Full wwPDB X-ray Structure Validation Report ⓘ

Jan 6, 2024 – 11:44 am GMT

PDB ID	:	5T4Y
Title	:	Crystal structure of BT1762-1763
Authors	:	van den Berg, B.
Deposited on	:	2016-08-30
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

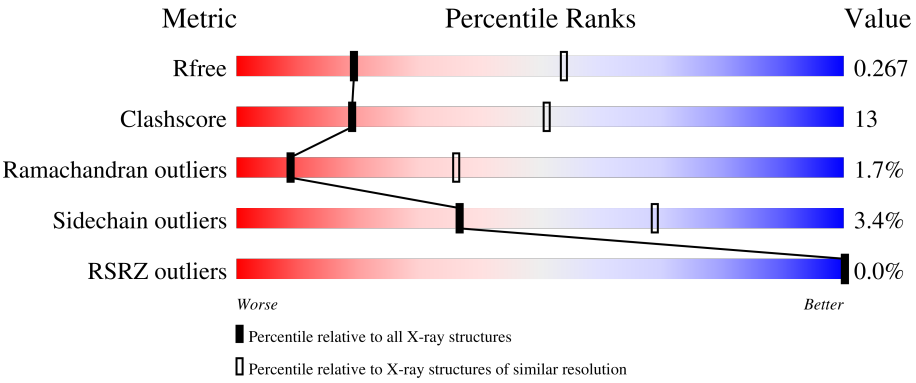
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	576	76% 19%
1	B	576	76% 20%
2	C	1041	48% 27% 22%
2	D	1041	48% 27% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 21727 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	2	0
			4450	2818	737	874	21			
1	B	553	Total	C	N	O	S	0	2	0
			4460	2824	740	875	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	HIS	-	expression tag	UNP Q8A6W4
A	554	HIS	-	expression tag	UNP Q8A6W4
A	555	HIS	-	expression tag	UNP Q8A6W4
A	556	HIS	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4
B	553	HIS	-	expression tag	UNP Q8A6W4
B	554	HIS	-	expression tag	UNP Q8A6W4
B	555	HIS	-	expression tag	UNP Q8A6W4
B	556	HIS	-	expression tag	UNP Q8A6W4
B	557	HIS	-	expression tag	UNP Q8A6W4
B	558	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			
2	C	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

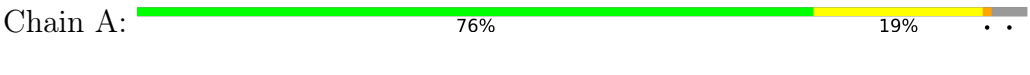
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	B	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0

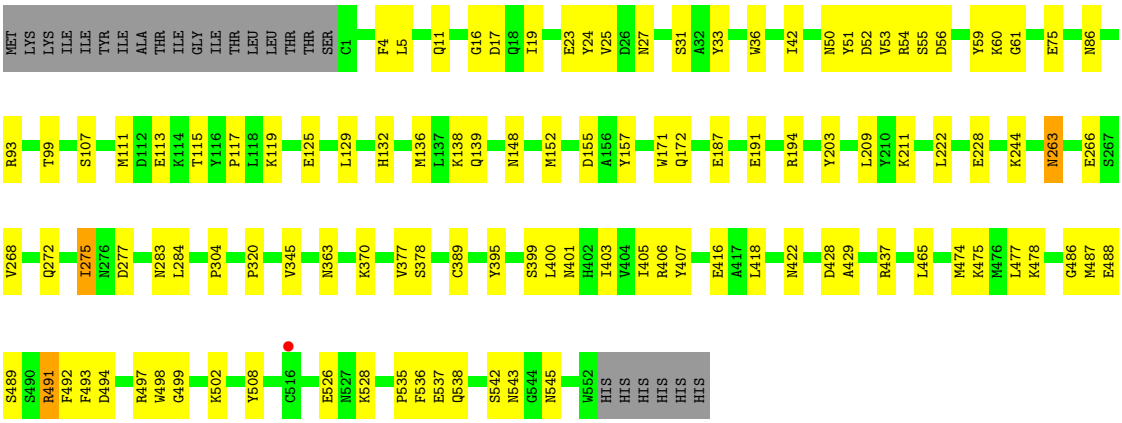
3 Residue-property plots (i)

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: SusD homolog

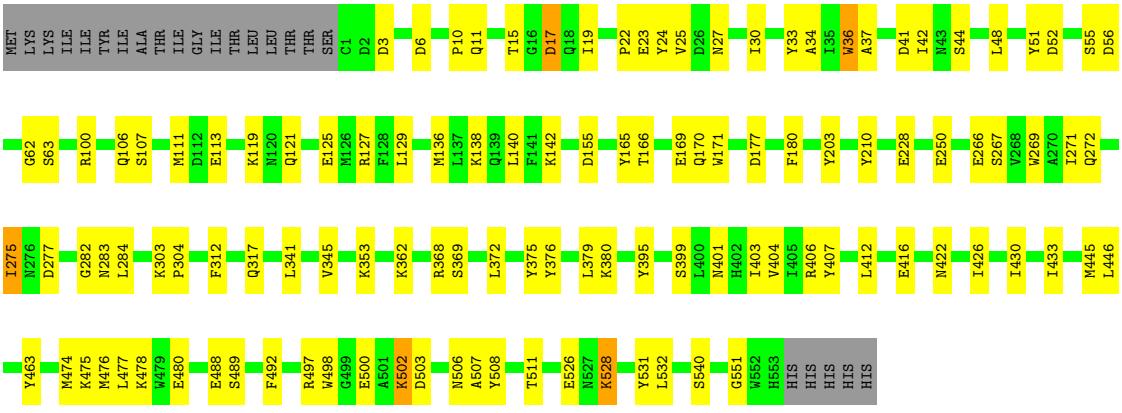
Chain A:





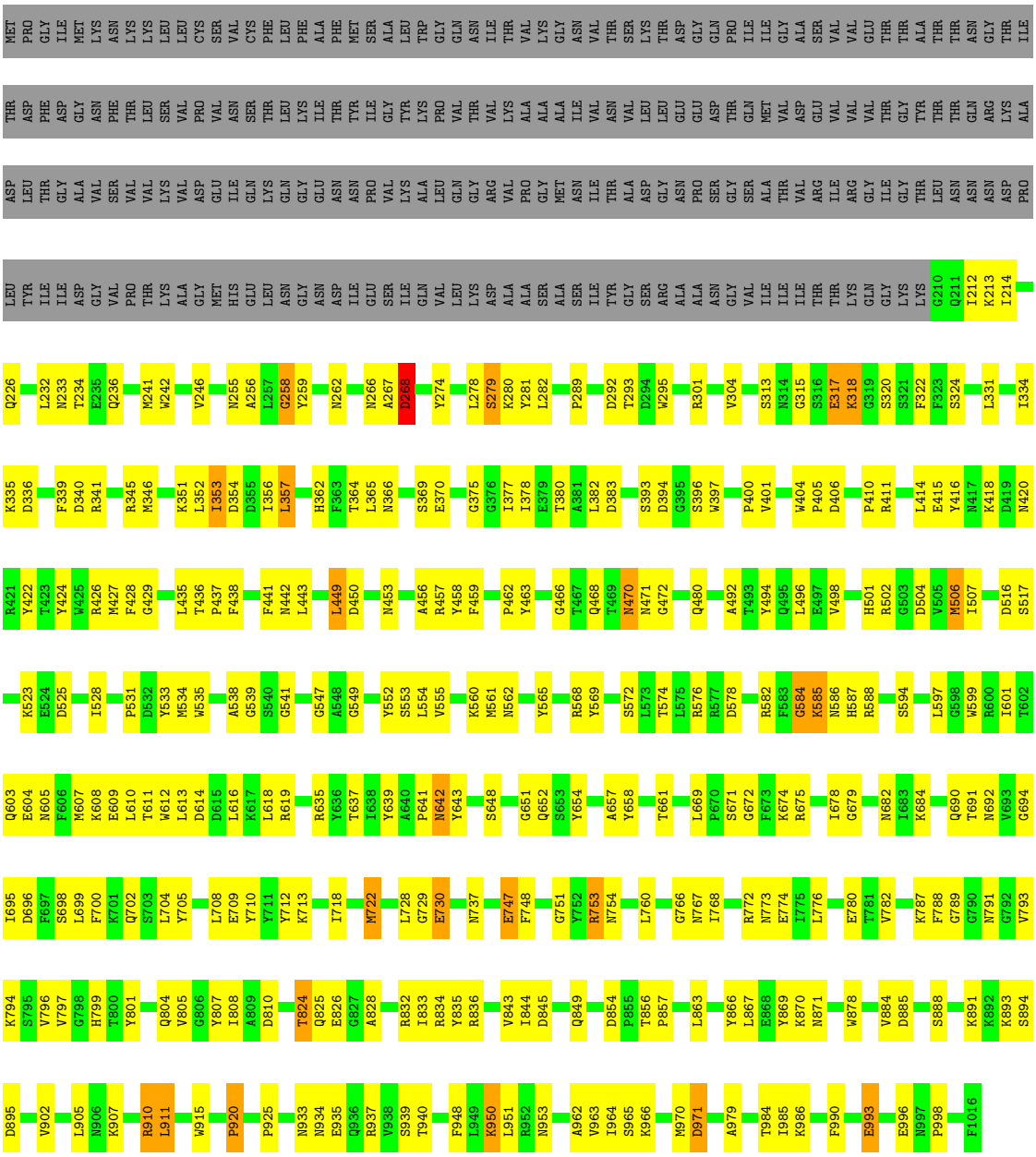
• Molecule 1: SusD homolog

Chain B:



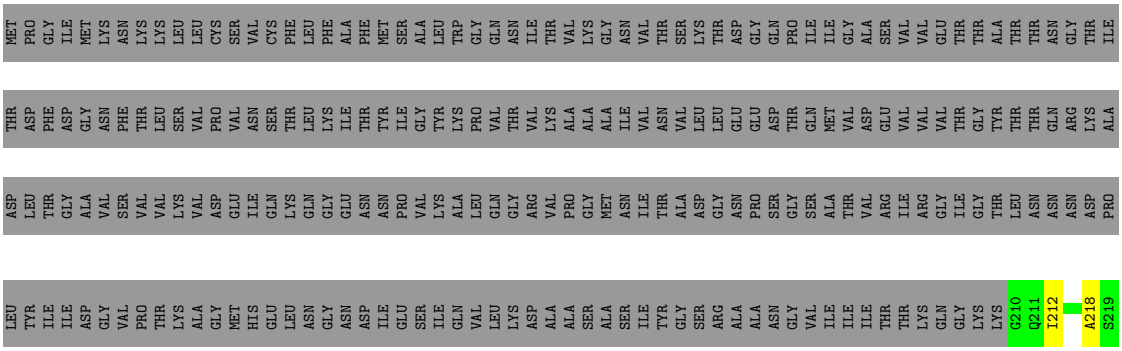
• Molecule 2: SusC homolog

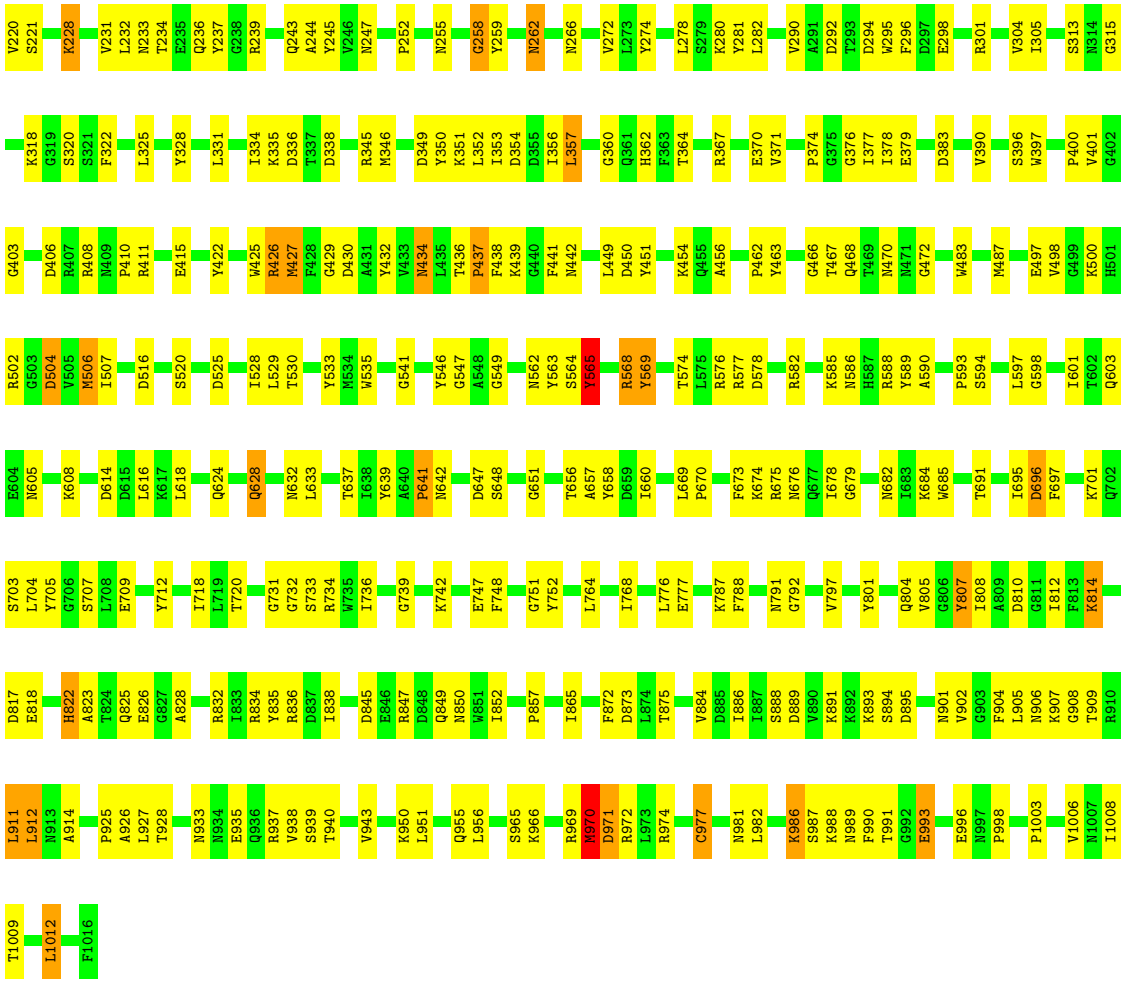
Chain D:



• Molecule 2: SusC homolog

Chain C:




V220 S221 K228 V231 L232 N233 T234 E235 Q236 Y237 G238 R239 Q243 A244 Y245 V246 N247 P252 N255 G258 Y259 N262 N266 V272 L273 Y274 L278 S279 K280 Y281 L282 V290 A291 D292 T293 D294 W295 F296 D297 E298 R301 V304 I305 S313 N314 G315
K318 G319 S320 S321 F322 L325 Y328 L331 I334 K335 D336 T337 D338 R345 M346 D349 Y350 K351 L352 I353 D354 D355 I356 L357 G360 Q361 H362 F363 T364 R367 E370 V371 P374 G375 G376 I377 I378 E379 D383 V390 S396 W397 P400 V401 G402
G403 D406 R407 R408 N409 P410 R411 E415 Y422 W425 R426 M427 F428 G429 D430 A431 Y432 V433 M434 L435 T436 P437 F438 K439 G440 F441 N442 L449 D450 Y451 K454 Q455 A456 P462 Y463 G466 T467 Q468 T469 N470 N471 G472 W483 M487 E497 V498 G499 K500 H501
R502 G503 D504 V505 M506 I507 D516 S520 D525 I528 L529 T530 Y533 M534 W535 G541 Y546 G547 A548 G549 N562 Y563 S564 Y565 R568 Y569 T574 L575 R576 R577 D578 R582 K585 N586 H587 R588 Y589 A590 P593 S594 L597 G598 I601 T602 Q603
E604 N605 K608 D614 D615 L616 K617 L618 Q624 Q628 N632 L633 T637 I638 Y639 A640 P641 N642 D647 S648 G651 T656 A657 Y658 D659 I660 L669 P670 F673 K674 R675 N676 Q677 I678 G679 N682 I683 K684 W685 T691 I695 D696 F697 K701 Q702
S703 L704 Y705 G706 S707 L708 E709 Y712 I718 L719 T720 G731 G732 S733 R734 W735 I736 G739 K742 E747 F748 G751 Y752 L764 I768 L776 E777 K787 F788 N791 G792 V797 Y801 Q804 V805 G806 Y807 I808 A809 D810 G811 I812 F813 K814
D817 E818 H822 A823 T824 Q825 E826 G827 A828 R832 I833 R834 Y835 R836 D837 I838 D845 E846 R847 D848 Q849 N850 W851 I852 P857 I865 F872 D873 L874 T875 V884 D885 I886 I887 S888 D889 V890 K891 K892 K893 S894 D895 N901 V902 G903 F904 L905 N906 K907 G908 T909 R910
L911 L912 N913 A914 P925 A926 L927 T928 N933 N934 E935 Q936 R937 V938 S939 T940 V943 K950 L951 Q955 L956 S965 K966 R969 M970 D971 R972 L973 R974 C977 N981 L982 K986 S987 K988 N989 F990 T991 G992 E993 E996 N997 P998 P1003 V1006 N1007 I1008
T1009 L1012 F1016

