



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 12:21 AM EST

PDB ID : 3OPB  
Title : Crystal structure of She4p  
Authors : Shi, H.; Blobel, G.  
Deposited on : 2010-08-31  
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](mailto: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>.

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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

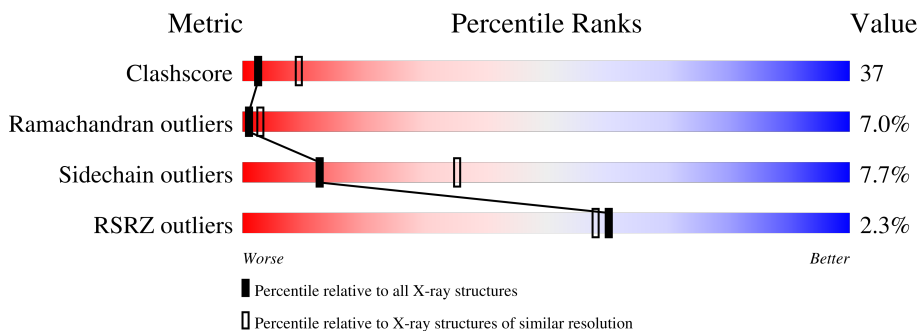
# 1 Overall quality at a glance

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))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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  $\geq 3$ , 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	778	 3% 36% 52% 8% . .
1	B	778	 % 41% 45% 8% . 5%

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 12015 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 SWI5-dependent HO expression protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	747	Total	C	N	O	S	0	0	0
			5954	3824	980	1124	26			
1	B	741	Total	C	N	O	S	0	0	0
			5920	3804	977	1113	26			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P51534
A	-3	SER	-	expression tag	UNP P51534
A	-2	PRO	-	expression tag	UNP P51534
A	-1	GLY	-	expression tag	UNP P51534
A	0	HIS	-	expression tag	UNP P51534
A	4	SER	CYS	engineered mutation	UNP P51534
A	?	-	MET	deletion	UNP P51534
A	?	-	PRO	deletion	UNP P51534
A	?	-	LYS	deletion	UNP P51534
A	?	-	ILE	deletion	UNP P51534
A	?	-	GLU	deletion	UNP P51534
A	?	-	ASN	deletion	UNP P51534
A	?	-	VAL	deletion	UNP P51534
A	?	-	ASN	deletion	UNP P51534
A	?	-	GLU	deletion	UNP P51534
A	?	-	SER	deletion	UNP P51534
A	?	-	ALA	deletion	UNP P51534
A	?	-	VAL	deletion	UNP P51534
A	?	-	LYS	deletion	UNP P51534
A	?	-	LEU	deletion	UNP P51534
A	?	-	GLU	deletion	UNP P51534
A	?	-	GLU	deletion	UNP P51534
A	406	UNK	SER	SEE REMARK 999	UNP P51534
A	407	UNK	ASN	SEE REMARK 999	UNP P51534
A	408	UNK	GLY	SEE REMARK 999	UNP P51534

