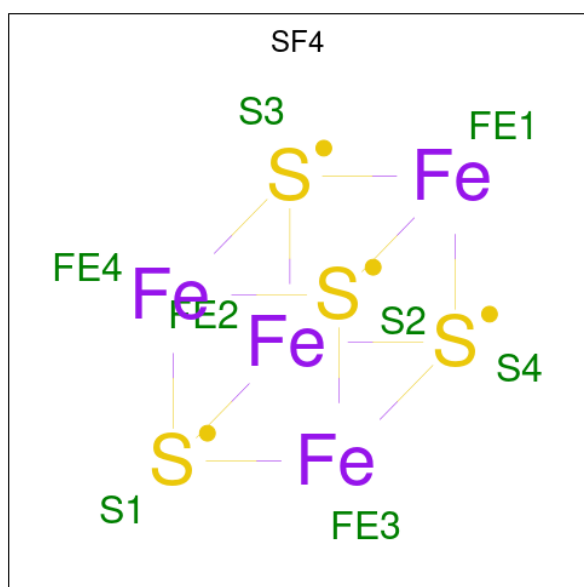
There are 4 unique types of molecules in this entry. The entry contains 27316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carbon monoxide dehydrogenase.

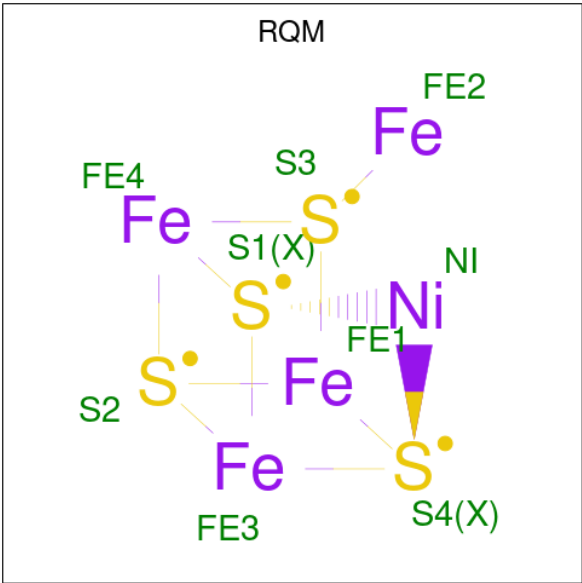
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	B	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	C	620	Total	C	N	O	S	0	0	0
			4538	2845	804	855	34			
1	D	621	Total	C	N	O	S	0	0	0
			4547	2850	805	858	34			
1	E	617	Total	C	N	O	S	0	0	0
			4514	2830	800	851	33			
1	F	617	Total	C	N	O	S	0	0	0
			4514	2830	800	851	33			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	C	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	E	1	Total	Fe	S	0	0
			8	4	4		
2	F	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is Fe(3)-Ni(1)-S(4) cluster (CCD ID: RQM) (formula: Fe₄NiS₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	B	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	C	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	E	1	Total	Fe	Ni	S	0	0
			9	4	1	4		
3	F	1	Total	Fe	Ni	S	0	0
			9	4	1	4		

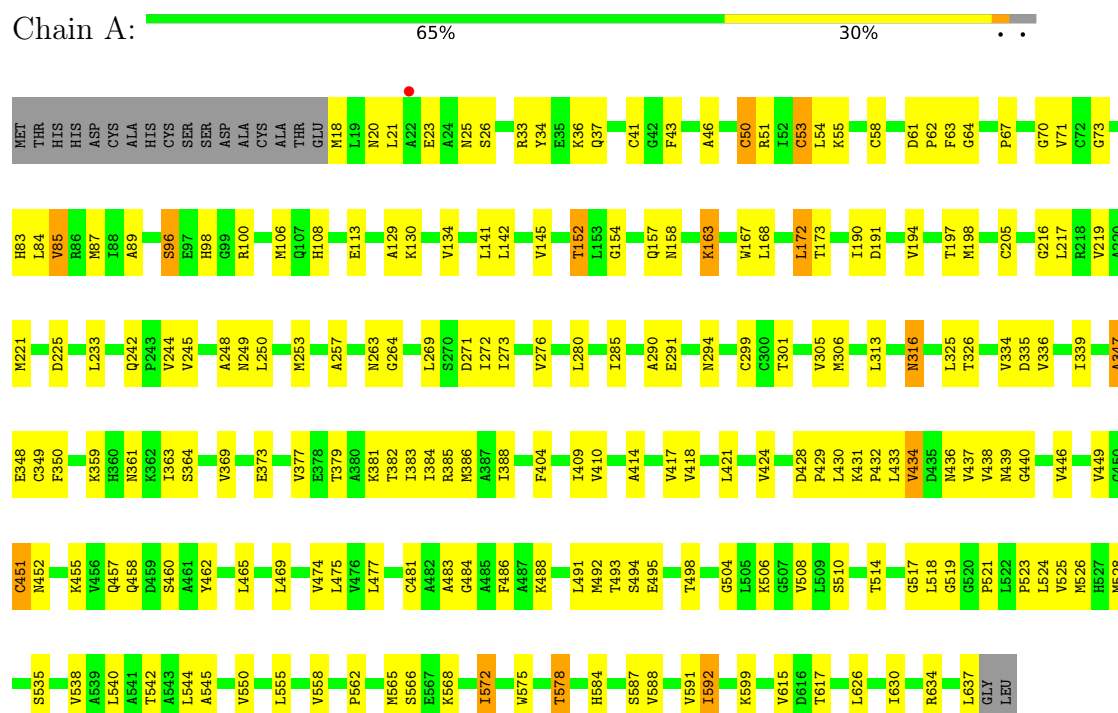
- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Na	0	0
			1	1		

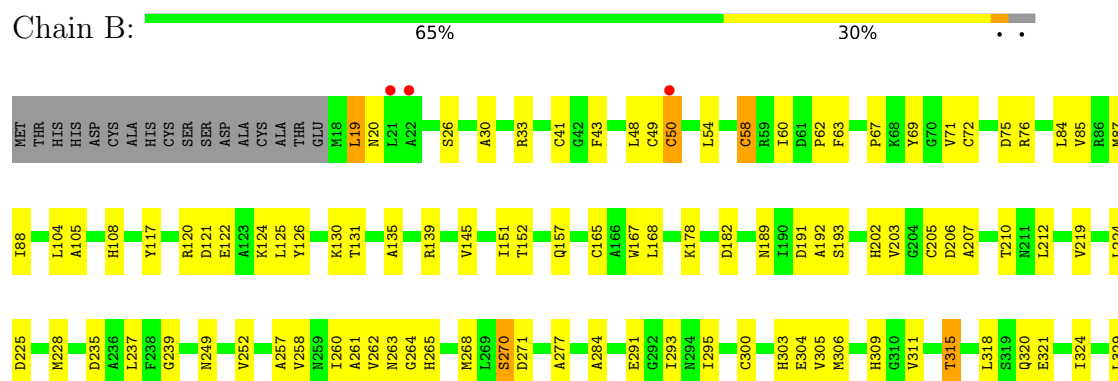
3 Residue-property plots [i](#)

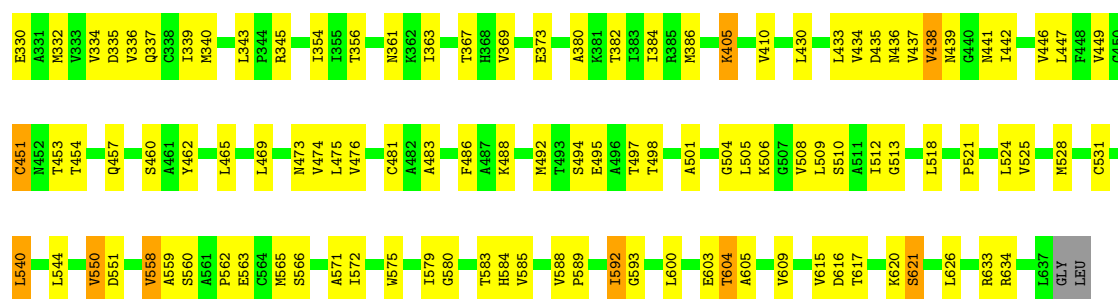
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