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.83Å 152.09Å 253.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.35 – 3.10 130.35 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (130.35-3.10) 98.6 (130.35-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.198 , 0.270 0.198 , 0.267	Depositor DCC
R_{free} test set	4357 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21727	wwPDB-VP
Average B, all atoms (Å^2)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0/4562	0.62	2/6190 (0.0%)
1	B	0.49	1/4573 (0.0%)	0.66	1/6205 (0.0%)
2	C	0.59	8/6571 (0.1%)	0.76	4/8909 (0.0%)
2	D	0.52	0/6571	0.76	3/8909 (0.0%)
All	All	0.52	9/22277 (0.0%)	0.71	10/30213 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	709	GLU	CG-CD	-6.93	1.41	1.51
2	C	565	TYR	CE1-CZ	-6.63	1.29	1.38
2	C	565	TYR	CE2-CZ	-6.15	1.30	1.38
2	C	565	TYR	CG-CD1	-6.06	1.31	1.39
1	B	36	TRP	CB-CG	-5.99	1.39	1.50
2	C	565	TYR	CG-CD2	-5.97	1.31	1.39
2	C	977	CYS	CB-SG	-5.38	1.73	1.81
2	C	709	GLU	CD-OE1	-5.30	1.19	1.25
2	C	262	ASN	CA-CB	5.18	1.66	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	911	LEU	CA-CB-CG	6.11	129.35	115.30
2	D	911	LEU	CB-CG-CD2	5.82	120.89	111.00
1	A	275	ILE	CG1-CB-CG2	-5.81	98.62	111.40
2	D	449	LEU	CA-CB-CG	5.42	127.77	115.30
2	C	565	TYR	CA-CB-CG	5.39	123.65	113.40
2	C	449	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	275	ILE	CG1-CB-CG2	-5.34	99.66	111.40
1	A	465	LEU	CB-CG-CD2	-5.20	102.16	111.00
2	D	911	LEU	CA-CB-CG	5.17	127.18	115.30
2	C	357	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	317	GLU	Peptide
2	D	353	ILE	Peptide
2	D	470	ASN	Peptide
2	D	584	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4450	0	4219	80	0
1	B	4460	0	4227	81	0
2	C	6406	0	6058	208	0
2	D	6406	0	6058	222	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	21727	0	20562	549	0

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 13.