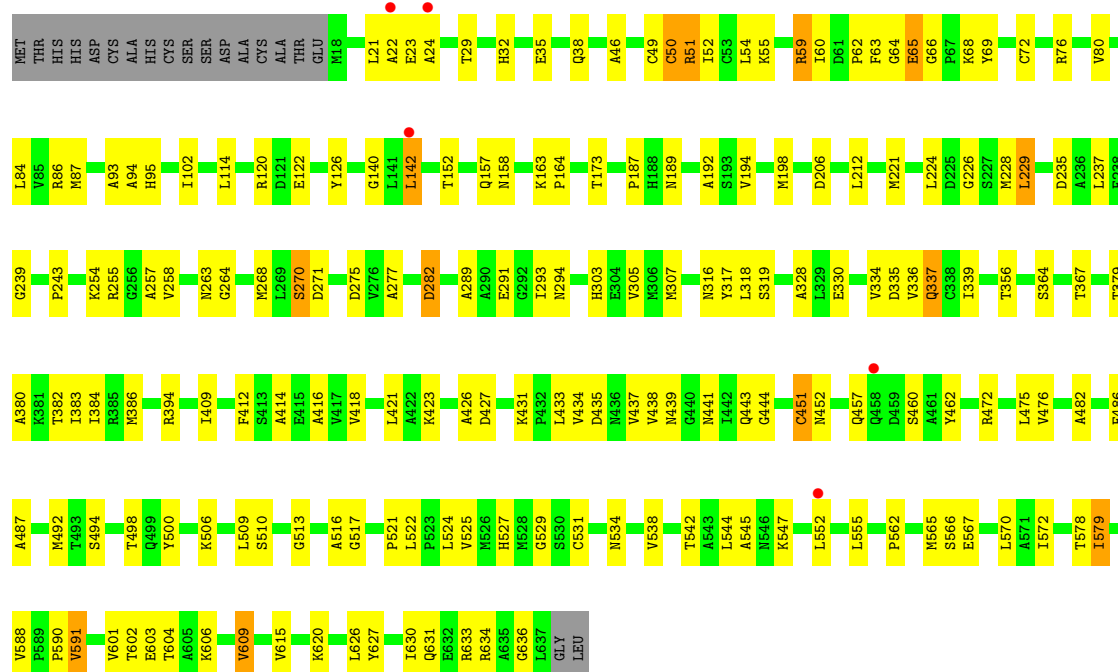


• Molecule 1: Carbon monoxide dehydrogenase

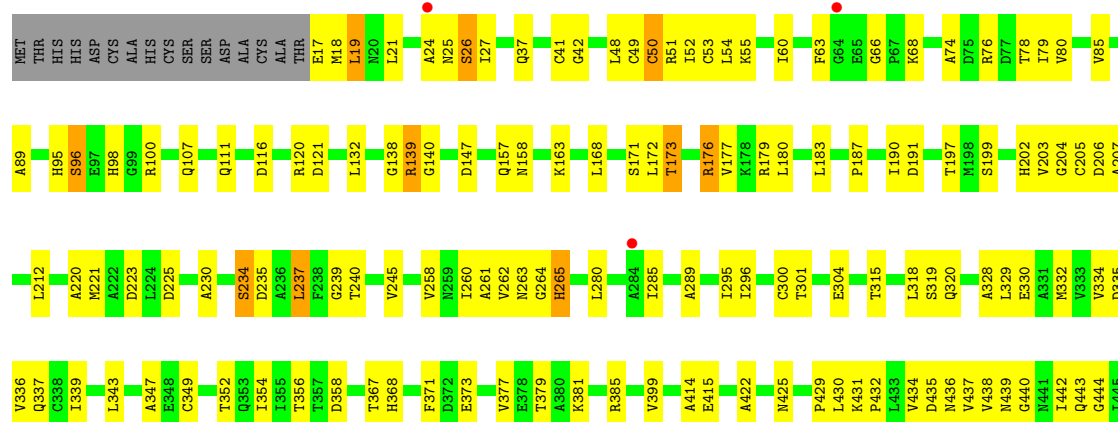


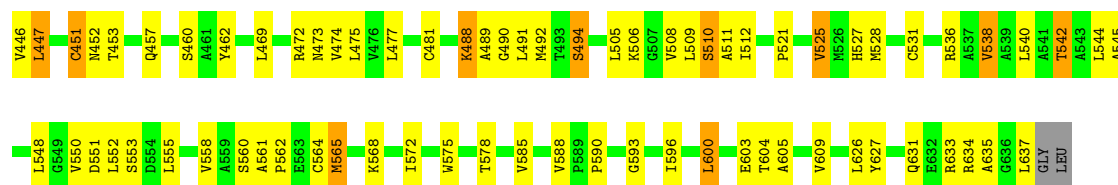


• Molecule 1: Carbon monoxide dehydrogenase

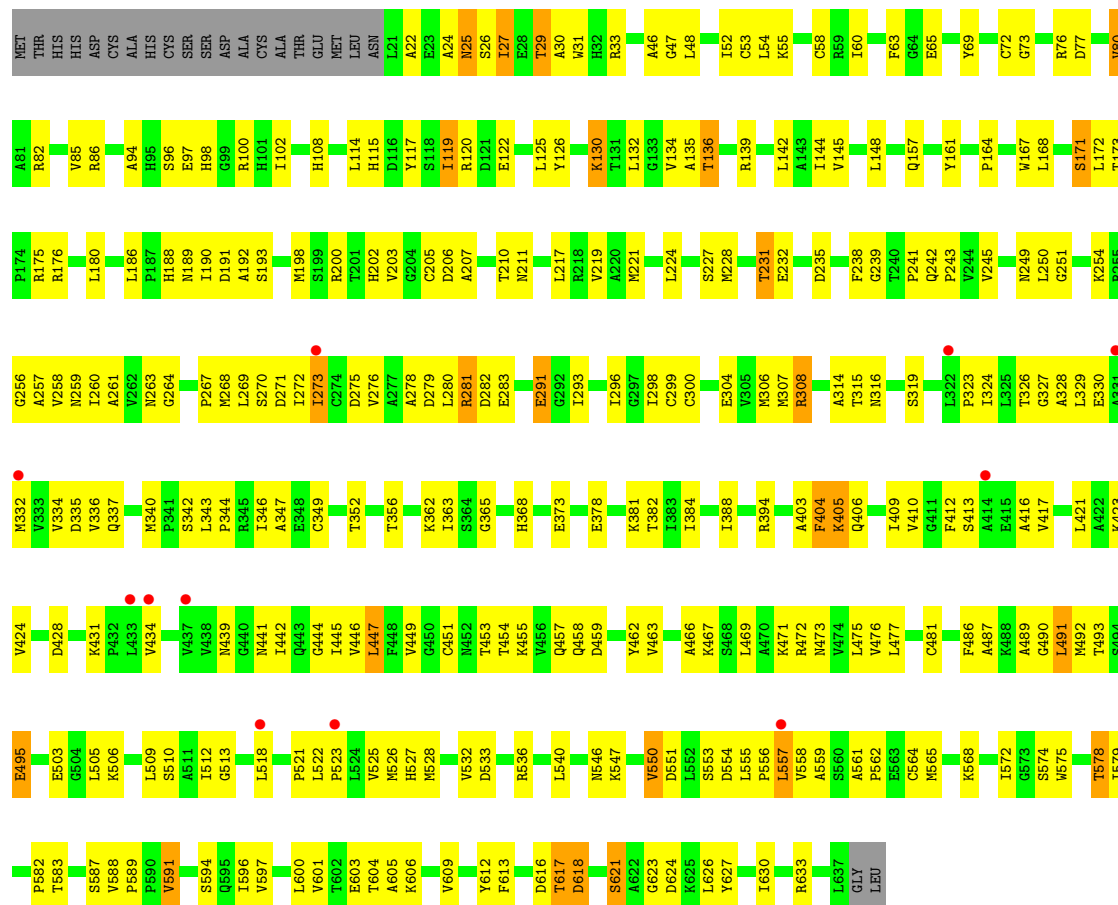


• Molecule 1: Carbon monoxide dehydrogenase

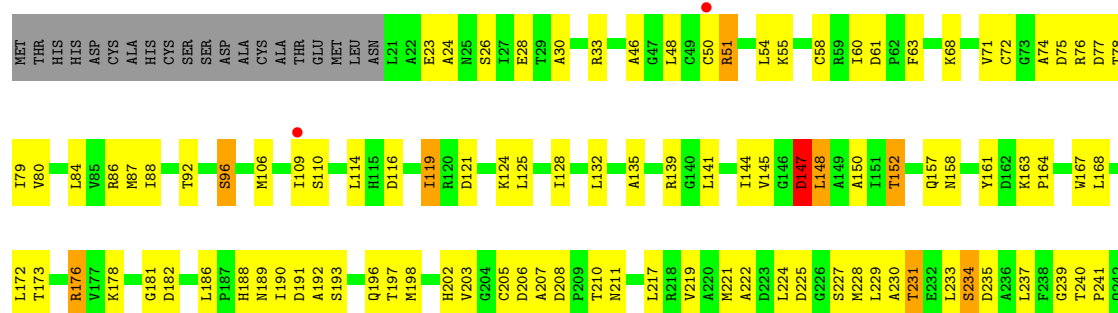




• Molecule 1: Carbon monoxide dehydrogenase



• Molecule 1: Carbon monoxide dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.45Å 200.57Å 116.37Å 90.00° 111.21° 90.00°	Depositor
Resolution (Å)	47.71 – 2.90 47.71 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.71-2.90) 99.1 (47.71-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.227 , 0.288 0.227 , 0.288	Depositor DCC
R_{free} test set	1100 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å ²)	81.6	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27316	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, NA, RQM

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	0.14	0/4611	0.39	0/6265
1	B	0.13	0/4611	0.38	0/6265
1	C	0.13	0/4611	0.38	0/6265
1	D	0.14	0/4620	0.38	0/6277
1	E	0.18	0/4587	0.47	0/6233
1	F	0.22	0/4587	0.53	0/6233
All	All	0.16	0/27627	0.42	0/37538