All (549) 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)
2:D:427:MET:CE	2:C:427:MET:SD	2.35	1.12
2:D:427:MET:HE2	2:C:427:MET:SD	1.95	1.04
2:D:427:MET:HE3	2:C:427:MET:SD	2.00	1.00
1:B:275:ILE:HG22	1:B:284:LEU:HD11	1.47	0.95
2:D:365:LEU:HD13	2:D:427:MET:SD	2.12	0.90
2:C:986:LYS:H	2:C:986:LYS:HD2	1.38	0.87
1:A:55:SER:HB3	1:A:492:PHE:HB2	1.59	0.84
2:C:873:ASP:OD2	2:C:974:ARG:NH2	2.11	0.83
2:C:832:ARG:NH1	2:C:935:GLU:OE2	2.12	0.81
2:C:243:GLN:O	2:C:247:ASN:OD1	1.99	0.81
2:C:232:LEU:H	2:C:906:ASN:HD21	1.27	0.81
2:C:434:ASN:HD21	2:C:442:ASN:HD22	1.28	0.80
2:D:352:LEU:HD12	2:D:357:LEU:HD13	1.63	0.78
2:C:520:SER:HB3	2:C:546:TYR:HB2	1.65	0.78
2:D:793:VAL:HG11	2:D:849:GLN:HE21	1.49	0.77
2:D:832:ARG:NH1	2:D:935:GLU:OE2	2.17	0.77
2:C:568:ARG:NH2	2:C:603:GLN:O	2.18	0.77
2:D:619:ARG:NH1	2:D:696:ASP:OD2	2.18	0.76
2:C:605:ASN:HA	2:C:608:LYS:HE3	1.66	0.75
2:C:462:PRO:HB3	2:C:472:GLY:HA2	1.67	0.75
1:B:113:GLU:HG3	1:B:119:LYS:HD3	1.66	0.75
1:A:275:ILE:HG23	1:A:399:SER:HB3	1.67	0.75
2:C:832:ARG:NH2	2:C:926:ALA:O	2.18	0.74
1:B:63:SER:HB3	2:C:904:PHE:CE2	2.23	0.74
2:D:568:ARG:HG2	2:D:603:GLN:HB3	1.69	0.73
1:B:478:LYS:NZ	1:B:500:GLU:OE2	2.15	0.72
2:D:825:GLN:HB3	2:D:828:ALA:HB2	1.72	0.71
1:B:282:GLY:HA2	1:B:284:LEU:HD13	1.70	0.71
1:B:42:ILE:HD13	1:B:395:TYR:CE2	2.26	0.70
2:D:963:VAL:HG13	2:D:964:ILE:HG23	1.71	0.70
1:B:528:LYS:HE2	1:B:551:GLY:O	1.92	0.70
2:D:504:ASP:HB2	2:D:562:ASN:HB2	1.72	0.70
2:C:383:ASP:HB3	2:C:893:LYS:HZ1	1.56	0.70
2:C:742:LYS:HE3	2:C:776:LEU:HD21	1.75	0.69
1:A:25:VAL:HG22	1:A:107:SER:HB3	1.73	0.69
2:D:825:GLN:HG3	2:D:844:ILE:HG13	1.75	0.69
2:C:506:MET:HG2	2:C:507:ILE:N	2.08	0.69
1:A:5:LEU:HD12	2:D:588:ARG:HD3	1.74	0.68
1:A:272:GLN:OE1	1:A:401:ASN:ND2	2.22	0.68
2:C:298:GLU:HG2	2:C:390:VAL:HG21	1.76	0.68
2:C:237:TYR:OH	2:C:904:PHE:HB3	1.94	0.68
2:D:607:MET:O	2:D:609:GLU:N	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASP:HA	1:B:508:TYR:CE2	2.30	0.67
2:D:810:ASP:OD2	2:D:836:ARG:HB3	1.94	0.67
2:C:304:VAL:HG12	2:C:331:LEU:HB2	1.77	0.67
2:C:674:LYS:HE2	2:C:676:ASN:OD1	1.95	0.67
1:B:55:SER:HB3	1:B:492:PHE:HB2	1.76	0.66
2:C:850:ASN:O	2:C:852:ILE:HG23	1.96	0.66
1:A:172:GLN:OE1	1:A:211:LYS:NZ	2.28	0.66
2:C:504:ASP:HB2	2:C:562:ASN:HB2	1.78	0.65
2:D:760:LEU:HD12	2:D:869:TYR:HB2	1.77	0.64
2:D:902:VAL:HG23	2:D:905:LEU:HD11	1.78	0.64
2:C:266:ASN:HB3	2:C:272:VAL:CG2	2.28	0.64
2:C:637:THR:HG22	2:C:678:ILE:HA	1.79	0.64
2:C:528:ILE:HG22	2:C:530:THR:HG22	1.79	0.64
2:C:374:PRO:HD2	2:C:377:ILE:HG13	1.78	0.64
1:A:275:ILE:CG2	1:A:399:SER:HB3	2.27	0.64
2:D:705:TYR:CZ	2:D:751:GLY:HA3	2.32	0.64
2:C:383:ASP:HB3	2:C:893:LYS:NZ	2.13	0.64
2:D:334:ILE:HD11	2:D:378:ILE:HD11	1.80	0.63
2:C:987:SER:O	2:C:989:ASN:N	2.31	0.63
1:A:19:ILE:HG13	2:D:639:TYR:CD2	2.34	0.63
2:D:794:LYS:HB2	2:D:805:VAL:HG21	1.80	0.63
2:D:301:ARG:HG3	2:D:335:LYS:HG2	1.80	0.63
2:D:453:ASN:OD1	2:D:480:GLN:NE2	2.29	0.63
1:B:275:ILE:HG22	1:B:284:LEU:CD1	2.27	0.62
2:C:282:LEU:HG	2:C:290:VAL:HG22	1.80	0.62
2:C:993:GLU:OE2	2:C:993:GLU:HA	1.97	0.62
1:A:535:PRO:HG2	1:A:538:GLN:HB2	1.81	0.62
2:D:377:ILE:HD13	2:D:414:LEU:HD21	1.82	0.62
2:C:221:SER:HB3	2:C:305:ILE:HB	1.81	0.62
1:A:125:GLU:OE1	1:A:194:ARG:NH2	2.29	0.62
2:C:601:ILE:HG21	2:C:616:LEU:HD23	1.81	0.62
2:C:810:ASP:OD2	2:C:836:ARG:HB3	2.00	0.62
1:B:416:GLU:CD	1:B:497:ARG:HH21	2.02	0.62
2:C:582:ARG:HD2	2:C:632:ASN:HA	1.83	0.61
2:C:593:PRO:HD2	2:C:624:GLN:HG3	1.83	0.61
1:A:24:TYR:O	1:A:27:ASN:HB2	2.01	0.61
1:A:138:LYS:HG2	1:A:171:TRP:CH2	2.36	0.61
2:C:301:ARG:HG3	2:C:335:LYS:HG2	1.82	0.60
2:C:818:GLU:O	2:C:822:HIS:HB2	2.01	0.60
2:D:365:LEU:CD1	2:D:427:MET:SD	2.87	0.60
2:C:886:ILE:HD13	2:C:998:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:370:GLU:HB3	2:D:422:TYR:CE2	2.37	0.59
2:C:682:ASN:ND2	2:C:682:ASN:O	2.35	0.59
2:D:279:SER:O	2:D:281:TYR:N	2.33	0.59
2:D:682:ASN:O	2:D:682:ASN:ND2	2.36	0.59
1:B:33:TYR:OH	1:B:125:GLU:OE1	2.15	0.59
2:C:232:LEU:HD22	2:C:907:LYS:O	2.02	0.59
2:C:295:TRP:CZ3	2:C:410:PRO:HD2	2.35	0.59
1:B:445:MET:HG2	1:B:446:LEU:HG	1.85	0.59
1:A:502:LYS:HG3	1:A:526:GLU:HB2	1.84	0.58
1:B:25:VAL:HG21	1:B:111:MET:SD	2.43	0.58
1:A:536:PHE:HZ	2:D:793:VAL:HG13	1.68	0.58
2:D:637:THR:HG23	2:D:679:GLY:H	1.68	0.58
1:B:416:GLU:OE1	1:B:497:ARG:NH2	2.36	0.58
2:D:986:LYS:HD2	2:D:990:PHE:HD2	1.67	0.58
2:D:214:ILE:HG12	2:C:352:LEU:HD22	1.85	0.58
1:A:42:ILE:HD13	1:A:395:TYR:CE2	2.38	0.58
2:C:791:ASN:HD21	2:C:804:GLN:CG	2.16	0.58
2:D:793:VAL:HG11	2:D:849:GLN:NE2	2.18	0.58
1:B:30:ILE:HG21	2:C:670:PRO:HB2	1.84	0.58
2:C:832:ARG:NH2	2:C:928:THR:HG23	2.19	0.58
2:C:894:SER:HA	2:C:908:GLY:HA3	1.85	0.57
2:D:962:ALA:O	2:D:966:LYS:HG3	2.03	0.57
2:D:233:ASN:HB2	2:D:236:GLN:OE1	2.05	0.57
2:D:618:LEU:HD23	2:D:695:ILE:HG13	1.86	0.57
1:A:51:TYR:OH	1:A:86:ASN:O	2.23	0.57
2:D:613:LEU:HD12	2:D:699:LEU:HD22	1.85	0.57
2:C:422:TYR:CG	2:C:454:LYS:HD2	2.39	0.57
2:C:691:THR:HG23	2:C:712:TYR:HB3	1.86	0.57
1:B:210:TYR:HA	1:B:497:ARG:HD2	1.86	0.57
2:D:610:LEU:O	2:D:611:THR:HG22	2.05	0.56
1:A:60:LYS:NZ	1:A:61:GLY:O	2.38	0.56
2:C:648:SER:HB3	2:C:651:GLY:O	2.05	0.56
2:C:825:GLN:HB3	2:C:828:ALA:HB2	1.87	0.56
2:D:587:HIS:CD2	2:D:684:LYS:HB3	2.41	0.56
1:B:34:ALA:O	1:B:37:ALA:N	2.39	0.56
2:C:739:GLY:HA3	2:C:777:GLU:O	2.06	0.56
2:D:766:GLY:HA2	2:D:863:LEU:HA	1.86	0.56
1:A:25:VAL:HG21	1:A:111:MET:SD	2.46	0.56
1:A:50:ASN:O	1:A:53:VAL:HG22	2.06	0.56
2:C:642:ASN:O	2:C:656:THR:OG1	2.20	0.56
2:C:832:ARG:HB3	2:C:933:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:HB3	1:A:157:TYR:CE2	2.40	0.55
2:D:336:ASP:OD2	2:D:411:ARG:NH2	2.39	0.55
2:C:748:PHE:HB3	2:C:768:ILE:HG23	1.88	0.55
2:D:420:ASN:HB3	2:D:458:TYR:CD1	2.41	0.55
1:A:377:VAL:HG12	1:A:378:SER:O	2.06	0.55
1:A:418:LEU:HB2	1:A:429:ALA:HB2	1.89	0.55
2:D:561:MET:O	2:D:572:SER:HA	2.07	0.55
2:D:394:ASP:OD1	2:D:394:ASP:N	2.37	0.55
2:D:835:TYR:CZ	2:D:937:ARG:HD3	2.41	0.55
2:C:298:GLU:O	2:C:335:LYS:NZ	2.39	0.55
2:C:436:THR:HG23	2:C:442:ASN:HB3	1.89	0.55
2:C:817:ASP:OD1	2:C:818:GLU:N	2.39	0.55
1:B:6:ASP:OD2	2:C:588:ARG:NH2	2.39	0.55
1:B:275:ILE:HG23	1:B:399:SER:HB3	1.89	0.55
2:D:400:PRO:O	2:D:466:GLY:HA3	2.06	0.55
2:D:498:VAL:HG12	2:D:498:VAL:O	2.06	0.55
2:D:776:LEU:O	2:D:797:VAL:HG13	2.06	0.55
2:D:637:THR:HG22	2:D:678:ILE:HA	1.88	0.55
2:D:318:LYS:HD2	2:C:212:ILE:HG13	1.87	0.55
1:A:113:GLU:CG	1:A:119:LYS:HD3	2.37	0.54
2:D:835:TYR:CE1	2:D:937:ARG:HD3	2.42	0.54
1:B:138:LYS:HG2	1:B:171:TRP:CZ2	2.41	0.54
2:C:965:SER:O	2:C:970:MET:HB2	2.08	0.54
1:A:56:ASP:OD1	1:A:56:ASP:N	2.41	0.54
2:D:808:ILE:HA	2:D:940:THR:HG23	1.90	0.54
2:C:914:ALA:HB1	2:C:925:PRO:O	2.08	0.54
2:C:875:THR:HG23	2:C:955:GLN:HB3	1.89	0.54
1:A:113:GLU:HG2	1:A:119:LYS:HD3	1.88	0.54
2:C:500:LYS:HG2	2:C:565:TYR:HB3	1.89	0.53
1:A:138:LYS:HG2	1:A:171:TRP:CZ2	2.43	0.53
1:A:543:ASN:ND2	2:D:780:GLU:HB2	2.23	0.53
2:D:574:THR:OG1	2:D:594:SER:HB3	2.08	0.53
2:C:497:GLU:OE2	2:C:502:ARG:HB3	2.08	0.53
2:C:528:ILE:HB	2:C:533:TYR:CG	2.43	0.53
2:C:981:ASN:O	2:C:1006:VAL:HG22	2.08	0.53
1:A:31:SER:HB2	2:D:672:GLY:HA3	1.90	0.53
2:D:791:ASN:HD21	2:D:804:GLN:HG2	1.74	0.53
2:C:353:ILE:HG22	2:C:356:ILE:HB	1.90	0.53
2:D:993:GLU:OE2	2:D:993:GLU:HA	2.09	0.53
2:C:228:LYS:HD3	2:C:296:PHE:CG	2.43	0.53
2:C:585:LYS:HA	2:C:588:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:420:ASN:HB3	2:D:458:TYR:HD1	1.74	0.53
2:D:613:LEU:HD12	2:D:699:LEU:CD2	2.39	0.53
2:D:747:GLU:OE1	2:D:767:ASN:ND2	2.42	0.53
1:B:24:TYR:O	1:B:27:ASN:HB2	2.08	0.53
2:C:231:VAL:HB	2:C:906:ASN:ND2	2.24	0.53
2:C:605:ASN:HA	2:C:608:LYS:CE	2.39	0.53
1:A:23:GLU:OE1	1:A:23:GLU:N	2.24	0.52
2:C:951:LEU:HD23	2:C:951:LEU:O	2.09	0.52
2:D:652:GLN:HB3	2:D:654:TYR:HE1	1.75	0.52
1:B:121:GLN:O	1:B:125:GLU:HG3	2.09	0.52
1:B:10:PRO:HB3	2:C:633:LEU:HD23	1.91	0.52
2:D:807:TYR:CD2	2:D:937:ARG:HG3	2.45	0.52
2:C:360:GLY:HA3	2:C:432:TYR:CZ	2.45	0.52
2:D:415:GLU:O	2:D:418:LYS:HG2	2.09	0.52
2:C:376:GLY:HA2	2:C:379:GLU:OE1	2.09	0.52
2:C:845:ASP:OD2	2:C:847:ARG:HG3	2.10	0.52
2:D:255:ASN:HD21	2:D:259:TYR:HB2	1.74	0.52