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	E	0	3
1	F	0	1
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	25	ASN	Peptide
1	E	423	LYS	Peptide
1	E	616	ASP	Peptide
1	F	348	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4538	0	4609	132	0
1	B	4538	0	4608	139	0
1	C	4538	0	4609	128	0
1	D	4547	0	4614	144	0
1	E	4514	0	4582	233	1
1	F	4514	0	4582	281	1
2	A	8	0	0	1	0
2	B	16	0	0	0	0
2	C	16	0	0	0	0
2	D	8	0	0	0	0
2	E	16	0	0	1	0
2	F	8	0	0	0	0
3	A	9	0	0	2	0
3	B	9	0	0	3	0
3	C	9	0	0	1	0
3	D	9	0	0	0	0
3	E	9	0	0	3	0
3	F	9	0	0	2	0
4	D	1	0	0	0	0
All	All	27316	0	27604	985	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (985) 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:503:GLU:HA	1:F:506:LYS:HD2	1.46	0.95
1:F:106:MET:HA	1:F:109:ILE:HG12	1.47	0.93
1:F:318:LEU:HD13	1:F:452:ASN:HB3	1.52	0.89
1:F:230:ALA:O	1:F:234:SER:OG	1.93	0.85
1:F:497:THR:OG1	1:F:522:LEU:O	1.94	0.85
1:F:512:ILE:HG13	1:F:522:LEU:HD11	1.58	0.85
1:E:447:LEU:HD23	1:E:477:LEU:HB2	1.58	0.85
1:D:472:ARG:HB3	1:D:627:TYR:HE1	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:HIS:HD1	1:D:223:ASP:CG	1.85	0.83
1:A:50:CYS:SG	1:A:51:ARG:N	2.52	0.82
1:B:332:MET:HE1	1:B:343:LEU:HD13	1.61	0.82
1:A:63:PHE:HD1	1:A:64:GLY:H	1.27	0.81
1:A:20:ASN:ND2	1:A:249:ASN:OD1	2.15	0.80
1:F:263:ASN:HB3	1:F:334:VAL:HG12	1.65	0.78
1:E:73:GLY:O	1:F:345:ARG:NH2	2.17	0.78
1:F:221:MET:HE2	1:F:578:THR:HB	1.65	0.78
1:F:510:SER:HA	1:F:521:PRO:HA	1.65	0.78
1:A:73:GLY:O	1:B:345:ARG:NH2	2.17	0.78
1:B:437:VAL:O	1:B:634:ARG:NH2	2.18	0.77
1:C:620:LYS:NZ	1:E:349:CYS:HA	1.99	0.76
1:D:176:ARG:NH2	1:D:609:VAL:O	2.18	0.75
1:C:487:ALA:HA	1:C:492:MET:HG3	1.69	0.75
1:E:327:GLY:O	1:E:394:ARG:NH1	2.19	0.75
1:B:262:VAL:HG11	1:B:270:SER:HB3	1.69	0.74
1:E:490:GLY:O	1:E:492:MET:N	2.21	0.74
1:D:230:ALA:O	1:D:234:SER:OG	2.06	0.74
1:F:280:LEU:HD21	1:F:381:LYS:HG2	1.69	0.74
1:F:473:ASN:HA	1:F:505:LEU:HB2	1.70	0.74
1:A:46:ALA:HB2	1:D:63:PHE:HB3	1.69	0.73
1:E:69:TYR:HB2	1:F:33:ARG:HD2	1.70	0.73
1:E:54:LEU:HB2	1:F:565:MET:HA	1.70	0.73
1:B:446:VAL:HG23	1:B:558:VAL:HG12	1.70	0.73
1:A:373:GLU:OE2	1:A:373:GLU:N	2.20	0.73
1:E:356:THR:OG1	1:E:368:HIS:ND1	2.20	0.72
1:B:585:VAL:HG11	1:B:589:PRO:HD3	1.72	0.72
1:F:438:VAL:O	1:F:439:ASN:ND2	2.23	0.72
1:F:190:ILE:HD11	1:F:225:ASP:HB3	1.70	0.72
1:D:139:ARG:NH2	1:D:147:ASP:OD2	2.23	0.71
1:E:210:THR:HG22	1:E:600:LEU:HD11	1.72	0.71
1:E:52:ILE:HG22	1:E:203:VAL:HG13	1.73	0.71
1:C:494:SER:HB3	1:C:521:PRO:HD2	1.73	0.71
1:F:445:ILE:HB	1:F:557:LEU:HD23	1.71	0.71
1:C:620:LYS:HZ1	1:E:349:CYS:HA	1.53	0.70
1:F:269:LEU:HD11	1:F:333:VAL:HG11	1.71	0.70
1:A:377:VAL:HG12	1:A:381:LYS:HE3	1.74	0.70
1:B:258:VAL:HB	1:B:293:ILE:HG22	1.72	0.70
1:E:555:LEU:O	1:E:557:LEU:N	2.25	0.70
1:E:356:THR:HG1	1:E:368:HIS:HD1	1.38	0.70
1:F:410:VAL:HG11	1:F:527:HIS:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:ASP:OD1	1:D:336:VAL:N	2.22	0.69
1:D:603:GLU:O	1:D:605:ALA:N	2.24	0.69
1:A:71:VAL:O	1:B:33:ARG:NH1	2.25	0.69
1:F:259:ASN:ND2	1:F:328:ALA:O	2.22	0.69
1:B:33:ARG:NH2	1:B:321:GLU:OE2	2.26	0.69
1:E:330:GLU:OE2	1:E:394:ARG:NH2	2.22	0.69
1:F:87:MET:HG2	1:F:567:GLU:HG2	1.74	0.69
1:F:276:VAL:HG22	1:F:280:LEU:HD23	1.75	0.69
1:F:167:TRP:CZ2	1:F:233:LEU:HD21	2.26	0.69
1:A:334:VAL:HB	1:A:339:ILE:HD13	1.75	0.68
1:A:428:ASP:HB3	1:A:431:LYS:HB2	1.73	0.68
1:F:501:ALA:HA	1:F:524:LEU:HD22	1.75	0.68
1:F:173:THR:HG23	1:F:176:ARG:HB2	1.74	0.68
1:F:603:GLU:O	1:F:605:ALA:N	2.26	0.68
1:E:337:GLN:HE22	1:E:568:LYS:HD3	1.59	0.68
1:C:54:LEU:HB2	1:D:565:MET:HA	1.76	0.67
1:C:443:GLN:HE22	1:C:631:GLN:HE21	1.40	0.67
1:B:528:MET:HE1	1:B:540:LEU:HD23	1.75	0.67
1:A:550:VAL:HG11	1:A:637:LEU:HD21	1.76	0.67
1:E:251:GLY:HA3	1:E:405:LYS:HG3	1.76	0.67
1:D:265:HIS:NE2	1:D:568:LYS:HE2	2.09	0.67
1:E:235:ASP:HA	1:E:308:ARG:HH12	1.60	0.67
1:E:623:GLY:HA2	1:E:626:LEU:HB2	1.76	0.67
1:E:346:ILE:HD12	1:E:347:ALA:H	1.60	0.67
1:F:74:ALA:HB1	1:F:78:THR:HB	1.75	0.67
1:E:114:LEU:HD11	1:E:373:GLU:HB3	1.76	0.66
1:F:462:TYR:HE2	1:F:562:PRO:HD2	1.58	0.66
1:C:317:TYR:HB3	1:C:452:ASN:HB2	1.78	0.66
1:F:119:ILE:HG21	1:F:141:LEU:HD12	1.77	0.66
1:E:249:ASN:OD1	1:E:250:LEU:N	2.26	0.66
1:C:35:GLU:HA	1:C:38:GLN:HG2	1.76	0.66
1:D:475:LEU:HD13	1:D:509:LEU:HD11	1.77	0.65
1:B:284:ALA:HB2	1:B:293:ILE:HG23	1.77	0.65
1:E:97:GLU:OE1	1:E:100:ARG:NH1	2.29	0.65
1:F:167:TRP:CH2	1:F:233:LEU:HD21	2.31	0.65
1:A:565:MET:HE3	1:A:566:SER:HB3	1.79	0.65
1:D:472:ARG:HB3	1:D:627:TYR:CE1	2.30	0.65
1:A:173:THR:HG23	1:A:542:THR:HG22	1.79	0.65
1:A:306:MET:HE1	1:A:313:LEU:HB2	1.78	0.65
1:D:318:LEU:HD23	1:D:452:ASN:CB	2.27	0.65
1:B:616:ASP:OD2	1:B:621:SER:OG	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:513:GLY:HA3	1:F:522:LEU:HG	1.77	0.65
1:E:82:ARG:NH2	2:E:701:SF4:S1	2.70	0.65
1:F:80:VAL:HG21	1:F:594:SER:HB3	1.78	0.65
1:D:508:VAL:HG12	1:D:512:ILE:HD11	1.79	0.64
1:E:293:ILE:HD13	1:E:384:ILE:HG21	1.79	0.64
1:C:500:TYR:HB2	1:C:524:LEU:HD11	1.78	0.64
1:F:110:SER:HB3	1:F:145:VAL:HG12	1.77	0.64
1:E:273:ILE:HA	1:E:276:VAL:HG22	1.79	0.64
1:F:147:ASP:O	1:F:150:ALA:N	2.31	0.64
1:F:577:VAL:HG21	1:F:613:PHE:HD2	1.61	0.64
1:A:449:VAL:HG11	1:A:572:ILE:HG21	1.78	0.64
1:A:477:LEU:HD23	1:A:526:MET:HB2	1.80	0.64
1:C:258:VAL:HG13	1:C:330:GLU:HG3	1.80	0.64
1:F:315:THR:OG1	1:F:316:ASN:N	2.31	0.64
1:F:152:THR:OG1	1:F:167:TRP:NE1	2.29	0.64
1:C:257:ALA:HB2	1:C:291:GLU:HB2	1.79	0.63
1:F:417:VAL:HG11	1:F:540:LEU:HD11	1.80	0.63
1:E:601:VAL:O	1:E:613:PHE:HB2	1.97	0.63
1:F:229:LEU:O	1:F:233:LEU:HB2	1.99	0.63
1:B:603:GLU:O	1:B:605:ALA:N	2.30	0.63
1:D:469:LEU:HD12	1:D:474:VAL:HG21	1.81	0.63
1:A:36:LYS:HE3	1:B:67:PRO:HA	1.80	0.63
1:C:527:HIS:HD2	1:C:529:GLY:H	1.45	0.63
1:F:491:LEU:HD23	1:F:524:LEU:HD23	1.80	0.63
1:E:446:VAL:HG12	1:E:558:VAL:HG22	1.80	0.63
1:A:510:SER:HA	1:A:521:PRO:HA	1.79	0.63
1:E:451:CYS:HB3	3:E:703:RQM:S2	2.38	0.63
1:F:409:ILE:HD11	1:F:523:PRO:HG3	1.80	0.63
1:A:584:HIS:HB2	1:A:626:LEU:HD21	1.81	0.62
1:F:28:GLU:H	1:F:28:GLU:CD	2.07	0.62
1:F:512:ILE:CG1	1:F:522:LEU:HD11	2.29	0.62
1:E:454:THR:HG21	1:F:71:VAL:HG11	1.82	0.62
1:F:227:SER:O	1:F:231:THR:OG1	2.17	0.62
1:F:328:ALA:HB2	1:F:399:VAL:HG13	1.80	0.62
1:A:62:PRO:HG3	1:D:63:PHE:HE1	1.62	0.62
1:A:498:THR:HG23	1:A:521:PRO:HG3	1.81	0.62
1:C:437:VAL:O	1:C:634:ARG:NH2	2.28	0.62
1:D:318:LEU:HD23	1:D:452:ASN:HB3	1.81	0.62
1:D:627:TYR:HE2	1:D:631:GLN:HE21	1.48	0.62
1:F:544:LEU:HD22	1:F:555:LEU:HD21	1.80	0.62
1:F:612:TYR:CE1	1:F:614:ILE:HD11	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:612:TYR:HE1	1:F:614:ILE:HD11	1.65	0.61
1:B:495:GLU:N	1:B:495:GLU:OE1	2.32	0.61
1:C:63:PHE:HB3	1:F:46:ALA:HB2	1.82	0.61
1:E:335:ASP:OD1	1:E:336:VAL:N	2.31	0.61
1:E:130:LYS:O	1:E:132:LEU:N	2.33	0.61
1:E:572:ILE:HA	1:E:575:TRP:NE1	2.16	0.61
1:F:125:LEU:HD23	1:F:141:LEU:HD13	1.81	0.61
1:F:546:ASN:O	1:F:548:LEU:N	2.33	0.61
1:E:164:PRO:HB3	1:E:186:LEU:HD23	1.81	0.61
1:B:481:CYS:HB2	3:B:703:RQM:S1	2.40	0.61
1:C:102:ILE:HD13	1:C:268:MET:HE2	1.82	0.61
1:D:173:THR:HG23	1:D:176:ARG:HB2	1.82	0.61
1:D:280:LEU:HD21	1:D:385:ARG:HE	1.65	0.61
1:E:315:THR:OG1	1:E:319:SER:OG	2.16	0.61
1:E:603:GLU:O	1:E:605:ALA:N	2.26	0.61
1:A:157:GLN:HB2	1:B:157:GLN:HB2	1.82	0.60
1:D:66:GLY:O	1:D:68:LYS:NZ	2.34	0.60
1:E:86:ARG:HG2	1:E:198:MET:HE1	1.83	0.60
1:E:492:MET:HG3	1:E:525:VAL:HG13	1.83	0.60
1:E:337:GLN:NE2	1:E:568:LYS:HD3	2.16	0.60
1:D:95:HIS:ND1	1:D:223:ASP:OD2	2.35	0.60
1:A:205:CYS:HA	1:B:361:ASN:HD21	1.67	0.60
1:D:437:VAL:O	1:D:634:ARG:NH2	2.33	0.60
1:F:410:VAL:HG22	1:F:412:PHE:CE1	2.35	0.60
1:F:509:LEU:O	1:F:522:LEU:HD12	2.02	0.60
1:A:409:ILE:HG23	1:A:523:PRO:HG3	1.84	0.60
1:B:320:GLN:HG2	1:B:340:MET:HE3	1.84	0.60
1:E:442:ILE:HG22	1:E:505:LEU:HD12	1.84	0.60
1:E:449:VAL:HG23	1:E:561:ALA:HB2	1.83	0.60
1:B:105:ALA:O	1:B:108:HIS:N	2.35	0.60
1:F:48:LEU:HB3	1:F:60:ILE:HB	1.84	0.60
1:F:410:VAL:HG11	1:F:527:HIS:CD2	2.37	0.59
1:B:252:VAL:HG12	1:B:405:LYS:HG3	1.85	0.59
1:F:418:VAL:HA	1:F:421:LEU:HB2	1.85	0.59
1:A:475:LEU:HD11	1:A:526:MET:HE2	1.84	0.59
1:C:226:GLY:HA2	1:C:229:LEU:HD22	1.83	0.59
1:C:426:ALA:O	1:C:427:ASP:HB2	2.01	0.59
1:E:98:HIS:HD1	1:E:532:VAL:HG21	1.67	0.59
1:E:135:ALA:HB3	1:E:139:ARG:HD2	1.84	0.59
1:E:239:GLY:O	1:E:308:ARG:NH1	2.33	0.59
1:E:119:ILE:HD13	1:E:125:LEU:HD13	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:559:ALA:HB3	1:E:583:THR:HG23	1.84	0.59
1:E:27:ILE:HG21	1:E:346:ILE:HD13	1.83	0.59
1:E:142:LEU:HA	1:E:145:VAL:HG12	1.84	0.59
1:F:181:GLY:HA2	1:F:186:LEU:HD13	1.84	0.59
1:F:410:VAL:HG22	1:F:412:PHE:HE1	1.68	0.59
1:D:492:MET:HG2	1:D:525:VAL:HG22	1.85	0.59
1:E:462:TYR:CE1	1:E:562:PRO:HD2	2.38	0.59
1:F:332:MET:HE1	1:F:343:LEU:HD13	1.85	0.59
1:A:336:VAL:HA	1:A:361:ASN:HD22	1.68	0.59
1:E:431:LYS:HA	1:E:434:VAL:HG12	1.85	0.59
1:E:475:LEU:HD22	1:E:476:VAL:H	1.66	0.59
1:A:347:ALA:O	1:A:349:CYS:N	2.36	0.58
1:A:528:MET:HE1	1:A:540:LEU:HD12	1.83	0.58
1:E:336:VAL:HG12	1:E:337:GLN:HG3	1.85	0.58
1:E:329:LEU:O	1:E:352:THR:OG1	2.19	0.58
1:E:558:VAL:HG21	1:E:626:LEU:HD22	1.84	0.58
1:F:259:ASN:HB2	1:F:296:ILE:HD11	1.84	0.58
1:A:572:ILE:HA	1:A:575:TRP:NE1	2.17	0.58
1:D:17:GLU:N	1:D:457:GLN:HG3	2.18	0.58
1:F:444:GLY:HA3	1:F:630:ILE:HD12	1.84	0.58
1:C:49:CYS:O	1:D:51:ARG:NH1	2.35	0.58
1:D:48:LEU:HD21	1:D:593:GLY:HA3	1.86	0.58
1:A:491:LEU:HD23	1:A:524:LEU:HD23	1.83	0.58
1:B:300:CYS:HA	1:B:303:HIS:HD2	1.69	0.58
1:B:451:CYS:SG	1:B:565:MET:HG3	2.44	0.58
1:C:264:GLY:HA3	1:C:335:ASP:OD1	2.02	0.58
1:E:231:THR:HG21	1:E:533:ASP:HA	1.86	0.58
1:F:577:VAL:HG21	1:F:613:PHE:CD2	2.39	0.58
1:A:46:ALA:HA	1:A:592:ILE:HG13	1.86	0.58
1:A:257:ALA:HB2	1:A:291:GLU:HB2	1.85	0.58
1:B:50:CYS:SG	1:B:58:CYS:SG	3.00	0.58
1:B:125:LEU:HD11	1:B:145:VAL:HG22	1.86	0.58
1:E:202:HIS:HB3	1:E:205:CYS:SG	2.44	0.58
1:E:279:ASP:O	1:E:281:ARG:NH1	2.36	0.58
1:F:245:VAL:HG13	1:F:409:ILE:HG22	1.83	0.58
1:B:339:ILE:HD12	1:B:363:ILE:HD11	1.86	0.58
1:E:328:ALA:HA	1:E:394:ARG:NH1	2.18	0.58
1:E:445:ILE:HG22	1:E:475:LEU:HB3	1.83	0.58
1:B:335:ASP:OD1	1:B:336:VAL:N	2.33	0.58
1:B:20:ASN:ND2	1:B:249:ASN:OD1	2.37	0.58
1:E:281:ARG:H	1:E:281:ARG:HD3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:VAL:HG13	1:F:491:LEU:HD11	1.85	0.57
1:C:120:ARG:NH2	1:C:275:ASP:OD2	2.36	0.57
1:E:587:SER:O	1:F:54:LEU:HD11	2.04	0.57
1:D:451:CYS:HA	1:D:481:CYS:HB2	1.87	0.57
1:F:241:PRO:HG2	1:F:413:SER:HB3	1.85	0.57
1:F:336:VAL:HA	1:F:361:ASN:ND2	2.19	0.57
1:F:528:MET:HE3	1:F:528:MET:HA	1.86	0.57
1:C:439:ASN:ND2	1:C:441:ASN:OD1	2.37	0.57
1:D:260:ILE:HB	1:D:295:ILE:HD13	1.86	0.57
1:E:340:MET:O	1:E:343:LEU:HG	2.04	0.57
1:F:421:LEU:HD22	1:F:432:PRO:HG2	1.87	0.57
1:F:606:LYS:NZ	1:F:607:ASP:OD2	2.35	0.57
1:A:498:THR:HA	1:A:506:LYS:HD3	1.86	0.57
1:F:339:ILE:HD11	1:F:363:ILE:HD11	1.87	0.57
1:C:60:ILE:HG21	1:C:76:ARG:HB3	1.87	0.57
1:E:259:ASN:N	1:E:330:GLU:OE1	2.38	0.57
1:F:124:LYS:NZ	1:F:240:THR:OG1	2.27	0.57
1:F:230:ALA:HB3	1:F:532:VAL:HG11	1.86	0.57
1:C:487:ALA:HB2	1:C:492:MET:HE2	1.86	0.57
1:E:256:GLY:C	1:E:291:GLU:HG3	2.30	0.57
1:A:108:HIS:HB3	1:A:113:GLU:HB2	1.86	0.57
1:D:560:SER:HB2	1:D:626:LEU:HD11	1.87	0.56