2:D:678:ILE:HD11	2:D:728:LEU:HD21	1.91	0.52
1:B:303:LYS:HE3	1:B:376:TYR:O	2.10	0.52
2:C:280:LYS:HB3	2:C:281:TYR:CD1	2.44	0.52
1:A:23:GLU:HG2	1:A:24:TYR:CD1	2.44	0.52
2:C:616:LEU:HD12	2:C:697:PHE:HB3	1.92	0.52
1:A:370:LYS:HG3	2:D:256:ALA:HA	1.91	0.52
1:B:36:TRP:NE1	1:B:129:LEU:HD22	2.25	0.52
2:C:345:ARG:C	2:C:346:MET:HG3	2.30	0.52
2:D:232:LEU:HD22	2:D:907:LYS:O	2.09	0.51
2:D:241:MET:CE	2:D:255:ASN:HD22	2.24	0.51
2:D:780:GLU:H	2:D:780:GLU:CD	2.13	0.51
2:C:578:ASP:O	2:C:589:TYR:HA	2.11	0.51
1:B:48:LEU:HD22	1:B:140:LEU:HD11	1.92	0.51
2:C:872:PHE:HD2	2:C:956:LEU:HD21	1.75	0.51
2:D:528:ILE:HB	2:D:533:TYR:CG	2.46	0.51
2:C:362:HIS:HB2	2:C:430:ASP:OD1	2.10	0.51
2:C:483:TRP:HA	2:C:516:ASP:HB3	1.93	0.51
2:C:628:GLN:HB2	2:C:685:TRP:CZ3	2.46	0.51
2:C:731:GLY:O	2:C:733:SER:N	2.44	0.51
2:D:718:ILE:O	2:D:737:ASN:HA	2.10	0.50
2:C:401:VAL:HA	2:C:467:THR:HG23	1.92	0.50
2:D:435:LEU:O	2:D:437:PRO:HD3	2.10	0.50
1:A:5:LEU:CD1	2:D:588:ARG:HD3	2.39	0.50
1:B:403:ILE:HG21	1:B:406:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:SER:O	2:D:279:SER:OG	2.21	0.50
2:D:353:ILE:HG22	2:D:356:ILE:HB	1.93	0.50
2:D:854:ASP:OD1	2:D:856:THR:OG1	2.30	0.50
2:C:901:ASN:O	2:C:901:ASN:ND2	2.45	0.50
2:D:854:ASP:O	2:D:885:ASP:HB2	2.12	0.50
1:B:177:ASP:O	1:B:180:PHE:N	2.43	0.50
1:A:155:ASP:OD1	1:A:155:ASP:N	2.45	0.50
2:D:255:ASN:HD21	2:D:258:GLY:HA2	1.77	0.50
1:B:272:GLN:OE1	1:B:401:ASN:ND2	2.40	0.50
2:C:266:ASN:HB3	2:C:272:VAL:HG21	1.93	0.50
2:D:345:ARG:HG2	2:D:345:ARG:HH11	1.77	0.50
2:D:401:VAL:O	2:D:404:TRP:HD1	1.95	0.50
2:D:416:TYR:CE2	2:D:463:TYR:HB3	2.46	0.50
2:D:774:GLU:HA	2:D:799:HIS:O	2.12	0.50
2:C:574:THR:OG1	2:C:594:SER:HB3	2.12	0.50
2:D:652:GLN:HB3	2:D:654:TYR:CE1	2.47	0.49
1:B:540:SER:OG	2:C:792:GLY:O	2.30	0.49
2:C:568:ARG:HD2	2:C:569:TYR:CE2	2.47	0.49
2:C:808:ILE:HG23	2:C:836:ARG:HG2	1.94	0.49
1:A:152:MET:HB3	1:A:157:TYR:HE2	1.76	0.49
2:D:547:GLY:O	2:C:535:TRP:HB3	2.11	0.49
1:B:369:SER:HB2	1:B:372:LEU:HB3	1.93	0.49
2:C:336:ASP:OD2	2:C:411:ARG:NH2	2.45	0.49
2:D:805:VAL:HG12	2:D:849:GLN:HG3	1.95	0.49
2:D:824:THR:OG1	2:D:843:VAL:HG12	2.12	0.49
2:D:377:ILE:O	2:D:380:THR:HG22	2.13	0.49
2:D:691:THR:HG23	2:D:712:TYR:HB3	1.93	0.49
1:B:41:ASP:HB3	1:B:44:SER:OG	2.13	0.49
2:D:258:GLY:HA2	2:D:259:TYR:HB2	1.94	0.49
2:D:705:TYR:HE1	2:D:753:ARG:HG2	1.77	0.49
2:C:647:ASP:OD1	2:C:648:SER:N	2.45	0.49
1:B:507:ALA:O	1:B:511:THR:HG23	2.12	0.49
2:C:362:HIS:O	2:C:429:GLY:HA3	2.13	0.49
2:D:788:PHE:N	2:D:789:GLY:HA3	2.27	0.49
2:C:318:LYS:O	2:C:351:LYS:HB2	2.12	0.49
2:C:788:PHE:HD1	2:C:801:TYR:CE2	2.31	0.49
2:D:586:ASN:N	2:D:586:ASN:OD1	2.46	0.49
2:D:266:ASN:O	2:D:268:ASP:N	2.46	0.49
2:D:457:ARG:NH1	2:D:534:MET:O	2.46	0.48
2:D:339:PHE:HD2	2:D:370:GLU:HB2	1.78	0.48
2:D:506:MET:HG2	2:D:507:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:O	1:A:117:PRO:HD3	2.14	0.48
2:D:449:LEU:HD22	2:C:425:TRP:HH2	1.79	0.48
1:A:542:SER:O	1:A:545:ASN:ND2	2.43	0.48
1:B:15:THR:O	1:B:17:ASP:N	2.47	0.48
2:D:293:THR:HG21	2:D:295:TRP:CE2	2.49	0.48
2:D:352:LEU:O	2:D:353:ILE:HG13	2.13	0.48
2:C:905:LEU:HB2	2:C:907:LYS:HE2	1.94	0.48
2:D:965:SER:O	2:D:970:MET:HB2	2.14	0.48
2:C:234:THR:HG22	2:C:292:ASP:CG	2.34	0.48
2:D:648:SER:HB3	2:D:651:GLY:O	2.14	0.48
2:D:891:LYS:HA	2:D:894:SER:OG	2.14	0.48
1:B:269:TRP:CZ3	1:B:404:VAL:HG21	2.49	0.48
2:C:218:ALA:HB3	2:C:1012:LEU:CD2	2.44	0.48
2:C:233:ASN:HB2	2:C:236:GLN:OE1	2.14	0.48
2:D:282:LEU:HD23	2:D:404:TRP:NE1	2.29	0.48
2:D:422:TYR:HA	2:D:456:ALA:HB2	1.95	0.48
2:D:613:LEU:CD1	2:D:699:LEU:HD22	2.44	0.48
1:B:283:ASN:ND2	2:C:657:ALA:O	2.45	0.48
2:C:422:TYR:CD1	2:C:454:LYS:HD2	2.48	0.48
2:C:601:ILE:CG2	2:C:616:LEU:HD23	2.43	0.48
2:C:734:ARG:HG3	2:C:736:ILE:HG23	1.95	0.48
1:A:363:ASN:OD1	1:A:363:ASN:N	2.47	0.47
2:D:953:ASN:ND2	2:D:979:ALA:O	2.38	0.47
1:B:52:ASP:CG	1:B:489:SER:HA	2.35	0.47
2:C:637:THR:CG2	2:C:679:GLY:H	2.26	0.47
1:A:99:THR:OG1	2:D:729:GLY:HA3	2.14	0.47
2:D:397:TRP:HZ2	2:D:415:GLU:HG3	1.79	0.47
2:D:902:VAL:CG2	2:D:905:LEU:HD11	2.43	0.47
2:C:252:PRO:O	2:C:255:ASN:ND2	2.41	0.47
2:C:902:VAL:HB	2:C:905:LEU:HD11	1.95	0.47
2:C:891:LYS:HA	2:C:894:SER:OG	2.15	0.47
2:C:906:ASN:C	2:C:907:LYS:HD2	2.35	0.47
1:A:478:LYS:HG2	1:A:498:TRP:CZ2	2.50	0.47
2:D:304:VAL:HG12	2:D:331:LEU:HB2	1.96	0.47
2:D:587:HIS:CD2	2:D:684:LYS:HD3	2.49	0.47
2:D:894:SER:O	2:D:910:ARG:HG3	2.14	0.47
1:B:30:ILE:HG13	2:C:660:ILE:HG13	1.97	0.47
2:C:791:ASN:HD21	2:C:804:GLN:HG2	1.79	0.47
2:D:364:THR:HB	2:D:428:PHE:CE1	2.50	0.47
2:D:383:ASP:HB2	2:D:905:LEU:HB3	1.97	0.47
1:B:19:ILE:HG13	2:C:639:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:462:PRO:HB3	2:D:472:GLY:HA2	1.97	0.47
1:B:22:PRO:HA	1:B:25:VAL:HG23	1.97	0.47
1:B:502:LYS:HG2	1:B:506:ASN:HD21	1.80	0.47
2:C:857:PRO:HA	2:C:884:VAL:HG12	1.97	0.47
1:B:266:GLU:HG3	1:B:407:TYR:H	1.79	0.47
1:B:275:ILE:HG21	1:B:275:ILE:HD13	1.51	0.47
1:B:138:LYS:HE2	1:B:170:GLN:HB3	1.97	0.46
2:C:703:SER:O	2:C:752:TYR:HD1	1.98	0.46
1:A:263:ASN:HD21	1:A:401:ASN:ND2	2.14	0.46
2:D:878:TRP:CZ3	2:D:951:LEU:HB2	2.50	0.46
1:B:380:LYS:NZ	1:B:488:GLU:OE2	2.47	0.46
2:C:886:ILE:HD11	2:C:990:PHE:HE1	1.81	0.46
1:A:56:ASP:HA	1:A:508:TYR:CE2	2.50	0.46
1:A:209:LEU:HD21	1:A:497:ARG:NE	2.29	0.46
2:D:289:PRO:HD3	2:D:393:SER:OG	2.16	0.46
2:D:441:PHE:HB2	2:D:494:TYR:CD1	2.50	0.46
2:D:576:ARG:HD3	2:D:578:ASP:OD1	2.15	0.46
2:C:352:LEU:HD12	2:C:357:LEU:HD13	1.96	0.46
2:C:397:TRP:HZ2	2:C:415:GLU:HG3	1.80	0.46
2:C:525:ASP:HB2	2:C:541:GLY:H	1.81	0.46
2:C:408:ARG:HG3	2:C:468:GLN:HG2	1.97	0.46
2:C:422:TYR:HA	2:C:456:ALA:HB2	1.95	0.46
1:B:502:LYS:O	1:B:506:ASN:ND2	2.47	0.46
2:C:262:ASN:O	2:C:274:TYR:HB2	2.14	0.46
2:D:525:ASP:HB2	2:D:541:GLY:H	1.79	0.46
2:D:280:LYS:HG2	2:D:281:TYR:CE1	2.51	0.46
2:D:404:TRP:HB3	2:D:405:PRO:HD2	1.96	0.46
1:B:304:PRO:HG2	1:B:345:VAL:HG13	1.98	0.46
1:B:312:PHE:CG	1:B:341:LEU:HB2	2.50	0.46
2:C:791:ASN:N	2:C:791:ASN:HD22	2.13	0.46
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.69	0.46
2:D:255:ASN:HD21	2:D:259:TYR:CB	2.28	0.46
2:D:459:PHE:CZ	2:D:531:PRO:HB3	2.50	0.46
2:D:950:LYS:NZ	2:D:996:GLU:OE2	2.45	0.46
2:C:530:THR:HG23	2:C:533:TYR:H	1.80	0.46
1:A:55:SER:HB2	1:A:491:ARG:HG3	1.97	0.46
1:B:433:ILE:HG23	1:B:480:GLU:HG2	1.99	0.46
2:C:258:GLY:HA2	2:C:259:TYR:O	2.16	0.46
2:C:891:LYS:HE3	2:C:991:THR:HG21	1.98	0.46
2:D:599:TRP:CE2	2:D:601:ILE:HG12	2.51	0.45
2:D:690:GLN:OE1	2:D:713:LYS:HE3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLY:O	1:A:488:GLU:N	2.50	0.45
2:C:822:HIS:CG	2:C:823:ALA:H	2.33	0.45
2:D:315:GLY:HA2	2:D:320:SER:HB3	1.98	0.45
2:D:340:ASP:OD1	2:D:369:SER:HB3	2.17	0.45
2:D:586:ASN:ND2	2:D:587:HIS:ND1	2.65	0.45
2:C:400:PRO:O	2:C:466:GLY:HA3	2.17	0.45
1:A:93:ARG:NH1	2:D:654:TYR:OH	2.48	0.45
2:D:698:SER:O	2:D:699:LEU:HD23	2.16	0.45
2:D:915:TRP:CD1	2:D:920:PRO:HA	2.51	0.45
1:B:15:THR:C	1:B:17:ASP:H	2.20	0.45
1:B:250:GLU:HG2	1:B:266:GLU:HB2	1.99	0.45
2:C:305:ILE:HD13	2:C:328:TYR:OH	2.16	0.45
2:C:315:GLY:HA2	2:C:320:SER:HB3	1.98	0.45
2:C:835:TYR:CZ	2:C:937:ARG:HD3	2.52	0.45
2:D:280:LYS:HG2	2:D:281:TYR:CD1	2.51	0.45
1:B:23:GLU:OE1	1:B:23:GLU:N	2.37	0.45
1:A:36:TRP:NE1	1:A:129:LEU:HD22	2.31	0.45
1:A:263:ASN:HD21	1:A:401:ASN:HD22	1.65	0.45
1:A:275:ILE:HG22	1:A:284:LEU:CD1	2.46	0.45
2:D:496:LEU:HD12	2:D:496:LEU:HA	1.66	0.45
2:D:722:MET:HE3	2:D:782:VAL:HG13	1.97	0.45
2:C:703:SER:O	2:C:752:TYR:CD1	2.69	0.45
2:D:585:LYS:HA	2:D:588:ARG:HG3	1.99	0.45
2:D:780:GLU:OE1	2:D:780:GLU:N	2.39	0.45
1:B:166:THR:O	1:B:170:GLN:N	2.45	0.45
2:D:610:LEU:HD12	2:D:612:TRP:CZ2	2.51	0.45
2:D:616:LEU:HA	2:D:696:ASP:O	2.17	0.45
2:D:808:ILE:HG23	2:D:836:ARG:HG2	1.98	0.45
2:D:905:LEU:O	2:D:907:LYS:HD3	2.17	0.45
2:C:437:PRO:HG2	2:C:441:PHE:HE2	1.82	0.45
2:D:262:ASN:O	2:D:274:TYR:HB2	2.17	0.45
2:C:705:TYR:CZ	2:C:751:GLY:HA3	2.52	0.45
2:C:720:THR:HG21	2:C:788:PHE:HZ	1.82	0.45
1:A:4:PHE:CE1	2:D:553:SER:HB3	2.52	0.44
1:A:389:CYS:HB2	1:A:399:SER:OG	2.17	0.44
2:D:613:LEU:CD1	2:D:699:LEU:CD2	2.95	0.44
2:C:950:LYS:NZ	2:C:996:GLU:HG2	2.32	0.44