1:A:285:ILE:HG22	1:A:290:ALA:HA	1.87	0.56
1:B:224:LEU:O	1:B:228:MET:HG3	2.05	0.56
1:B:497:THR:HA	1:B:524:LEU:HD13	1.86	0.56
1:E:621:SER:HA	1:E:624:ASP:HB2	1.86	0.56
1:F:121:ASP:HB2	1:F:239:GLY:HA2	1.86	0.56
1:F:501:ALA:CA	1:F:524:LEU:HD22	2.34	0.56
1:C:95:HIS:HE1	1:C:572:ILE:HD11	1.71	0.56
1:C:423:LYS:NZ	1:C:516:ALA:HA	2.20	0.56
1:E:55:LYS:HA	1:F:455:LYS:HE3	1.87	0.56
1:E:227:SER:O	1:E:231:THR:OG1	2.24	0.56
1:F:233:LEU:O	1:F:237:LEU:HD12	2.06	0.56
1:E:96:SER:HB2	1:E:190:ILE:HG21	1.87	0.56
1:F:28:GLU:N	1:F:28:GLU:OE1	2.37	0.56
1:F:79:ILE:HD12	1:F:79:ILE:H	1.71	0.56
1:B:473:ASN:HA	1:B:505:LEU:HB2	1.88	0.56
1:C:255:ARG:O	1:C:394:ARG:NH2	2.38	0.56
1:E:189:ASN:HB3	1:E:192:ALA:HB3	1.88	0.56
1:D:443:GLN:OE1	1:D:631:GLN:NE2	2.37	0.56
1:F:408:SER:HB3	1:F:492:MET:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LYS:HZ3	1:F:317:TYR:HE2	1.52	0.56
1:E:241:PRO:HD2	1:E:413:SER:HB3	1.86	0.56
1:C:22:ALA:O	1:C:24:ALA:N	2.39	0.56
1:D:265:HIS:CD2	1:D:568:LYS:HZ3	2.24	0.56
1:F:333:VAL:HG22	1:F:355:ILE:HD11	1.88	0.56
1:F:428:ASP:HB3	1:F:431:LYS:HB2	1.88	0.56
1:B:261:ALA:HB3	1:B:332:MET:HG3	1.87	0.56
1:A:263:ASN:HB3	1:A:334:VAL:HG12	1.87	0.56
1:D:414:ALA:HA	1:D:540:LEU:HD11	1.88	0.56
1:E:463:VAL:HG23	1:E:491:LEU:HD11	1.87	0.56
1:A:55:LYS:HG3	1:B:565:MET:HE2	1.87	0.55
1:D:168:LEU:HG	1:D:225:ASP:HB2	1.87	0.55
1:D:442:ILE:HD11	1:D:475:LEU:H	1.71	0.55
1:F:54:LEU:HD13	1:F:54:LEU:O	2.06	0.55
1:F:476:VAL:HG12	1:F:525:VAL:HG13	1.87	0.55
1:C:472:ARG:HD2	1:C:627:TYR:CD2	2.42	0.55
1:E:202:HIS:CE1	1:F:567:GLU:HB2	2.42	0.55
1:C:443:GLN:HE22	1:C:631:GLN:NE2	2.04	0.55
1:F:401:ILE:HD12	1:F:401:ILE:H	1.71	0.55
1:B:580:GLY:O	1:B:633:ARG:NH2	2.37	0.55
1:E:481:CYS:N	3:E:703:RQM:S1	2.65	0.55
1:F:469:LEU:HD22	1:F:474:VAL:HG21	1.88	0.55
1:C:498:THR:HA	1:C:506:LYS:HD3	1.87	0.55
1:D:96:SER:HB2	1:D:190:ILE:HG21	1.89	0.55
1:B:441:ASN:HD22	1:B:504:GLY:HA2	1.72	0.55
1:B:501:ALA:HB1	1:B:505:LEU:HD12	1.87	0.55
1:C:330:GLU:OE2	1:C:394:ARG:NH1	2.38	0.55
1:D:572:ILE:HA	1:D:575:TRP:NE1	2.22	0.55
1:F:124:LYS:HE3	1:F:235:ASP:HB3	1.89	0.55
1:F:555:LEU:O	1:F:557:LEU:N	2.40	0.55
1:F:561:ALA:HB1	1:F:564:CYS:HB3	1.89	0.55
1:E:243:PRO:HD3	1:E:416:ALA:HB1	1.89	0.55
1:F:106:MET:HE2	1:F:237:LEU:HD11	1.89	0.55
1:B:462:TYR:CE1	1:B:562:PRO:HD2	2.41	0.55
1:F:409:ILE:H	1:F:493:THR:HA	1.72	0.55
1:A:62:PRO:HG3	1:D:63:PHE:CE1	2.41	0.54
1:F:583:THR:O	1:F:613:PHE:HB2	2.07	0.54
1:E:421:LEU:HA	1:E:512:ILE:HD11	1.90	0.54
1:F:258:VAL:HG11	1:F:388:ILE:HG22	1.88	0.54
1:B:501:ALA:HB3	1:B:506:LYS:HB2	1.88	0.54
1:C:570:LEU:HD21	1:D:54:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:TRP:O	1:E:171:SER:OG	2.25	0.54
1:B:433:LEU:HD23	1:B:544:LEU:HD13	1.90	0.54
1:D:138:GLY:O	1:D:140:GLY:N	2.41	0.54
1:F:225:ASP:O	1:F:229:LEU:HD23	2.07	0.54
1:F:235:ASP:OD2	1:F:536:ARG:NH1	2.30	0.54
1:C:62:PRO:HG3	1:F:63:PHE:HE2	1.73	0.54
1:F:270:SER:HA	1:F:273:ILE:HG13	1.90	0.54
1:B:62:PRO:HA	1:B:76:ARG:HH21	1.72	0.54
1:C:93:ALA:HB2	1:C:194:VAL:HG21	1.89	0.54
1:D:300:CYS:O	1:D:304:GLU:HG2	2.08	0.54
1:F:75:ASP:O	1:F:78:THR:N	2.41	0.54
1:F:330:GLU:OE2	1:F:394:ARG:NH2	2.33	0.54
1:A:89:ALA:HB2	1:A:197:THR:HG21	1.90	0.54
1:A:301:THR:O	1:A:305:VAL:HG22	2.07	0.54
1:F:264:GLY:HA3	1:F:335:ASP:OD1	2.08	0.54
1:A:363:ILE:HA	1:B:207:ALA:HB3	1.89	0.53
1:D:202:HIS:HB3	1:D:205:CYS:SG	2.47	0.53
1:D:561:ALA:HB1	1:D:564:CYS:HB3	1.89	0.53
1:E:224:LEU:HD22	1:E:579:ILE:HD11	1.90	0.53
1:A:439:ASN:OD1	1:A:440:GLY:N	2.42	0.53
1:A:565:MET:HA	1:B:54:LEU:HB2	1.89	0.53
1:B:206:ASP:HB3	1:B:212:LEU:HD21	1.91	0.53
1:B:324:ILE:HD11	1:B:354:ILE:HD11	1.89	0.53
1:E:492:MET:SD	1:E:527:HIS:HB2	2.48	0.53
1:E:627:TYR:HA	1:E:630:ILE:HG22	1.91	0.53
1:F:334:VAL:HG22	1:F:355:ILE:O	2.08	0.53
1:B:210:THR:HA	1:B:600:LEU:HD11	1.89	0.53
1:F:148:LEU:O	1:F:152:THR:HB	2.09	0.53
1:A:462:TYR:CE1	1:A:562:PRO:HD2	2.44	0.53
1:A:336:VAL:HA	1:A:361:ASN:ND2	2.23	0.53
1:E:114:LEU:HD12	1:E:117:TYR:CD1	2.43	0.53
1:B:121:ASP:HB2	1:B:239:GLY:HA2	1.91	0.53
1:B:270:SER:HB2	1:B:305:VAL:HG11	1.90	0.53
1:B:451:CYS:HA	3:B:703:RQM:S1	2.49	0.53
1:B:584:HIS:HB2	1:B:626:LEU:HD21	1.90	0.53
1:C:80:VAL:O	1:C:84:LEU:HD23	2.09	0.53
1:D:315:THR:HG21	1:D:320:GLN:HA	1.91	0.53
1:D:462:TYR:CE1	1:D:562:PRO:HD2	2.43	0.53
1:D:473:ASN:HA	1:D:505:LEU:HB2	1.91	0.53
1:E:473:ASN:HA	1:E:505:LEU:HB2	1.90	0.53
1:E:513:GLY:O	1:E:518:LEU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:CYS:HB2	3:F:702:RQM:S2	2.36	0.53
1:F:487:ALA:O	1:F:488:LYS:HB3	2.08	0.53
1:A:141:LEU:O	1:A:145:VAL:HG12	2.08	0.53
1:B:566:SER:OG	3:B:703:RQM:S4	2.61	0.53
1:A:483:ALA:HB1	1:A:492:MET:HE1	1.90	0.53
1:B:189:ASN:HB3	1:B:192:ALA:HB3	1.90	0.53
1:E:362:LYS:HD2	1:E:363:ILE:N	2.24	0.53
1:A:248:ALA:HB1	1:A:488:LYS:HG2	1.91	0.52
1:D:439:ASN:OD1	1:D:440:GLY:N	2.42	0.52
1:F:176:ARG:NH2	1:F:609:VAL:O	2.41	0.52
1:B:202:HIS:HB3	1:B:205:CYS:SG	2.49	0.52
1:C:157:GLN:HB2	1:D:157:GLN:HB2	1.92	0.52
1:D:50:CYS:HB2	1:D:79:ILE:HG23	1.91	0.52
1:A:64:GLY:HA3	1:D:42:GLY:HA2	1.91	0.52
1:B:508:VAL:O	1:B:512:ILE:HD12	2.10	0.52
1:C:69:TYR:O	1:D:37:GLN:NE2	2.43	0.52
1:C:544:LEU:HD23	1:C:555:LEU:HD13	1.90	0.52
1:D:446:VAL:HG23	1:D:558:VAL:HG23	1.91	0.52
1:D:53:CYS:HB3	1:D:203:VAL:CG2	2.39	0.52
1:F:116:ASP:OD2	1:F:376:ALA:N	2.40	0.52
1:F:260:ILE:HD13	1:F:331:ALA:HB3	1.91	0.52
1:E:477:LEU:HA	1:E:525:VAL:O	2.09	0.52
1:F:75:ASP:O	1:F:77:ASP:N	2.43	0.52
1:F:106:MET:HE1	1:F:233:LEU:HB3	1.92	0.52
1:F:584:HIS:HB2	1:F:626:LEU:HD21	1.92	0.52
1:B:48:LEU:HB3	1:B:60:ILE:HB	1.92	0.52
1:D:538:VAL:O	1:D:542:THR:OG1	2.27	0.52
1:A:517:GLY:C	1:A:519:GLY:H	2.18	0.52
1:B:572:ILE:HA	1:B:575:TRP:NE1	2.25	0.52
1:E:250:LEU:HB2	1:E:404:PHE:HD2	1.74	0.52
1:F:258:VAL:HG21	1:F:293:ILE:HD13	1.92	0.52
1:A:96:SER:HB2	1:A:190:ILE:HG21	1.92	0.51
1:E:503:GLU:HA	1:E:506:LYS:HG2	1.93	0.51
1:A:54:LEU:HD13	1:B:87:MET:HE1	1.90	0.51
1:C:527:HIS:CD2	1:C:529:GLY:H	2.26	0.51
1:D:180:LEU:HD21	1:D:609:VAL:HG23	1.92	0.51
1:E:406:GLN:HE21	1:E:490:GLY:HA2	1.76	0.51
1:F:572:ILE:HA	1:F:575:TRP:NE1	2.25	0.51
1:B:382:THR:O	1:B:386:MET:HG3	2.10	0.51
1:E:257:ALA:HB2	1:E:291:GLU:HB2	1.92	0.51
1:E:555:LEU:C	1:E:633:ARG:HD3	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:ILE:HG12	1:F:222:ALA:HB1	1.91	0.51
1:F:243:PRO:HD3	1:F:416:ALA:HB1	1.92	0.51
1:F:272:ILE:O	1:F:276:VAL:HG12	2.11	0.51
1:B:263:ASN:O	1:B:334:VAL:HA	2.10	0.51
1:B:300:CYS:O	1:B:304:GLU:HG2	2.10	0.51
1:D:494:SER:HB3	1:D:521:PRO:HD2	1.92	0.51
1:E:76:ARG:HH11	1:E:594:SER:HA	1.75	0.51
1:E:324:ILE:HG21	1:E:347:ALA:HB2	1.91	0.51
1:B:260:ILE:HB	1:B:295:ILE:HG22	1.92	0.51
1:E:476:VAL:HG13	1:E:525:VAL:HA	1.93	0.51
1:A:54:LEU:HD11	1:B:589:PRO:HA	1.93	0.51
1:B:513:GLY:O	1:B:518:LEU:HB2	2.11	0.51
1:F:260:ILE:HG23	1:F:295:ILE:HD13	1.92	0.51
1:F:403:ALA:O	1:F:405:LYS:N	2.44	0.51
1:F:505:LEU:HA	1:F:508:VAL:HG22	1.92	0.51
1:F:597:VAL:O	1:F:601:VAL:HG22	2.10	0.51
1:A:41:CYS:SG	1:A:43:PHE:HB2	2.51	0.51
1:A:382:THR:O	1:A:386:MET:HG3	2.11	0.51
1:B:277:ALA:HA	1:B:293:ILE:HD11	1.93	0.51
1:D:447:LEU:HD23	1:D:477:LEU:HB2	1.92	0.51
1:E:33:ARG:NH2	1:F:71:VAL:O	2.34	0.51
1:F:335:ASP:OD1	1:F:336:VAL:N	2.41	0.51
1:A:37:GLN:NE2	1:B:69:TYR:O	2.44	0.51
1:E:617:THR:OG1	1:E:618:ASP:N	2.42	0.51
1:F:258:VAL:CG2	1:F:293:ILE:HD13	2.41	0.51
1:A:630:ILE:O	1:A:634:ARG:HG3	2.10	0.50
1:C:603:GLU:OE1	1:C:606:LYS:NZ	2.43	0.50
1:B:336:VAL:HA	1:B:361:ASN:ND2	2.27	0.50
1:E:206:ASP:OD1	1:E:211:ASN:ND2	2.43	0.50
1:F:158:ASN:HD21	1:F:163:LYS:HB3	1.77	0.50
1:B:152:THR:OG1	1:B:167:TRP:NE1	2.40	0.50
1:B:483:ALA:HB1	1:B:492:MET:HE1	1.93	0.50
1:D:381:LYS:O	1:D:385:ARG:HG2	2.10	0.50
1:D:506:LYS:O	1:D:510:SER:OG	2.20	0.50
1:F:269:LEU:HD23	1:F:371:PHE:CD2	2.47	0.50
1:C:235:ASP:O	1:C:239:GLY:N	2.38	0.50
1:E:180:LEU:HD12	1:E:180:LEU:H	1.76	0.50
1:F:355:ILE:HA	1:F:367:THR:O	2.12	0.50
1:A:335:ASP:OD1	1:A:336:VAL:N	2.34	0.50
1:B:498:THR:HA	1:B:506:LYS:HE2	1.94	0.50
1:C:51:ARG:NH1	1:D:49:CYS:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:CYS:SG	1:D:52:ILE:HD12	2.52	0.50
1:E:136:THR:HA	1:E:144:ILE:HG12	1.93	0.50
1:F:392:GLY:C	1:F:393:ARG:HD2	2.37	0.50
1:B:261:ALA:HB2	1:B:329:LEU:HD11	1.94	0.50
1:C:303:HIS:O	1:C:307:MET:HG2	2.12	0.50
1:D:235:ASP:O	1:D:239:GLY:N	2.39	0.50
1:A:152:THR:OG1	1:A:167:TRP:NE1	2.39	0.50
1:F:78:THR:HG23	1:F:207:ALA:HA	1.93	0.50
1:F:443:GLN:O	1:F:474:VAL:HA	2.11	0.50
1:A:436:ASN:HA	1:A:439:ASN:ND2	2.26	0.50
1:B:41:CYS:SG	1:B:43:PHE:HB2	2.52	0.50
1:E:55:LYS:NZ	1:F:317:TYR:HE2	2.10	0.50
1:F:577:VAL:HG13	1:F:612:TYR:N	2.27	0.50
1:B:193:SER:HB3	1:B:219:VAL:HG23	1.93	0.50
1:B:592:ILE:HD12	1:E:63:PHE:HA	1.93	0.50
1:D:328:ALA:HB2	1:D:399:VAL:HG13	1.93	0.50
1:F:281:ARG:O	1:F:285:ILE:HD12	2.11	0.50
1:B:124:LYS:NZ	1:B:235:ASP:OD2	2.36	0.49
1:D:332:MET:HE3	1:D:343:LEU:HD22	1.94	0.49
1:E:47:GLY:HA2	1:F:51:ARG:NH2	2.27	0.49
1:E:200:ARG:HH21	1:F:360:HIS:HA	1.76	0.49
1:E:254:LYS:N	1:E:259:ASN:HD21	2.10	0.49
1:F:327:GLY:HA3	1:F:398:ARG:O	2.11	0.49
1:E:202:HIS:ND1	1:F:567:GLU:OE1	2.41	0.49
1:F:507:GLY:O	1:F:510:SER:OG	2.26	0.49
1:B:380:ALA:O	1:B:384:ILE:HD12	2.13	0.49
1:C:94:ALA:HA	1:D:199:SER:HB2	1.94	0.49
1:B:453:THR:HG22	1:B:563:GLU:HB3	1.93	0.49
1:A:106:MET:HE2	1:A:233:LEU:HD22	1.93	0.49
1:F:493:THR:H	1:F:496:ALA:HB2	1.77	0.49
1:A:157:GLN:HB2	1:B:157:GLN:CB	2.43	0.49
1:B:75:ASP:OD1	1:B:75:ASP:N	2.39	0.49
1:C:475:LEU:HD12	1:C:476:VAL:H	1.77	0.49
1:D:431:LYS:HE3	1:D:435:ASP:OD1	2.13	0.49
1:C:431:LYS:NZ	1:C:435:ASP:OD2	2.39	0.49
1:F:307:MET:HE2	1:F:529:GLY:HA2	1.95	0.49
1:A:306:MET:CE	1:A:313:LEU:HB2	2.41	0.49
1:C:339:ILE:H	1:D:204:GLY:HA3	1.78	0.49
1:D:116:ASP:CG	1:D:377:VAL:HG23	2.37	0.49
1:A:545:ALA:HB2	1:A:555:LEU:HD11	1.95	0.49
1:B:120:ARG:NH2	1:B:271:ASP:OD1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:HD13	1:B:509:LEU:HD21	1.94	0.49
1:C:542:THR:HA	1:C:552:LEU:HD21	1.94	0.49
1:E:29:THR:HG23	1:E:31:TRP:H	1.77	0.49
1:E:486:PHE:HB3	1:E:525:VAL:HG11	1.94	0.49
1:F:193:SER:O	1:F:197:THR:OG1	2.30	0.49
1:A:272:ILE:O	1:A:276:VAL:HG23	2.13	0.49
1:E:509:LEU:HG	1:E:522:LEU:HB2	1.95	0.49
1:F:152:THR:HG23	1:F:229:LEU:HD13	1.94	0.49
1:F:494:SER:O	1:F:521:PRO:HG2	2.13	0.49
1:F:596:ILE:HD12	1:F:596:ILE:H	1.78	0.49
1:A:190:ILE:HD11	1:A:225:ASP:OD2	2.13	0.48
1:C:451:CYS:HB2	3:C:703:RQM:S2	2.52	0.48
1:C:513:GLY:HA3	1:C:521:PRO:HA	1.94	0.48
1:E:486:PHE:CD2	1:E:525:VAL:HG21	2.47	0.48
1:F:84:LEU:O	1:F:88:ILE:HG13	2.13	0.48
1:F:409:ILE:O	1:F:410:VAL:HB	2.11	0.48
1:F:434:VAL:O	1:F:438:VAL:HG23	2.13	0.48
1:F:451:CYS:HB2	1:F:452:ASN:H	1.50	0.48
1:A:249:ASN:HB3	1:A:404:PHE:O	2.12	0.48
1:C:243:PRO:HD3	1:C:416:ALA:HB1	1.95	0.48
1:D:492:MET:SD	1:D:527:HIS:HB2	2.53	0.48
1:E:157:GLN:HB2	1:F:157:GLN:HB3	1.94	0.48
1:E:202:HIS:HE1	1:F:567:GLU:HB2	1.77	0.48
1:F:86:ARG:HD3	1:F:198:MET:HE1	1.95	0.48
1:B:550:VAL:HG22	1:B:551:ASP:H	1.78	0.48
1:E:403:ALA:O	1:E:405:LYS:N	2.45	0.48
1:E:589:PRO:O	1:E:591:VAL:N	2.40	0.48
1:A:34:TYR:HA	1:B:71:VAL:HG22	1.94	0.48
1:B:508:VAL:HG22	1:B:512:ILE:HD11	1.94	0.48
1:C:318:LEU:HG	1:C:452:ASN:HB3	1.94	0.48
1:C:634:ARG:C	1:C:636:GLY:H	2.20	0.48
1:D:551:ASP:OD1	1:D:552:LEU:N	2.46	0.48
1:F:193:SER:HB3	1:F:219:VAL:HG23	1.95	0.48
1:F:253:MET:HB3	1:F:259:ASN:HD22	1.79	0.48
1:F:273:ILE:HA	1:F:276:VAL:HG12	1.94	0.48
1:A:421:LEU:HD23	1:A:432:PRO:HB2	1.95	0.48
1:E:323:PRO:O	1:E:326:THR:OG1	2.30	0.48
1:E:550:VAL:HG12	1:E:551:ASP:H	1.78	0.48
1:F:462:TYR:CE1	1:F:482:ALA:HA	2.48	0.48
1:C:509:LEU:HG	1:C:522:LEU:HB2	1.94	0.48
1:F:462:TYR:CE2	1:F:562:PRO:HD2	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:PHE:HA	1:F:592:ILE:HD12	1.95	0.48
1:D:462:TYR:HE1	1:D:562:PRO:HD2	1.77	0.48
1:D:627:TYR:HE2	1:D:631:GLN:NE2	2.09	0.48
1:E:168:LEU:HD13	1:E:172:LEU:HD21	1.95	0.48
1:E:442:ILE:HG13	1:E:442:ILE:O	2.14	0.48
1:F:561:ALA:N	1:F:584:HIS:O	2.27	0.48
1:B:560:SER:HB2	1:B:626:LEU:HD11	1.94	0.48
1:D:100:ARG:NH2	1:D:191:ASP:OD1	2.47	0.48
1:D:202:HIS:CG	1:D:203:VAL:H	2.32	0.48
1:F:206:ASP:OD2	1:F:211:ASN:ND2	2.44	0.48
1:E:24:ALA:C	1:E:26:SER:H	2.22	0.48
1:E:447:LEU:HD13	1:E:449:VAL:HG13	1.96	0.48
1:E:568:LYS:NZ	3:E:703:RQM:S4	2.83	0.48
1:F:351:HIS:O	1:F:352:THR:OG1	2.27	0.48
1:E:29:THR:HG23	1:E:30:ALA:N	2.29	0.48
1:F:30:ALA:HB2	1:F:340:MET:HE1	1.96	0.48
1:C:337:GLN:HG3	1:D:205:CYS:SG	2.54	0.47
1:E:384:ILE:O	1:E:388:ILE:HG12	2.14	0.47
1:F:106:MET:HB2	1:F:106:MET:HE3	1.70	0.47
1:F:410:VAL:HG11	1:F:527:HIS:HD2	1.77	0.47
1:B:436:ASN:HA	1:B:439:ASN:HD21	1.79	0.47
1:C:380:ALA:O	1:C:384:ILE:HG13	2.13	0.47
1:C:486:PHE:HB3	1:C:525:VAL:HG21	1.96	0.47
1:C:566:SER:HB2	1:D:202:HIS:CE1	2.50	0.47
1:F:276:VAL:HG11	1:F:380:ALA:HB1	1.96	0.47
1:B:117:TYR:OH	1:B:268:MET:O	2.25	0.47
1:C:120:ARG:NH1	1:C:271:ASP:OD1	2.47	0.47
1:C:189:ASN:HB3	1:C:192:ALA:HB3	1.97	0.47
1:C:335:ASP:CG	1:C:336:VAL:H	2.23	0.47
1:E:108:HIS:HB3	1:E:114:LEU:HD23	1.95	0.47
1:E:439:ASN:HD22	1:E:441:ASN:H	1.62	0.47
1:C:492:MET:HE1	1:C:527:HIS:HB2	1.96	0.47
1:E:306:MET:HG2	1:E:410:VAL:HG21	1.96	0.47
1:E:597:VAL:O	1:E:601:VAL:HG22	2.15	0.47
1:A:517:GLY:O	1:A:519:GLY:N	2.47	0.47
1:B:306:MET:HE2	1:B:410:VAL:HG11	1.97	0.47
1:E:509:LEU:HD21	1:E:523:PRO:O	2.13	0.47
1:C:66:GLY:H	1:C:68:LYS:HE2	1.79	0.47
1:C:435:ASP:O	1:C:438:VAL:HG12	2.15	0.47
1:E:221:MET:SD	1:E:578:THR:OG1	2.73	0.47
1:E:575:TRP:HA	1:E:578:THR:HG23	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:125:LEU:HD22	1:F:145:VAL:HG23	1.96	0.47
1:F:257:ALA:HA	1:F:289:ALA:HB1	1.97	0.47
1:A:33:ARG:NH1	1:B:71:VAL:O	2.48	0.47
1:A:205:CYS:HA	1:B:361:ASN:ND2	2.30	0.47
1:B:167:TRP:HB3	1:B:228:MET:HE3	1.97	0.47
1:C:334:VAL:HG23	1:C:356:THR:HA	1.96	0.47
1:D:158:ASN:HD21	1:D:163:LYS:HB3	1.78	0.47
1:E:102:ILE:HG13	1:E:268:MET:SD	2.54	0.47
1:E:205:CYS:SG	1:F:337:GLN:HA	2.55	0.47
1:F:564:CYS:HB2	1:F:569:ALA:HB1	1.96	0.47
1:C:462:TYR:HE1	1:C:562:PRO:HD2	1.80	0.47
1:D:89:ALA:HB2	1:D:197:THR:HG21	1.97	0.47
1:D:436:ASN:HA	1:D:439:ASN:ND2	2.30	0.47
1:E:122:GLU:O	1:E:126:TYR:HD2	1.97	0.47
1:E:238:PHE:HB2	1:E:308:ARG:HD2	1.96	0.47
1:E:272:ILE:O	1:E:275:ASP:HB3	2.15	0.47
1:E:458:GLN:O	1:E:458:GLN:HG2	2.15	0.47
1:F:77:ASP:OD1	1:F:596:ILE:HD13	2.15	0.47
1:F:545:ALA:HB1	1:F:550:VAL:O	2.14	0.47
1:B:451:CYS:HA	1:B:481:CYS:HB2	1.96	0.47
1:E:77:ASP:OD1	1:E:594:SER:OG	2.33	0.47
1:E:409:ILE:HG12	1:E:492:MET:O	2.15	0.47
1:A:54:LEU:HB3	1:B:565:MET:HA	1.97	0.46
1:B:305:VAL:HG23	1:B:311:VAL:HB	1.97	0.46
1:E:378:GLU:OE1	1:E:378:GLU:N	2.37	0.46
1:F:497:THR:O	1:F:506:LYS:HE3	2.15	0.46
1:A:385:ARG:HA	1:A:388:ILE:HG12	1.97	0.46
1:C:334:VAL:HB	1:C:339:ILE:HD13	1.96	0.46
1:C:379:THR:O	1:C:383:ILE:HG12	2.15	0.46
1:F:463:VAL:HG12	1:F:467:LYS:HE2	1.98	0.46
1:C:282:ASP:OD1	1:C:282:ASP:N	2.43	0.46
1:D:264:GLY:C	1:D:301:THR:HB	2.40	0.46
1:E:47:GLY:O	1:E:80:VAL:HG12	2.15	0.46
1:E:344:PRO:HB3	1:E:365:GLY:C	2.40	0.46
1:F:68:LYS:O	1:F:68:LYS:HG3	2.14	0.46
1:F:335:ASP:CG	1:F:336:VAL:H	2.22	0.46
1:F:409:ILE:HD11	1:F:523:PRO:CG	2.46	0.46
1:A:264:GLY:HA3	1:A:335:ASP:OD1	2.15	0.46
1:B:49:CYS:SG	1:B:50:CYS:N	2.88	0.46
1:C:50:CYS:SG	1:C:52:ILE:HG13	2.55	0.46
1:C:254:LYS:HB2	1:C:257:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ALA:HB2	1:D:329:LEU:HD11	1.96	0.46
1:D:371:PHE:HA	1:D:379:THR:HG21	1.98	0.46
1:E:94:ALA:HB1	1:E:337:GLN:NE2	2.31	0.46
1:E:624:ASP:HA	1:E:627:TYR:CZ	2.50	0.46
1:F:609:VAL:C	1:F:611:GLY:H	2.22	0.46
1:C:476:VAL:HG11	1:C:525:VAL:HG12	1.97	0.46
1:E:120:ARG:NH1	1:E:271:ASP:OD1	2.47	0.46
1:F:161:TYR:HA	1:F:188:HIS:CG	2.51	0.46
1:F:317:TYR:HB2	3:F:702:RQM:S2	2.56	0.46
1:F:430:LEU:O	1:F:434:VAL:HG12	2.16	0.46
1:A:194:VAL:O	1:A:198:MET:HG2	2.15	0.46
1:A:484:GLY:O	1:A:488:LYS:HG3	2.16	0.46
1:B:19:LEU:HG	1:B:20:ASN:H	1.81	0.46
1:C:457:GLN:HB2	1:C:460:SER:OG	2.16	0.46
1:F:379:THR:O	1:F:383:ILE:HG12	2.16	0.46
1:F:486:PHE:CD1	1:F:525:VAL:HG11	2.50	0.46
1:D:347:ALA:C	1:D:349:CYS:H	2.24	0.46
1:E:428:ASP:HB3	1:E:431:LYS:HB2	1.97	0.46
1:F:446:VAL:HG12	1:F:476:VAL:HA	1.96	0.46
1:A:446:VAL:HG23	1:A:558:VAL:HG12	1.97	0.46
1:D:329:LEU:O	1:D:352:THR:OG1	2.26	0.46
1:E:207:ALA:HB3	1:F:363:ILE:HG23	1.97	0.46
1:F:327:GLY:HA2	1:F:350:PHE:CD1	2.50	0.46
1:F:602:THR:O	1:F:612:TYR:HB2	2.15	0.46
1:A:142:LEU:HA	1:A:145:VAL:CG1	2.46	0.46
1:A:154:GLY:HA2	1:A:157:GLN:HG2	1.97	0.46
1:D:85:VAL:HG12	1:D:197:THR:HG23	1.97	0.46
1:E:454:THR:HG22	1:F:55:LYS:HG2	1.98	0.46
1:E:555:LEU:O	1:E:633:ARG:HD3	2.16	0.46
1:B:579:ILE:HD13	1:B:579:ILE:HA	1.81	0.45
1:F:124:LYS:HE2	1:F:124:LYS:HB2	1.49	0.45
1:A:158:ASN:HD21	1:A:163:LYS:HB3	1.81	0.45
1:A:535:SER:HA	1:A:538:VAL:HG22	1.98	0.45
1:D:472:ARG:HD2	1:D:627:TYR:CD1	2.52	0.45
1:E:263:ASN:O	1:E:334:VAL:HA	2.16	0.45
1:F:132:LEU:HD23	1:F:132:LEU:HA	1.81	0.45
1:F:443:GLN:O	1:F:474:VAL:HG12	2.16	0.45
1:A:129:ALA:HB1	1:A:134:VAL:HB	1.98	0.45
1:A:481:CYS:CB	3:A:702:RQM:S1	3.04	0.45
1:B:373:GLU:CD	1:B:373:GLU:H	2.24	0.45
1:F:471:LYS:HA	1:F:502:GLY:HA3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:LEU:O	1:A:434:VAL:HG12	2.17	0.45
1:B:19:LEU:HG	1:B:20:ASN:N	2.31	0.45
1:C:114:LEU:HD23	1:C:114:LEU:HA	1.85	0.45
1:D:356:THR:OG1	1:D:368:HIS:ND1	2.38	0.45
1:D:508:VAL:O	1:D:512:ILE:HD12	2.15	0.45
1:B:264:GLY:HA3	1:B:335:ASP:OD1	2.16	0.45
1:C:54:LEU:HD21	1:D:590:PRO:HD3	1.98	0.45
1:C:552:LEU:HD12	1:C:579:ILE:CG2	2.47	0.45
1:E:180:LEU:HB2	1:E:186:LEU:CD1	2.45	0.45
1:F:202:HIS:HB3	1:F:205:CYS:SG	2.56	0.45
1:A:494:SER:HB3	1:A:521:PRO:HD2	1.99	0.45
1:C:601:VAL:HG23	1:C:602:THR:HG23	1.97	0.45
1:D:78:THR:OG1	1:D:207:ALA:O	2.32	0.45
1:E:193:SER:HB3	1:E:219:VAL:HG23	1.98	0.45
1:F:324:ILE:HG23	1:F:325:LEU:HD23	1.98	0.45
1:A:433:LEU:O	1:A:437:VAL:HG23	2.16	0.45
1:A:544:LEU:HD23	1:A:555:LEU:HD13	1.99	0.45
1:B:434:VAL:O	1:B:438:VAL:HG22	2.16	0.45
1:E:217:LEU:HD13	1:E:578:THR:HG22	1.98	0.45
1:F:273:ILE:HA	1:F:276:VAL:CG1	2.46	0.45
1:F:601:VAL:HB	1:F:613:PHE:CE2	2.51	0.45
1:A:306:MET:HG2	1:A:410:VAL:HG21	1.99	0.45
1:C:270:SER:HB2	1:C:305:VAL:HG11	1.99	0.45
1:D:422:ALA:HA	1:D:425:ASN:C	2.41	0.45
1:F:260:ILE:HD11	1:F:333:VAL:HG23	1.98	0.45
1:F:498:THR:HA	1:F:506:LYS:HE2	1.98	0.45
1:F:577:VAL:O	1:F:611:GLY:HA3	2.16	0.45
1:A:421:LEU:HB3	1:A:429:PRO:O	2.17	0.45
1:D:53:CYS:HB3	1:D:203:VAL:HG22	1.98	0.45
1:D:53:CYS:SG	1:D:55:LYS:HB2	2.56	0.45
1:E:269:LEU:O	1:E:273:ILE:HG22	2.17	0.45
1:E:315:THR:HG21	1:E:319:SER:O	2.16	0.45
1:E:606:LYS:HB3	1:E:612:TYR:CD2	2.52	0.45
1:C:87:MET:O	1:C:567:GLU:HB3	2.17	0.45
1:C:382:THR:O	1:C:386:MET:HG3	2.17	0.45
1:D:508:VAL:O	1:D:511:ALA:N	2.50	0.45
1:E:175:ARG:NH2	1:E:546:ASN:OD1	2.50	0.45
1:F:46:ALA:HA	1:F:592:ILE:HG13	1.98	0.45
1:F:274:CYS:SG	1:F:295:ILE:HG21	2.57	0.45
1:C:443:GLN:HA	1:C:634:ARG:HH21	1.82	0.44
1:D:422:ALA:HA	1:D:425:ASN:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:ALA:HB2	1:D:555:LEU:HD11	1.99	0.44
1:E:424:VAL:HG21	1:E:512:ILE:HD12	1.99	0.44
1:F:96:SER:HB2	1:F:190:ILE:HG21	1.99	0.44
1:F:273:ILE:HD12	1:F:274:CYS:N	2.32	0.44
1:F:582:PRO:HA	1:F:612:TYR:O	2.18	0.44
1:A:481:CYS:HB2	3:A:702:RQM:S1	2.56	0.44
1:E:167:TRP:HZ3	1:E:232:GLU:HG3	1.82	0.44
1:E:235:ASP:HA	1:E:308:ARG:NH1	2.29	0.44
1:E:332:MET:SD	1:E:343:LEU:HD13	2.58	0.44
1:A:384:ILE:O	1:A:388:ILE:HG23	2.17	0.44
1:A:469:LEU:O	1:A:474:VAL:HG22	2.18	0.44
1:B:257:ALA:HB2	1:B:291:GLU:HB2	1.99	0.44
1:C:510:SER:HA	1:C:521:PRO:HB3	1.99	0.44
1:C:620:LYS:HZ3	1:E:349:CYS:HA	1.81	0.44
1:F:409:ILE:HG13	1:F:492:MET:O	2.18	0.44
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.71	0.44
1:D:187:PRO:HD3	1:D:221:MET:HB2	1.98	0.44
1:E:307:MET:HB3	1:E:307:MET:HE3	1.72	0.44
1:E:413:SER:HA	1:E:536:ARG:HD3	1.99	0.44
1:B:88:ILE:HG23	1:B:571:ALA:HA	1.98	0.44
1:B:168:LEU:HD22	1:B:228:MET:HE2	1.98	0.44
1:F:497:THR:HG23	1:F:506:LYS:HA	1.99	0.44
1:A:221:MET:SD	1:A:578:THR:HB	2.58	0.44
1:A:379:THR:O	1:A:383:ILE:HG12	2.17	0.44
1:B:63:PHE:CG	1:E:46:ALA:HB2	2.52	0.44
1:B:315:THR:HG22	1:B:488:LYS:NZ	2.33	0.44
1:B:559:ALA:HB3	1:B:583:THR:HG23	2.00	0.44
1:C:55:LYS:HG2	1:D:453:THR:OG1	2.17	0.44
1:E:53:CYS:HB3	1:E:55:LYS:HG2	1.99	0.44
1:F:269:LEU:HD23	1:F:371:PHE:HD2	1.81	0.44
1:B:30:ALA:HA	1:B:33:ARG:NH1	2.32	0.44
1:E:76:ARG:O	1:E:80:VAL:HG13	2.18	0.44
1:E:472:ARG:HD2	1:E:627:TYR:CD2	2.53	0.44
1:E:495:GLU:H	1:E:495:GLU:HG2	1.46	0.44
1:F:106:MET:HA	1:F:109:ILE:CG1	2.33	0.44
1:F:124:LYS:CE	1:F:235:ASP:HB3	2.47	0.44
1:A:242:GLN:O	1:A:244:VAL:HG23	2.18	0.44
1:B:130:LYS:HE3	1:B:130:LYS:HB3	1.85	0.44
1:B:135:ALA:O	1:B:139:ARG:HD3	2.17	0.44
1:C:152:THR:HG23	1:C:229:LEU:HD12	1.98	0.44
1:C:258:VAL:O	1:C:294:ASN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:547:LYS:O	1:E:547:LYS:HD3	2.18	0.44
1:F:382:THR:O	1:F:386:MET:HE3	2.18	0.44
1:F:443:GLN:OE1	1:F:631:GLN:NE2	2.51	0.44
1:A:70:GLY:HA3	2:A:701:SF4:S2	2.58	0.44
1:A:457:GLN:O	1:A:460:SER:OG	2.27	0.44
1:C:84:LEU:HD21	1:C:590:PRO:O	2.16	0.44
1:C:421:LEU:HD21	1:C:433:LEU:HD22	1.99	0.44
1:F:164:PRO:HB3	1:F:186:LEU:HB3	2.00	0.44
1:F:189:ASN:HB3	1:F:192:ALA:HB3	2.00	0.44
1:A:493:THR:OG1	1:A:495:GLU:OE1	2.32	0.43
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.87	0.43
1:B:334:VAL:HG23	1:B:356:THR:HA	1.99	0.43
1:C:433:LEU:O	1:C:437:VAL:HG23	2.18	0.43
1:C:443:GLN:HA	1:C:634:ARG:HE	1.82	0.43
1:C:578:THR:HA	1:C:609:VAL:HG11	2.00	0.43
1:D:600:LEU:HD23	1:D:600:LEU:HA	1.84	0.43
1:E:330:GLU:CD	1:E:394:ARG:HH21	2.20	0.43
1:F:339:ILE:CD1	1:F:363:ILE:HD11	2.48	0.43
1:A:269:LEU:O	1:A:273:ILE:HG12	2.18	0.43
1:A:451:CYS:HB2	1:A:452:ASN:H	1.58	0.43
1:B:435:ASP:O	1:B:439:ASN:ND2	2.51	0.43
1:C:173:THR:HG23	1:C:542:THR:HG22	2.00	0.43
1:D:18:MET:O	1:D:19:LEU:HB2	2.18	0.43
1:D:21:LEU:HD21	1:D:488:LYS:NZ	2.33	0.43
1:D:95:HIS:ND1	1:D:223:ASP:OD1	2.49	0.43
1:E:148:LEU:HD23	1:E:148:LEU:HA	1.89	0.43
1:E:463:VAL:CG2	1:E:467:LYS:HE3	2.49	0.43
1:A:85:VAL:HG22	1:A:216:GLY:HA3	2.00	0.43
1:C:545:ALA:HB2	1:C:555:LEU:HD11	1.99	0.43
1:D:280:LEU:HD11	1:D:381:LYS:HG2	2.00	0.43
1:E:161:TYR:HA	1:E:188:HIS:CG	2.53	0.43
1:E:264:GLY:HA3	1:E:335:ASP:OD1	2.18	0.43
1:E:300:CYS:O	1:E:304:GLU:HG2	2.17	0.43
1:F:486:PHE:CD2	1:F:491:LEU:HD13	2.53	0.43
1:A:253:MET:HA	1:A:294:ASN:ND2	2.33	0.43
1:B:457:GLN:HG2	1:B:460:SER:HB3	2.00	0.43
1:C:140:GLY:O	1:C:142:LEU:N	2.44	0.43
1:E:597:VAL:HA	1:E:600:LEU:HB2	2.01	0.43