2:D:424:TYR:HA	2:D:453:ASN:O	2.17	0.44
2:D:950:LYS:HD2	2:D:984:THR:CG2	2.46	0.44
2:C:325:LEU:HD23	2:C:325:LEU:HA	1.80	0.44
1:A:191:GLU:HG2	2:D:661:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:643:TYR:HD2	2:D:671:SER:HB2	1.81	0.44
1:B:62:GLY:O	1:B:369:SER:HB3	2.17	0.44
2:C:808:ILE:HG21	2:C:838:ILE:HD11	1.98	0.44
1:A:139:GLN:HB3	1:A:493:PHE:CD2	2.53	0.44
2:D:295:TRP:CZ3	2:D:410:PRO:HD2	2.53	0.44
2:D:400:PRO:HG2	2:D:468:GLN:HE21	1.82	0.44
2:C:641:PRO:HB3	2:C:673:PHE:CE1	2.52	0.44
1:A:54:ARG:HH21	1:A:493:PHE:HE1	1.64	0.44
2:D:807:TYR:O	2:D:939:SER:HA	2.17	0.44
1:B:478:LYS:HG2	1:B:498:TRP:CH2	2.52	0.44
2:C:888:SER:OG	2:C:889:ASP:N	2.49	0.44
1:A:277:ASP:HB2	2:D:669:LEU:HG	2.00	0.44
2:D:370:GLU:HB3	2:D:422:TYR:CZ	2.53	0.44
2:D:948:PHE:HA	2:D:985:ILE:O	2.17	0.44
2:C:498:VAL:HG23	2:C:498:VAL:O	2.17	0.44
1:A:19:ILE:HG13	2:D:639:TYR:CG	2.53	0.44
1:A:148:ASN:OD1	1:A:148:ASN:N	2.51	0.44
1:A:491:ARG:O	1:A:494:ASP:HB2	2.17	0.44
2:D:789:GLY:N	2:D:796:VAL:HG21	2.33	0.44
1:A:33:TYR:HB3	2:D:658:TYR:CD2	2.53	0.43
1:A:403:ILE:HG21	1:A:406:ARG:HG2	2.00	0.43
2:C:220:VAL:O	2:C:1009:THR:HG23	2.18	0.43
2:C:345:ARG:HG2	2:C:364:THR:HG23	2.00	0.43
2:C:695:ILE:O	2:C:707:SER:HA	2.18	0.43
2:D:313:SER:HB3	2:D:322:PHE:HD1	1.83	0.43
2:D:569:TYR:OH	2:D:604:GLU:OE2	2.27	0.43
2:C:313:SER:HB3	2:C:322:PHE:HD1	1.83	0.43
2:C:675:ARG:HD2	2:C:678:ILE:HG12	2.00	0.43
1:B:36:TRP:HE1	1:B:129:LEU:HD22	1.82	0.43
1:B:51:TYR:CD1	1:B:532:LEU:HD11	2.53	0.43
1:B:362:LYS:HA	1:B:375:TYR:CD1	2.54	0.43
2:D:523:LYS:HG2	2:D:539:GLY:HA3	2.00	0.43
2:D:748:PHE:HB3	2:D:768:ILE:HG23	2.01	0.43
1:B:11:GLN:HB2	2:C:549:GLY:O	2.18	0.43
1:A:138:LYS:HE3	1:A:171:TRP:CE2	2.52	0.43
2:C:352:LEU:HD12	2:C:357:LEU:CD1	2.47	0.43
2:C:577:ARG:HA	2:C:590:ALA:O	2.18	0.43
1:A:486:GLY:C	1:A:488:GLU:H	2.22	0.43
2:D:870:LYS:O	2:D:871:ASN:HB2	2.18	0.43
2:D:902:VAL:HG23	2:D:905:LEU:CD1	2.48	0.43
2:C:367:ARG:HG3	2:C:425:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:427:MET:SD	2:D:427:MET:N	2.92	0.43
2:D:698:SER:C	2:D:699:LEU:HD23	2.39	0.43
1:B:25:VAL:HG22	1:B:107:SER:OG	2.18	0.43
1:B:100:ARG:NH2	2:C:674:LYS:HB2	2.34	0.43
2:C:370:GLU:HG2	2:C:371:VAL:N	2.34	0.43
2:C:751:GLY:HA2	2:C:764:LEU:O	2.19	0.43
2:C:807:TYR:O	2:C:939:SER:HA	2.18	0.43
2:C:872:PHE:CD2	2:C:956:LEU:HD21	2.53	0.43
2:C:966:LYS:HE3	2:C:966:LYS:HB3	1.82	0.43
2:D:436:THR:HA	2:D:442:ASN:HB3	2.01	0.43
2:C:370:GLU:HB3	2:C:422:TYR:CE2	2.54	0.43
2:C:568:ARG:CG	2:C:603:GLN:HB3	2.48	0.43
2:D:242:TRP:O	2:D:246:VAL:HG13	2.19	0.43
1:B:56:ASP:OD1	1:B:56:ASP:N	2.52	0.43
2:C:576:ARG:HD3	2:C:578:ASP:OD1	2.19	0.43
2:C:637:THR:HG22	2:C:679:GLY:H	1.84	0.43
1:A:42:ILE:HG21	1:A:395:TYR:CD2	2.54	0.42
1:A:222:LEU:HD13	1:A:499:GLY:HA3	2.01	0.42
1:A:474:MET:O	1:A:478:LYS:HG3	2.19	0.42
2:D:324:SER:HB3	2:D:345:ARG:HB2	2.01	0.42
2:D:915:TRP:HE1	2:D:920:PRO:HB3	1.84	0.42
1:B:502:LYS:HG3	1:B:526:GLU:HB2	2.01	0.42
2:C:462:PRO:HD2	2:C:529:LEU:HD13	2.00	0.42
2:C:463:TYR:CD2	2:C:470:ASN:HB2	2.54	0.42
2:D:365:LEU:HD12	2:D:366:ASN:N	2.34	0.42
2:D:857:PRO:HB3	2:D:884:VAL:HG22	1.99	0.42
1:B:127:ARG:NH2	1:B:177:ASP:OD1	2.49	0.42
1:B:142:LYS:HD2	1:B:531:TYR:CE2	2.54	0.42
2:C:426:ARG:NH1	2:C:450:ASP:OD2	2.52	0.42
2:C:563:TYR:CG	2:C:564:SER:N	2.87	0.42
2:C:712:TYR:OH	2:C:742:LYS:HE2	2.19	0.42
2:C:852:ILE:HD13	2:C:940:THR:HG22	2.00	0.42
2:D:318:LYS:O	2:D:351:LYS:N	2.45	0.42
2:D:560:LYS:HG3	2:D:574:THR:HG22	2.01	0.42
2:C:221:SER:HA	2:C:1008:ILE:O	2.20	0.42
2:C:894:SER:O	2:C:911:LEU:HB3	2.19	0.42
1:A:416:GLU:HB2	1:A:477:LEU:HD11	2.01	0.42
2:D:426:ARG:NH1	2:D:450:ASP:OD2	2.51	0.42
1:A:5:LEU:HD21	2:D:555:VAL:HG12	2.01	0.42
1:A:16:GLY:HA3	2:D:637:THR:OG1	2.20	0.42
2:D:950:LYS:HD2	2:D:984:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:LYS:NZ	1:B:503:ASP:OD1	2.45	0.42
2:C:951:LEU:HD22	2:C:982:LEU:HB3	2.01	0.42
1:A:132:HIS:O	1:A:136:MET:HE2	2.20	0.42
2:D:586:ASN:HD22	2:D:587:HIS:CE1	2.38	0.42
2:D:278:LEU:HD23	2:D:278:LEU:HA	1.86	0.42
2:D:832:ARG:HB3	2:D:933:ASN:ND2	2.34	0.42
1:B:412:LEU:HD23	1:B:412:LEU:HA	1.85	0.42
2:C:970:MET:HB3	2:C:971:ASP:H	1.40	0.42
1:A:11:GLN:HB2	2:D:549:GLY:O	2.19	0.42
2:D:345:ARG:C	2:D:346:MET:HG3	2.40	0.42
2:D:362:HIS:O	2:D:429:GLY:HA3	2.20	0.42
2:D:950:LYS:HD3	2:D:984:THR:HB	2.02	0.42
1:B:353:LYS:NZ	1:B:379:LEU:O	2.52	0.42
1:A:320:PRO:HD3	1:A:437:ARG:NH2	2.34	0.42
2:D:234:THR:HG22	2:D:292:ASP:CG	2.40	0.42
2:D:443:LEU:H	2:D:443:LEU:HG	1.76	0.42
2:D:535:TRP:HB3	2:C:547:GLY:O	2.20	0.42
2:C:805:VAL:HG12	2:C:849:GLN:HG3	2.02	0.42
2:D:255:ASN:ND2	2:D:259:TYR:HB2	2.35	0.42
2:D:331:LEU:HD23	2:D:331:LEU:HA	1.69	0.42
2:D:643:TYR:CD2	2:D:671:SER:HB2	2.55	0.42
2:D:708:LEU:HD12	2:D:747:GLU:O	2.19	0.42
2:D:878:TRP:CE2	2:D:951:LEU:HD13	2.55	0.42
2:C:764:LEU:HD22	2:C:865:ILE:HG12	2.02	0.42
2:C:812:ILE:HG13	2:C:814:LYS:HE2	2.01	0.42
2:C:852:ILE:HD12	2:C:943:VAL:HG21	2.02	0.42
2:D:748:PHE:HB3	2:D:768:ILE:CG2	2.49	0.41
1:A:266:GLU:HG3	1:A:407:TYR:H	1.84	0.41
2:C:608:LYS:H	2:C:608:LYS:HG2	1.58	0.41
2:D:888:SER:HB2	2:D:998:PRO:HB2	2.01	0.41
1:B:368:ARG:HG2	2:C:403:GLY:HA2	2.02	0.41
1:B:475:LYS:HE2	1:B:475:LYS:HB3	1.92	0.41
1:B:277:ASP:HB2	2:C:669:LEU:HG	2.01	0.41
2:C:377:ILE:HD13	2:C:377:ILE:HA	1.98	0.41
2:D:293:THR:HG21	2:D:295:TRP:CD2	2.56	0.41
2:C:236:GLN:O	2:C:239:ARG:N	2.53	0.41
2:C:258:GLY:CA	2:C:259:TYR:HB2	2.51	0.41
2:C:601:ILE:HG22	2:C:616:LEU:HB3	2.02	0.41
2:C:788:PHE:CD1	2:C:801:TYR:CE2	3.08	0.41
1:A:475:LYS:HB3	1:A:475:LYS:HE2	1.90	0.41
1:B:416:GLU:HB2	1:B:477:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:O	1:B:430:ILE:HG12	2.21	0.41
2:C:598:GLY:HA2	2:C:618:LEU:O	2.21	0.41
2:D:498:VAL:O	2:D:501:HIS:HB2	2.20	0.41
2:D:789:GLY:CA	2:D:796:VAL:HG21	2.50	0.41
1:B:42:ILE:HG21	1:B:395:TYR:CD2	2.56	0.41
1:B:136:MET:HE2	1:B:136:MET:HB2	1.89	0.41
2:C:244:ALA:HB2	2:C:927:LEU:HB3	2.03	0.41
2:C:720:THR:HG21	2:C:788:PHE:CZ	2.55	0.41
1:A:59:TYR:HA	1:A:75:GLU:OE2	2.21	0.41
1:A:304:PRO:HG2	1:A:345:VAL:HG13	2.02	0.41
2:D:528:ILE:HD12	2:D:533:TYR:CD1	2.56	0.41
2:D:694:GLY:HA2	2:D:709:GLU:HA	2.02	0.41
2:D:699:LEU:N	2:D:704:LEU:O	2.49	0.41
2:C:808:ILE:HG21	2:C:808:ILE:HD13	1.77	0.41
2:C:986:LYS:HD2	2:C:986:LYS:N	2.19	0.41
1:A:52:ASP:CG	1:A:489:SER:HA	2.41	0.41
1:A:187:GLU:OE2	1:A:244:LYS:HD3	2.21	0.41
1:A:268:VAL:HB	1:A:405:ILE:O	2.21	0.41
2:D:212:ILE:HD11	2:C:318:LYS:HB3	2.03	0.41
2:D:233:ASN:HB2	2:D:236:GLN:CD	2.41	0.41
2:D:241:MET:HE1	2:D:255:ASN:HD22	1.85	0.41
2:D:414:LEU:HD23	2:D:414:LEU:HA	1.88	0.41
2:D:552:TYR:HE2	2:D:554:LEU:HD11	1.86	0.41
2:D:614:ASP:OD2	2:D:702:GLN:HG2	2.21	0.41
2:D:833:ILE:HD11	2:D:925:PRO:HG3	2.03	0.41
1:B:155:ASP:OD1	1:B:155:ASP:N	2.38	0.41
2:C:334:ILE:HD11	2:C:378:ILE:HD11	2.03	0.41
2:C:338:ASP:O	2:C:370:GLU:HG3	2.21	0.41
2:C:616:LEU:HA	2:C:696:ASP:O	2.20	0.41
2:D:453:ASN:ND2	2:C:451:TYR:OH	2.54	0.41
2:D:866:TYR:O	2:D:867:LEU:HD12	2.21	0.41
2:C:349:ASP:C	2:C:350:TYR:CD1	2.95	0.41
1:A:400:LEU:HA	1:A:400:LEU:HD12	1.75	0.40
2:D:934:ASN:O	2:D:937:ARG:HD2	2.20	0.40
1:B:474:MET:HE3	1:B:478:LYS:HE3	2.03	0.40
2:C:704:LEU:HD12	2:C:704:LEU:HA	1.86	0.40
1:A:283:ASN:ND2	2:D:657:ALA:O	2.53	0.40
2:D:538:ALA:HA	2:C:641:PRO:HG2	2.03	0.40
2:D:588:ARG:HH11	2:D:588:ARG:HG2	1.86	0.40
2:D:639:TYR:CZ	2:D:675:ARG:HB2	2.56	0.40
2:D:674:LYS:HG3	2:D:730:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:TYR:CD1	1:B:476:MET:HE3	2.57	0.40
2:C:232:LEU:N	2:C:906:ASN:HD21	2.06	0.40
2:C:245:TYR:CD2	2:C:252:PRO:HA	2.57	0.40
2:C:891:LYS:HG2	2:C:895:ASP:OD2	2.20	0.40
2:C:909:THR:O	2:C:912:LEU:HB2	2.20	0.40
2:D:443:LEU:HA	2:D:492:ALA:HA	2.03	0.40
2:D:641:PRO:O	2:D:642:ASN:C	2.59	0.40
2:D:705:TYR:CE2	2:D:751:GLY:HA3	2.56	0.40
1:B:165:TYR:HB3	1:B:169:GLU:HB3	2.02	0.40
2:C:808:ILE:HA	2:C:940:THR:HG23	2.02	0.40
2:C:852:ILE:HB	2:C:940:THR:HG22	2.03	0.40
2:D:318:LYS:HA	2:D:318:LYS:HD3	1.50	0.40
2:D:382:LEU:HB3	2:D:893:LYS:NZ	2.37	0.40
1:B:271:ILE:HA	2:C:658:TYR:OH	2.22	0.40
2:C:462:PRO:HD2	2:C:529:LEU:CD1	2.52	0.40