1:F:324:ILE:HD11	1:F:352:THR:OG1	2.19	0.43
1:F:408:SER:HB3	1:F:492:MET:CG	2.48	0.43
1:F:567:GLU:HA	1:F:570:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:LYS:HE2	1:B:54:LEU:O	2.18	0.43
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.86	0.43
1:C:444:GLY:HA3	1:C:630:ILE:HD13	2.00	0.43
1:C:565:MET:HA	1:D:54:LEU:HB2	1.99	0.43
1:D:489:ALA:O	1:D:491:LEU:N	2.51	0.43
1:E:378:GLU:H	1:E:378:GLU:CD	2.23	0.43
1:E:444:GLY:HA3	1:E:630:ILE:HD11	2.00	0.43
1:D:98:HIS:C	1:D:98:HIS:CD2	2.95	0.43
1:F:178:LYS:NZ	1:F:182:ASP:OD2	2.45	0.43
1:A:462:TYR:HE1	1:A:562:PRO:HD2	1.84	0.43
1:A:486:PHE:CD2	1:A:525:VAL:HG11	2.54	0.43
1:C:86:ARG:HD3	1:C:198:MET:HE1	2.00	0.43
1:E:260:ILE:CD1	1:E:384:ILE:HG23	2.49	0.43
1:F:119:ILE:HG23	1:F:119:ILE:O	2.18	0.43
1:F:225:ASP:HA	1:F:228:MET:HG3	2.00	0.43
1:F:329:LEU:O	1:F:351:HIS:NE2	2.52	0.43
1:F:349:CYS:O	1:F:350:PHE:HB2	2.18	0.43
1:F:392:GLY:O	1:F:393:ARG:NH1	2.41	0.43
1:C:46:ALA:HB2	1:F:63:PHE:HB3	2.00	0.43
1:C:472:ARG:HD2	1:C:627:TYR:HD2	1.84	0.43
1:D:434:VAL:O	1:D:437:VAL:HG22	2.18	0.43
1:D:469:LEU:HB3	1:D:474:VAL:CG2	2.49	0.43
1:D:528:MET:O	1:D:536:ARG:HD2	2.19	0.43
1:E:82:ARG:HA	1:E:85:VAL:HG22	1.99	0.43
1:F:217:LEU:HB3	1:F:578:THR:HG21	1.99	0.43
1:F:579:ILE:HD13	1:F:579:ILE:HA	1.86	0.43
1:A:306:MET:HE1	1:A:313:LEU:CB	2.47	0.43
1:C:63:PHE:O	1:C:65:GLU:N	2.39	0.43
1:C:95:HIS:CE1	1:C:572:ILE:HD11	2.52	0.43
1:D:120:ARG:HB2	1:D:237:LEU:O	2.19	0.43
1:E:130:LYS:HD3	1:E:130:LYS:HA	1.69	0.43
1:E:280:LEU:HD13	1:E:282:ASP:OD1	2.19	0.43
1:E:550:VAL:HG12	1:E:551:ASP:N	2.33	0.43
1:E:306:MET:HE2	1:E:410:VAL:HG11	2.00	0.43
1:F:538:VAL:O	1:F:542:THR:HG23	2.19	0.43
1:F:620:LYS:HD2	1:F:620:LYS:HA	1.84	0.43
1:A:142:LEU:HA	1:A:145:VAL:HG12	2.00	0.42
1:B:469:LEU:O	1:B:474:VAL:HG22	2.19	0.42
1:B:476:VAL:HG11	1:B:525:VAL:HG12	2.01	0.42
1:C:431:LYS:HE3	1:C:431:LYS:HB3	1.91	0.42
1:D:139:ARG:HH22	1:D:147:ASP:CG	2.25	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:ALA:HB2	1:D:429:PRO:HG3	2.01	0.42
1:E:462:TYR:HB3	1:E:486:PHE:CE1	2.53	0.42
1:F:334:VAL:HG23	1:F:356:THR:HA	2.01	0.42
1:F:336:VAL:HA	1:F:361:ASN:HD22	1.84	0.42
1:F:473:ASN:C	1:F:505:LEU:HD13	2.44	0.42
1:F:558:VAL:HG11	1:F:626:LEU:HD22	2.00	0.42
1:F:578:THR:HG23	1:F:609:VAL:HG21	2.00	0.42
1:A:250:LEU:HD12	1:A:326:THR:HG21	2.00	0.42
1:B:63:PHE:HB3	1:E:46:ALA:HB2	2.01	0.42
1:C:122:GLU:O	1:C:126:TYR:HD1	2.02	0.42
1:D:553:SER:O	1:D:633:ARG:NE	2.52	0.42
1:E:224:LEU:HG	1:E:228:MET:SD	2.59	0.42
1:A:18:MET:HG2	1:A:458:GLN:O	2.19	0.42
1:A:55:LYS:HE3	1:A:71:VAL:CG1	2.49	0.42
1:B:462:TYR:HB3	1:B:486:PHE:CE1	2.54	0.42
1:C:29:THR:H	1:C:32:HIS:HB2	1.84	0.42
1:D:18:MET:HB2	1:D:460:SER:HB3	2.02	0.42
1:D:27:ILE:HD12	1:D:27:ILE:HA	1.92	0.42
1:E:231:THR:CG2	1:E:533:ASP:HA	2.49	0.42
1:E:261:ALA:HA	1:E:296:ILE:O	2.19	0.42
1:E:263:ASN:OD1	1:E:298:ILE:HB	2.18	0.42
1:F:321:GLU:O	1:F:324:ILE:HG22	2.20	0.42
1:C:434:VAL:HG21	1:C:547:LYS:HG2	2.02	0.42
1:D:429:PRO:O	1:D:432:PRO:HD2	2.19	0.42
1:E:409:ILE:HG13	1:E:523:PRO:HG3	2.02	0.42
1:E:463:VAL:HG22	1:E:467:LYS:HE3	2.01	0.42
1:E:510:SER:HA	1:E:521:PRO:HA	2.02	0.42
1:A:168:LEU:O	1:A:172:LEU:HD22	2.20	0.42
1:C:263:ASN:HB3	1:C:334:VAL:HG12	2.02	0.42
1:D:318:LEU:HD23	1:D:452:ASN:HB2	2.01	0.42
1:D:415:GLU:OE1	1:D:415:GLU:N	2.51	0.42
1:E:267:PRO:HA	1:E:270:SER:OG	2.20	0.42
1:A:504:GLY:O	1:A:508:VAL:HG23	2.20	0.42
1:B:510:SER:HA	1:B:521:PRO:HA	2.01	0.42
1:D:451:CYS:HB2	1:D:452:ASN:H	1.76	0.42
1:E:296:ILE:HD12	1:E:314:ALA:HB2	2.02	0.42
1:E:378:GLU:O	1:E:381:LYS:HG3	2.19	0.42
1:F:252:VAL:HA	1:F:405:LYS:HE2	2.00	0.42
1:F:258:VAL:HG23	1:F:293:ILE:HA	2.02	0.42
1:F:510:SER:HA	1:F:521:PRO:CA	2.44	0.42
1:F:596:ILE:O	1:F:600:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:CYS:HB3	1:B:225:ASP:OD2	2.19	0.42
1:C:206:ASP:HB3	1:C:212:LEU:HD21	2.02	0.42
1:C:486:PHE:CB	1:C:525:VAL:HG21	2.50	0.42
1:D:53:CYS:HB3	1:D:203:VAL:HG21	2.02	0.42
1:D:262:VAL:HG23	1:D:301:THR:HG23	2.01	0.42
1:D:285:ILE:HA	1:D:289:ALA:O	2.19	0.42
1:E:453:THR:HG23	1:E:455:LYS:H	1.83	0.42
1:F:167:TRP:CH2	1:F:233:LEU:CD2	3.01	0.42
1:F:520:GLY:HA3	1:F:521:PRO:HD3	1.83	0.42
1:F:527:HIS:HE1	1:F:529:GLY:O	2.01	0.42
1:A:53:CYS:O	1:B:565:MET:HB2	2.19	0.42
1:B:465:LEU:HD12	1:B:562:PRO:HG3	2.01	0.42
1:B:486:PHE:CB	1:B:525:VAL:HG21	2.49	0.42
1:C:163:LYS:HE2	1:C:164:PRO:O	2.20	0.42
1:C:277:ALA:O	1:C:293:ILE:HD12	2.20	0.42
1:E:445:ILE:HA	1:E:475:LEU:O	2.20	0.42
1:F:92:THR:O	1:F:96:SER:HB3	2.19	0.42
1:F:114:LEU:HD12	1:F:114:LEU:HA	1.87	0.42
1:B:442:ILE:HD11	1:B:508:VAL:HG11	2.02	0.42
1:C:158:ASN:HD21	1:C:163:LYS:HB3	1.85	0.42
1:C:187:PRO:HD3	1:C:221:MET:HB2	2.01	0.42
1:C:224:LEU:O	1:C:228:MET:HG3	2.19	0.42
1:C:414:ALA:O	1:C:418:VAL:HG23	2.20	0.42
1:D:263:ASN:HB3	1:D:334:VAL:HG12	2.01	0.42
1:D:347:ALA:C	1:D:349:CYS:N	2.78	0.42
1:A:217:LEU:O	1:A:221:MET:HG2	2.20	0.42
1:D:430:LEU:HD13	1:D:430:LEU:HA	1.89	0.42
1:E:299:CYS:HB3	1:E:300:CYS:H	1.76	0.42
1:E:381:LYS:HD2	1:E:382:THR:N	2.34	0.42
1:E:574:SER:O	1:E:578:THR:HG23	2.20	0.42
1:F:276:VAL:O	1:F:280:LEU:HD23	2.20	0.42
1:F:406:GLN:OE1	1:F:406:GLN:N	2.53	0.42
1:F:621:SER:O	1:F:625:LYS:HG3	2.20	0.42
1:A:100:ARG:NH2	1:A:191:ASP:OD1	2.53	0.41
1:A:216:GLY:HA2	1:A:219:VAL:HG12	2.02	0.41
1:A:250:LEU:O	1:A:253:MET:HG3	2.20	0.41
1:A:316:ASN:OD1	1:A:458:GLN:NE2	2.53	0.41
1:B:76:ARG:HD3	1:B:593:GLY:O	2.20	0.41
1:B:340:MET:O	1:B:343:LEU:HD12	2.20	0.41
1:B:430:LEU:O	1:B:434:VAL:HG23	2.20	0.41
1:D:107:GLN:O	1:D:111:GLN:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:172:LEU:HB2	1:D:177:VAL:HG23	2.01	0.41
1:D:179:ARG:O	1:D:183:LEU:HG	2.20	0.41
1:E:100:ARG:NH1	1:F:196:GLN:HE21	2.17	0.41
1:E:280:LEU:HD12	1:E:283:GLU:CG	2.50	0.41
1:A:263:ASN:OD1	1:A:299:CYS:HB2	2.20	0.41
1:B:258:VAL:HG13	1:B:330:GLU:HG2	2.01	0.41
1:B:447:LEU:HG	1:B:449:VAL:HG13	2.02	0.41
1:B:620:LYS:HA	1:B:620:LYS:HD3	1.80	0.41
1:E:445:ILE:HD11	1:E:557:LEU:HD12	2.03	0.41
1:E:550:VAL:CG1	1:E:554:ASP:HB2	2.50	0.41
1:F:480:GLY:N	1:F:529:GLY:O	2.46	0.41
1:F:535:SER:HA	1:F:538:VAL:HG22	2.02	0.41
1:A:172:LEU:HA	1:A:542:THR:HG21	2.03	0.41
1:C:317:TYR:HE2	1:D:55:LYS:HZ3	1.67	0.41
1:E:342:SER:O	1:E:346:ILE:HG22	2.19	0.41
1:E:412:PHE:O	1:E:528:MET:HG2	2.20	0.41
1:F:518:LEU:HD12	1:F:518:LEU:HA	1.90	0.41
1:F:623:GLY:HA2	1:F:626:LEU:HB2	2.01	0.41
1:A:568:LYS:HG3	1:B:202:HIS:CE1	2.55	0.41
1:B:122:GLU:O	1:B:126:TYR:HD1	2.04	0.41
1:C:328:ALA:HA	1:C:394:ARG:HD2	2.01	0.41
1:D:258:VAL:HG13	1:D:330:GLU:HG2	2.01	0.41
1:D:343:LEU:HB3	1:D:354:ILE:HD13	2.02	0.41
1:F:61:ASP:OD2	1:F:63:PHE:N	2.47	0.41
1:F:135:ALA:O	1:F:139:ARG:NH1	2.53	0.41
1:F:359:LYS:HG3	1:F:360:HIS:CD2	2.56	0.41
1:F:470:ALA:CB	1:F:524:LEU:HD11	2.50	0.41
1:B:104:LEU:HD23	1:B:104:LEU:HA	1.89	0.41
1:B:592:ILE:H	1:B:592:ILE:HG12	1.61	0.41
1:C:59:ARG:HH21	1:D:41:CYS:HB2	1.86	0.41
1:D:528:MET:HE1	1:D:540:LEU:HD13	2.03	0.41
1:E:72:CYS:SG	1:E:73:GLY:N	2.93	0.41
1:E:254:LYS:H	1:E:259:ASN:HD21	1.68	0.41
1:E:444:GLY:CA	1:E:630:ILE:HD11	2.50	0.41
1:E:445:ILE:C	1:E:445:ILE:HD12	2.44	0.41
1:E:558:VAL:HB	1:E:582:PRO:O	2.20	0.41
1:F:139:ARG:HB2	1:F:144:ILE:HD11	2.02	0.41
1:F:408:SER:HA	1:F:493:THR:HG22	2.03	0.41
1:A:25:ASN:O	1:A:26:SER:OG	2.35	0.41
1:A:83:HIS:O	1:A:87:MET:HG3	2.20	0.41
1:B:339:ILE:CD1	1:B:363:ILE:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:ARG:NH2	1:E:191:ASP:OD2	2.54	0.41
1:E:471:LYS:HB3	1:E:471:LYS:HE3	1.69	0.41
1:F:172:LEU:HG	1:F:176:ARG:HB3	2.03	0.41
1:F:324:ILE:CD1	1:F:352:THR:HG21	2.51	0.41
1:F:410:VAL:CG1	1:F:527:HIS:HD2	2.34	0.41
1:A:325:LEU:HA	1:A:350:PHE:CZ	2.55	0.41
1:A:417:VAL:O	1:A:421:LEU:HD12	2.21	0.41
1:C:409:ILE:HG22	1:C:412:PHE:CE1	2.56	0.41
1:C:487:ALA:CA	1:C:492:MET:HG3	2.46	0.41
1:E:191:ASP:HB3	1:F:191:ASP:HB3	2.03	0.41
1:E:575:TRP:O	1:E:579:ILE:HG13	2.21	0.41
1:F:269:LEU:HD11	1:F:333:VAL:CG1	2.47	0.41
1:F:497:THR:C	1:F:499:GLN:H	2.29	0.41
1:B:178:LYS:HE3	1:B:182:ASP:OD2	2.21	0.41
1:C:84:LEU:HD11	1:C:591:VAL:HG13	2.03	0.41
1:C:626:LEU:HD23	1:C:626:LEU:HA	1.91	0.41
1:D:121:ASP:HB2	1:D:239:GLY:HA2	2.03	0.41
1:D:206:ASP:HB3	1:D:212:LEU:HD21	2.03	0.41
1:D:334:VAL:HB	1:D:339:ILE:HD13	2.02	0.41
1:E:462:TYR:HB3	1:E:486:PHE:CZ	2.56	0.41
1:A:191:ASP:HB3	1:B:191:ASP:HB3	2.03	0.41
1:A:414:ALA:O	1:A:418:VAL:HG23	2.21	0.41
1:A:592:ILE:H	1:A:592:ILE:HG12	1.57	0.41
1:B:462:TYR:HE1	1:B:562:PRO:HD2	1.85	0.41
1:C:534:ASN:O	1:C:538:VAL:HG23	2.21	0.41
1:C:633:ARG:HD3	1:C:633:ARG:HA	1.83	0.41
1:D:220:ALA:O	1:D:223:ASP:HB3	2.20	0.41
1:D:635:ALA:C	1:D:637:LEU:H	2.28	0.41
1:E:48:LEU:HB3	1:E:60:ILE:HB	2.02	0.41
1:E:164:PRO:CB	1:E:186:LEU:HD23	2.50	0.41
1:E:258:VAL:HG13	1:E:293:ILE:HA	2.03	0.41
1:E:565:MET:HE3	1:E:565:MET:HB3	1.81	0.41
1:E:454:THR:H	1:F:55:LYS:HG2	1.85	0.41
1:E:459:ASP:OD1	1:E:459:ASP:N	2.54	0.41
1:E:486:PHE:HB2	1:E:492:MET:HE3	2.02	0.41
1:F:542:THR:HA	1:F:552:LEU:HD11	2.01	0.41
1:B:334:VAL:HB	1:B:339:ILE:HD13	2.03	0.40
1:D:596:ILE:HD12	1:D:596:ILE:H	1.85	0.40
1:E:242:GLN:HG3	1:E:243:PRO:HD2	2.03	0.40
1:F:282:ASP:OD1	1:F:282:ASP:N	2.53	0.40
1:A:61:ASP:HB2	1:A:67:PRO:HD2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:LEU:HD12	1:C:21:LEU:HA	1.92	0.40
1:D:434:VAL:HG22	1:D:548:LEU:HD21	2.03	0.40
1:D:442:ILE:HD11	1:D:444:GLY:O	2.22	0.40
1:D:510:SER:HA	1:D:521:PRO:HB3	2.03	0.40
1:E:24:ALA:C	1:E:26:SER:N	2.80	0.40
1:E:278:ALA:O	1:E:281:ARG:HD3	2.21	0.40
1:F:231:THR:HG21	1:F:533:ASP:HA	2.04	0.40
1:F:265:HIS:N	1:F:301:THR:OG1	2.54	0.40
1:F:409:ILE:HD11	1:F:523:PRO:HD3	2.03	0.40
1:F:475:LEU:HD23	1:F:476:VAL:N	2.37	0.40
1:C:157:GLN:CB	1:D:157:GLN:HB2	2.50	0.40
1:C:462:TYR:CE2	1:C:482:ALA:HA	2.56	0.40
1:C:579:ILE:HD13	1:C:579:ILE:HA	1.82	0.40
1:E:245:VAL:HG22	1:E:409:ILE:HG22	2.03	0.40
1:E:316:ASN:OD1	1:E:316:ASN:N	2.54	0.40
1:F:144:ILE:H	1:F:144:ILE:HD12	1.86	0.40
1:F:230:ALA:CB	1:F:532:VAL:HG11	2.52	0.40
1:F:371:PHE:CE1	1:F:373:GLU:HA	2.57	0.40
1:F:465:LEU:HD21	1:F:622:ALA:HB3	2.04	0.40
1:F:490:GLY:O	1:F:493:THR:HG23	2.21	0.40
1:F:551:ASP:OD1	1:F:552:LEU:N	2.51	0.40
1:D:60:ILE:HG21	1:D:76:ARG:HB3	2.04	0.40
1:E:362:LYS:HG3	1:F:208:ASP:HB2	2.03	0.40
1:E:404:PHE:HD1	1:E:404:PHE:HA	1.74	0.40
1:F:355:ILE:O	1:F:355:ILE:HD12	2.21	0.40
1:F:577:VAL:C	1:F:579:ILE:H	2.28	0.40
1:A:98:HIS:CD2	1:A:98:HIS:C	3.00	0.40
1:E:176:ARG:HG2	1:E:551:ASP:OD1	2.22	0.40
1:E:466:ALA:HB2	1:E:486:PHE:CE1	2.57	0.40
1:E:487:ALA:O	1:E:489:ALA:N	2.45	0.40
1:E:490:GLY:O	1:E:493:THR:HG23	2.21	0.40
1:E:626:LEU:HD23	1:E:626:LEU:HA	1.91	0.40
1:F:124:LYS:O	1:F:128:ILE:HG23	2.22	0.40
1:F:139:ARG:HE	1:F:139:ARG:HB3	1.72	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:LYS:NZ	1:F:291:GLU:OE2[1_655]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	618/639 (97%)	558 (90%)	53 (9%)	7 (1%)	11	36
1	B	618/639 (97%)	553 (90%)	58 (9%)	7 (1%)	11	36
1	C	618/639 (97%)	561 (91%)	49 (8%)	8 (1%)	9	32
1	D	619/639 (97%)	556 (90%)	51 (8%)	12 (2%)	6	23
1	E	615/639 (96%)	527 (86%)	73 (12%)	15 (2%)	4	18
1	F	615/639 (96%)	523 (85%)	64 (10%)	28 (5%)	2	7
All	All	3703/3834 (97%)	3278 (88%)	348 (9%)	77 (2%)	5	21

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	SER
1	C	65	GLU
1	D	265	HIS
1	D	490	GLY
1	E	27	ILE
1	E	405	LYS
1	E	457	GLN
1	E	491	LEU
1	E	617	THR
1	F	352	THR
1	F	404	PHE
1	F	410	VAL
1	F	444	GLY
1	F	488	LYS
1	F	521	PRO
1	F	604	THR
1	F	612	TYR
1	A	23	GLU
1	C	23	GLU
1	C	517	GLY

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Mol	Chain	Res	Type
1	D	24	ALA
1	E	65	GLU
1	E	404	PHE
1	E	556	PRO
1	F	23	GLU
1	F	26	SER
1	F	51	ARG
1	F	76	ARG
1	F	531	CYS
1	A	21	LEU
1	A	347	ALA
1	A	518	LEU
1	B	588	VAL
1	C	142	LEU
1	D	74	ALA
1	D	139	ARG
1	D	604	THR
1	E	25	ASN
1	F	147	ASP
1	F	254	LYS
1	F	588	VAL
1	F	603	GLU
1	B	19	LEU
1	B	405	LYS
1	C	289	ALA
1	C	588	VAL
1	D	19	LEU
1	D	26	SER
1	D	565	MET
1	D	588	VAL
1	E	526	MET
1	E	588	VAL
1	F	148	LEU
1	F	337	GLN
1	F	556	PRO
1	A	130	LYS
1	B	337	GLN
1	C	337	GLN
1	D	25	ASN
1	E	604	THR
1	F	24	ALA
1	F	395	ASP