There are no symmetry-related clashes.

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	552/576 (96%)	500 (91%)	48 (9%)	4 (1%)	22 57
1	B	553/576 (96%)	514 (93%)	36 (6%)	3 (0%)	29 64
2	C	805/1041 (77%)	716 (89%)	68 (8%)	21 (3%)	5 26
2	D	805/1041 (77%)	714 (89%)	72 (9%)	19 (2%)	6 27
All	All	2715/3234 (84%)	2444 (90%)	224 (8%)	47 (2%)	9 36

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	608	LYS
2	D	826	GLU
2	D	993	GLU
2	C	732	GLY
2	C	971	ASP
2	C	988	LYS
2	C	993	GLU
1	A	422	ASN
2	D	258	GLY
2	D	268	ASP
2	D	318	LYS
2	D	471	ASN
2	D	642	ASN
2	D	700	PHE
2	C	258	GLY
2	C	294	ASP
2	C	396	SER
2	C	406	ASP
2	C	826	GLU
2	C	970	MET
1	A	487	MET
1	A	491	ARG
2	D	375	GLY
2	D	845	ASP
1	B	267	SER
1	B	422	ASN
1	B	528	LYS
2	C	807	TYR
1	A	528	LYS
2	D	267	ALA
2	D	824	THR
2	D	971	ASP
2	C	437	PRO
2	C	797	VAL
2	C	822	HIS
2	D	396	SER
2	D	406	ASP
2	D	438	PHE
2	D	584	GLY
2	C	354	ASP
2	C	787	LYS
2	C	912	LEU
2	D	920	PRO

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Mol	Chain	Res	Type
2	C	718	ILE
2	C	1003	PRO
2	C	938	VAL
2	C	641	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	475/495 (96%)	469 (99%)	6 (1%)	69	87
1	B	476/495 (96%)	469 (98%)	7 (2%)	65	85
2	C	673/869 (77%)	644 (96%)	29 (4%)	29	62
2	D	673/869 (77%)	637 (95%)	36 (5%)	22	54
All	All	2297/2728 (84%)	2219 (97%)	78 (3%)	37	69

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	203	TYR
1	A	228	GLU
1	A	263	ASN
1	A	428	ASP
1	A	537	GLU
2	D	213	LYS
2	D	226	GLN
2	D	268	ASP
2	D	279	SER
2	D	317	GLU
2	D	341	ARG
2	D	354	ASP
2	D	357	LEU
2	D	470	ASN
2	D	502	ARG
2	D	506	MET

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Mol	Chain	Res	Type
2	D	516	ASP
2	D	517	SER
2	D	565	TYR
2	D	582	ARG
2	D	585	LYS
2	D	597	LEU
2	D	605	ASN
2	D	635	ARG
2	D	692	ASN
2	D	710	TYR
2	D	722	MET
2	D	730	GLU
2	D	747	GLU
2	D	753	ARG
2	D	754	ASN
2	D	772	ARG
2	D	773	ASN
2	D	787	LYS
2	D	801	TYR
2	D	834	ARG
2	D	895	ASP
2	D	910	ARG
2	D	911	LEU
2	D	950	LYS
2	D	971	ASP
1	B	3	ASP
1	B	17	ASP
1	B	106	GLN
1	B	203	TYR
1	B	228	GLU
1	B	317	GLN
1	B	502	LYS
2	C	228	LYS
2	C	278	LEU
2	C	426	ARG
2	C	427	MET
2	C	434	ASN
2	C	438	PHE
2	C	439	LYS
2	C	487	MET
2	C	504	ASP
2	C	506	MET

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Mol	Chain	Res	Type
2	C	565	TYR
2	C	568	ARG
2	C	569	TYR
2	C	586	ASN
2	C	597	LEU
2	C	614	ASP
2	C	628	GLN
2	C	684	LYS
2	C	696	ASP
2	C	701	LYS
2	C	747	GLU
2	C	814	LYS
2	C	834	ARG
2	C	969	ARG
2	C	970	MET
2	C	972	ARG
2	C	977	CYS
2	C	986	LYS
2	C	1012	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
2	D	255	ASN
2	D	849	GLN
1	B	106	GLN
1	B	110	GLN
2	C	442	ASN
2	C	791	ASN
2	C	906	ASN
2	C	913	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	552/576 (95%)	-0.38	1 (0%) 95 90	47, 83, 111, 146	0
1	B	553/576 (96%)	-0.33	0 100 100	37, 65, 95, 124	0
2	C	807/1041 (77%)	-0.44	0 100 100	37, 64, 104, 150	0
2	D	807/1041 (77%)	-0.39	0 100 100	35, 71, 111, 146	0
All	All	2719/3234 (84%)	-0.39	1 (0%) 100 100	35, 70, 108, 150	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	CYS	2.1

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

There are no monosaccharides in this entry.

6.4 Ligands

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, 95^{th} 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	MG	A	602	1/1	0.84	0.09	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	B	602	1/1	0.94	0.17	113,113,113,113	0
3	MG	B	601	1/1	0.96	0.12	4,4,4,4	0
3	MG	C	1101	1/1	0.96	0.22	47,47,47,47	0
3	MG	A	601	1/1	0.97	0.16	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.