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Mol	Chain	Res	Type
1	F	530	SER
1	F	547	LYS
1	A	348	GLU
1	A	588	VAL
1	B	604	THR
1	D	337	GLN
1	E	22	ALA
1	E	618	ASP
1	F	518	LEU
1	E	550	VAL
1	F	409	ILE
1	C	64	GLY
1	F	258	VAL
1	F	550	VAL
1	B	550	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	475/490 (97%)	446 (94%)	29 (6%)	17	46
1	B	475/490 (97%)	447 (94%)	28 (6%)	18	48
1	C	475/490 (97%)	456 (96%)	19 (4%)	28	62
1	D	476/490 (97%)	444 (93%)	32 (7%)	15	43
1	E	472/490 (96%)	444 (94%)	28 (6%)	18	48
1	F	472/490 (96%)	438 (93%)	34 (7%)	13	39
All	All	2845/2940 (97%)	2675 (94%)	170 (6%)	17	47

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	CYS
1	A	53	CYS
1	A	58	CYS

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Mol	Chain	Res	Type
1	A	84	LEU
1	A	85	VAL
1	A	96	SER
1	A	152	THR
1	A	163	LYS
1	A	172	LEU
1	A	245	VAL
1	A	271	ASP
1	A	316	ASN
1	A	359	LYS
1	A	364	SER
1	A	369	VAL
1	A	424	VAL
1	A	434	VAL
1	A	438	VAL
1	A	451	CYS
1	A	465	LEU
1	A	514	THR
1	A	572	ILE
1	A	578	THR
1	A	587	SER
1	A	591	VAL
1	A	592	ILE
1	A	599	LYS
1	A	615	VAL
1	A	617	THR
1	B	50	CYS
1	B	58	CYS
1	B	72	CYS
1	B	84	LEU
1	B	85	VAL
1	B	131	THR
1	B	151	ILE
1	B	203	VAL
1	B	237	LEU
1	B	265	HIS
1	B	270	SER
1	B	309	HIS
1	B	315	THR
1	B	367	THR
1	B	369	VAL
1	B	438	VAL

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Mol	Chain	Res	Type
1	B	451	CYS
1	B	454	THR
1	B	494	SER
1	B	531	CYS
1	B	540	LEU
1	B	558	VAL
1	B	592	ILE
1	B	604	THR
1	B	609	VAL
1	B	615	VAL
1	B	617	THR
1	B	621	SER
1	C	50	CYS
1	C	51	ARG
1	C	59	ARG
1	C	72	CYS
1	C	229	LEU
1	C	237	LEU
1	C	270	SER
1	C	282	ASP
1	C	316	ASN
1	C	319	SER
1	C	364	SER
1	C	367	THR
1	C	451	CYS
1	C	531	CYS
1	C	579	ILE
1	C	591	VAL
1	C	604	THR
1	C	609	VAL
1	C	615	VAL
1	D	26	SER
1	D	50	CYS
1	D	80	VAL
1	D	96	SER
1	D	132	LEU
1	D	171	SER
1	D	173	THR
1	D	176	ARG
1	D	234	SER
1	D	237	LEU
1	D	240	THR

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Mol	Chain	Res	Type
1	D	245	VAL
1	D	296	ILE
1	D	319	SER
1	D	358	ASP
1	D	367	THR
1	D	373	GLU
1	D	438	VAL
1	D	447	LEU
1	D	451	CYS
1	D	488	LYS
1	D	494	SER
1	D	510	SER
1	D	525	VAL
1	D	531	CYS
1	D	538	VAL
1	D	542	THR
1	D	544	LEU
1	D	550	VAL
1	D	578	THR
1	D	585	VAL
1	D	600	LEU
1	E	29	THR
1	E	58	CYS
1	E	80	VAL
1	E	115	HIS
1	E	119	ILE
1	E	130	LYS
1	E	134	VAL
1	E	136	THR
1	E	171	SER
1	E	173	THR
1	E	231	THR
1	E	273	ILE
1	E	281	ARG
1	E	291	GLU
1	E	308	ARG
1	E	417	VAL
1	E	447	LEU
1	E	469	LEU
1	E	495	GLU
1	E	540	LEU
1	E	553	SER

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Mol	Chain	Res	Type
1	E	557	LEU
1	E	564	CYS
1	E	578	THR
1	E	591	VAL
1	E	596	ILE
1	E	609	VAL
1	E	621	SER
1	F	50	CYS
1	F	58	CYS
1	F	72	CYS
1	F	96	SER
1	F	119	ILE
1	F	147	ASP
1	F	152	THR
1	F	168	LEU
1	F	176	ARG
1	F	203	VAL
1	F	210	THR
1	F	224	LEU
1	F	231	THR
1	F	234	SER
1	F	258	VAL
1	F	315	THR
1	F	319	SER
1	F	369	VAL
1	F	377	VAL
1	F	418	VAL
1	F	435	ASP
1	F	446	VAL
1	F	451	CYS
1	F	456	VAL
1	F	468	SER
1	F	498	THR
1	F	506	LYS
1	F	512	ILE
1	F	531	CYS
1	F	550	VAL
1	F	557	LEU
1	F	578	THR
1	F	599	LYS
1	F	600	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	98	HIS
1	A	353	GLN
1	A	361	ASN
1	A	452	ASN
1	A	631	GLN
1	B	20	ASN
1	B	40	GLN
1	B	83	HIS
1	B	202	HIS
1	B	337	GLN
1	B	361	ASN
1	B	441	ASN
1	C	40	GLN
1	C	98	HIS
1	C	107	GLN
1	C	303	HIS
1	C	443	GLN
1	C	457	GLN
1	C	527	HIS
1	D	98	HIS
1	D	111	GLN
1	D	337	GLN
1	D	353	GLN
1	D	595	GLN
1	E	25	ASN
1	E	38	GLN
1	E	158	ASN
1	E	196	GLN
1	E	337	GLN
1	E	351	HIS
1	E	353	GLN
1	E	406	GLN
1	E	439	ASN
1	E	527	HIS
1	E	595	GLN
1	F	101	HIS
1	F	196	GLN
1	F	361	ASN
1	F	443	GLN
1	F	457	GLN
1	F	631	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	RQM	E	703	1	0,12,12	-	-	-		
3	RQM	F	702	1	0,12,12	-	-	-		
2	SF4	E	701	1	0,12,12	-	-	-		
2	SF4	D	701	1	0,12,12	-	-	-		
3	RQM	B	703	1	0,12,12	-	-	-		
2	SF4	F	701	1	0,12,12	-	-	-		
2	SF4	C	702	1	0,12,12	-	-	-		
3	RQM	D	702	1	0,12,12	-	-	-		
2	SF4	C	701	1	0,12,12	-	-	-		
2	SF4	B	702	1	0,12,12	-	-	-		
3	RQM	A	702	1	0,12,12	-	-	-		
3	RQM	C	703	1	0,12,12	-	-	-		
2	SF4	A	701	1	0,12,12	-	-	-		
2	SF4	E	702	1	0,12,12	-	-	-		
2	SF4	B	701	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	RQM	E	703	1	-	-	0/4/4/4
3	RQM	F	702	1	-	-	0/4/4/4
2	SF4	E	701	1	-	-	0/6/5/5
2	SF4	D	701	1	-	-	0/6/5/5
3	RQM	B	703	1	-	-	0/4/4/4
2	SF4	F	701	1	-	-	0/6/5/5
2	SF4	C	702	1	-	-	0/6/5/5
3	RQM	D	702	1	-	-	0/4/4/4
2	SF4	C	701	1	-	-	0/6/5/5
2	SF4	B	702	1	-	-	0/6/5/5
3	RQM	A	702	1	-	-	0/4/4/4
3	RQM	C	703	1	-	-	0/4/4/4
2	SF4	A	701	1	-	-	0/6/5/5
2	SF4	E	702	1	-	-	0/6/5/5
2	SF4	B	701	1	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	703	RQM	3	0
3	F	702	RQM	2	0
2	E	701	SF4	1	0
3	B	703	RQM	3	0
3	A	702	RQM	2	0
3	C	703	RQM	1	0
2	A	701	SF4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	620/639 (97%)	-0.10	1 (0%) 91 89	43, 69, 90, 110	0
1	B	620/639 (97%)	-0.19	3 (0%) 87 83	44, 67, 87, 107	0
1	C	620/639 (97%)	-0.18	5 (0%) 82 77	47, 68, 90, 116	0
1	D	621/639 (97%)	-0.22	3 (0%) 87 83	43, 67, 88, 108	0
1	E	617/639 (96%)	0.31	11 (1%) 67 59	72, 103, 129, 146	0
1	F	617/639 (96%)	0.48	33 (5%) 32 25	76, 109, 135, 149	0
All	All	3715/3834 (96%)	0.01	56 (1%) 72 64	43, 75, 123, 149	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	50	CYS	4.6
1	F	520	GLY	4.2
1	F	512	ILE	4.0
1	F	544	LEU	3.9
1	F	487	ALA	3.7
1	E	414	ALA	3.7
1	F	540	LEU	3.3
1	E	332	MET	3.3
1	D	64	GLY	3.1
1	F	328	ALA	3.0
1	F	525	VAL	3.0
1	F	420	ALA	3.0
1	E	273	ILE	2.9
1	F	498	THR	2.9
1	E	557	LEU	2.9
1	F	354	ILE	2.9
1	E	437	VAL	2.8
1	F	505	LEU	2.8
1	D	24	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	433	LEU	2.8
1	F	526	MET	2.8
1	F	518	LEU	2.7
1	C	22	ALA	2.7
1	F	331	ALA	2.7
1	F	500	TYR	2.7
1	E	331	ALA	2.6
1	F	502	GLY	2.6
1	F	508	VAL	2.5
1	F	524	LEU	2.4
1	B	22	ALA	2.4
1	F	493	THR	2.4
1	F	491	LEU	2.4
1	F	527	HIS	2.4
1	C	142	LEU	2.4
1	F	109	ILE	2.4
1	B	50	CYS	2.3
1	E	523	PRO	2.3
1	D	284	ALA	2.2
1	F	261	ALA	2.2
1	F	260	ILE	2.2
1	E	434	VAL	2.2
1	F	494	SER	2.2
1	E	322	LEU	2.2
1	F	548	LEU	2.1
1	E	518	LEU	2.1
1	C	24	ALA	2.1
1	F	355	ILE	2.1
1	F	541	ALA	2.1
1	F	418	VAL	2.1
1	B	21	LEU	2.1
1	F	404	PHE	2.1
1	C	458	GLN	2.0
1	A	22	ALA	2.0
1	C	552	LEU	2.0
1	F	447	LEU	2.0
1	F	444	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	RQM	A	702	9/9	0.82	0.13	72,80,95,97	9
3	RQM	F	702	9/9	0.85	0.10	92,104,115,118	9
3	RQM	D	702	9/9	0.87	0.09	61,79,94,107	9
3	RQM	C	703	9/9	0.91	0.09	71,88,98,108	9
2	SF4	C	701	8/8	0.91	0.16	89,110,130,132	0
3	RQM	B	703	9/9	0.91	0.08	62,74,84,97	9
3	RQM	E	703	9/9	0.93	0.07	84,105,115,125	9
2	SF4	F	701	8/8	0.93	0.12	93,116,127,132	0
2	SF4	A	701	8/8	0.95	0.11	64,87,94,96	0
2	SF4	B	701	8/8	0.96	0.10	79,93,111,115	0
2	SF4	C	702	8/8	0.96	0.10	73,91,107,109	0
2	SF4	D	701	8/8	0.96	0.11	62,86,95,101	0
2	SF4	E	701	8/8	0.96	0.10	76,83,90,102	8
2	SF4	E	702	8/8	0.96	0.10	75,114,125,129	0
2	SF4	B	702	8/8	0.96	0.10	64,84,97,98	0
4	NA	D	703	1/1	0.96	0.13	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.