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Chain	Residue	Modelled	Actual	Comment	Reference
A	409	UNK	SER	SEE REMARK 999	UNP P51534
A	410	UNK	SER	SEE REMARK 999	UNP P51534
A	411	UNK	GLN	SEE REMARK 999	UNP P51534
A	412	UNK	SER	SEE REMARK 999	UNP P51534
A	413	UNK	ILE	SEE REMARK 999	UNP P51534
A	414	UNK	ASN	SEE REMARK 999	UNP P51534
A	415	UNK	ASP	SEE REMARK 999	UNP P51534
A	416	UNK	LEU	SEE REMARK 999	UNP P51534
A	417	UNK	LYS	SEE REMARK 999	UNP P51534
A	418	UNK	ASN	SEE REMARK 999	UNP P51534
A	419	UNK	TYR	SEE REMARK 999	UNP P51534
A	420	UNK	ALA	SEE REMARK 999	UNP P51534
A	421	UNK	ASP	SEE REMARK 999	UNP P51534
A	422	UNK	LEU	SEE REMARK 999	UNP P51534
A	423	UNK	LYS	SEE REMARK 999	UNP P51534
A	424	UNK	GLY	SEE REMARK 999	UNP P51534
A	426	ALA	GLY	engineered mutation	UNP P51534
A	435	ALA	GLU	engineered mutation	UNP P51534
A	436	ALA	SER	engineered mutation	UNP P51534
A	475	ILE	VAL	engineered mutation	UNP P51534
A	489	LEU	CYS	engineered mutation	UNP P51534
A	490	ALA	ILE	engineered mutation	UNP P51534
A	491	GLN	SER	engineered mutation	UNP P51534
A	494	ALA	GLY	engineered mutation	UNP P51534
A	495	VAL	THR	engineered mutation	UNP P51534
A	496	LYS	THR	engineered mutation	UNP P51534
B	-4	GLY	-	expression tag	UNP P51534
B	-3	SER	-	expression tag	UNP P51534
B	-2	PRO	-	expression tag	UNP P51534
B	-1	GLY	-	expression tag	UNP P51534
B	0	HIS	-	expression tag	UNP P51534
B	4	SER	CYS	engineered mutation	UNP P51534
B	?	-	MET	deletion	UNP P51534
B	?	-	PRO	deletion	UNP P51534
B	?	-	LYS	deletion	UNP P51534
B	?	-	ILE	deletion	UNP P51534
B	?	-	GLU	deletion	UNP P51534
B	?	-	ASN	deletion	UNP P51534
B	?	-	VAL	deletion	UNP P51534
B	?	-	ASN	deletion	UNP P51534
B	?	-	GLU	deletion	UNP P51534
B	?	-	SER	deletion	UNP P51534

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP P51534
B	?	-	VAL	deletion	UNP P51534
B	?	-	LYS	deletion	UNP P51534
B	?	-	LEU	deletion	UNP P51534
B	?	-	GLU	deletion	UNP P51534
B	?	-	GLU	deletion	UNP P51534
B	406	UNK	SER	SEE REMARK 999	UNP P51534
B	407	UNK	ASN	SEE REMARK 999	UNP P51534
B	408	UNK	GLY	SEE REMARK 999	UNP P51534
B	409	UNK	SER	SEE REMARK 999	UNP P51534
B	410	UNK	SER	SEE REMARK 999	UNP P51534
B	411	UNK	GLN	SEE REMARK 999	UNP P51534
B	412	UNK	SER	SEE REMARK 999	UNP P51534
B	413	UNK	ILE	SEE REMARK 999	UNP P51534
B	414	UNK	ASN	SEE REMARK 999	UNP P51534
B	415	UNK	ASP	SEE REMARK 999	UNP P51534
B	416	UNK	LEU	SEE REMARK 999	UNP P51534
B	417	UNK	LYS	SEE REMARK 999	UNP P51534
B	418	UNK	ASN	SEE REMARK 999	UNP P51534
B	419	UNK	TYR	SEE REMARK 999	UNP P51534
B	420	UNK	ALA	SEE REMARK 999	UNP P51534
B	421	UNK	ASP	SEE REMARK 999	UNP P51534
B	422	UNK	LEU	SEE REMARK 999	UNP P51534
B	423	UNK	LYS	SEE REMARK 999	UNP P51534
B	424	UNK	GLY	SEE REMARK 999	UNP P51534
B	426	ALA	GLY	engineered mutation	UNP P51534
B	435	ALA	GLU	engineered mutation	UNP P51534
B	436	ALA	SER	engineered mutation	UNP P51534
B	475	ILE	VAL	engineered mutation	UNP P51534
B	489	LEU	CYS	engineered mutation	UNP P51534
B	490	ALA	ILE	engineered mutation	UNP P51534
B	491	GLN	SER	engineered mutation	UNP P51534
B	494	ALA	GLY	engineered mutation	UNP P51534
B	495	VAL	THR	engineered mutation	UNP P51534
B	496	LYS	THR	engineered mutation	UNP P51534

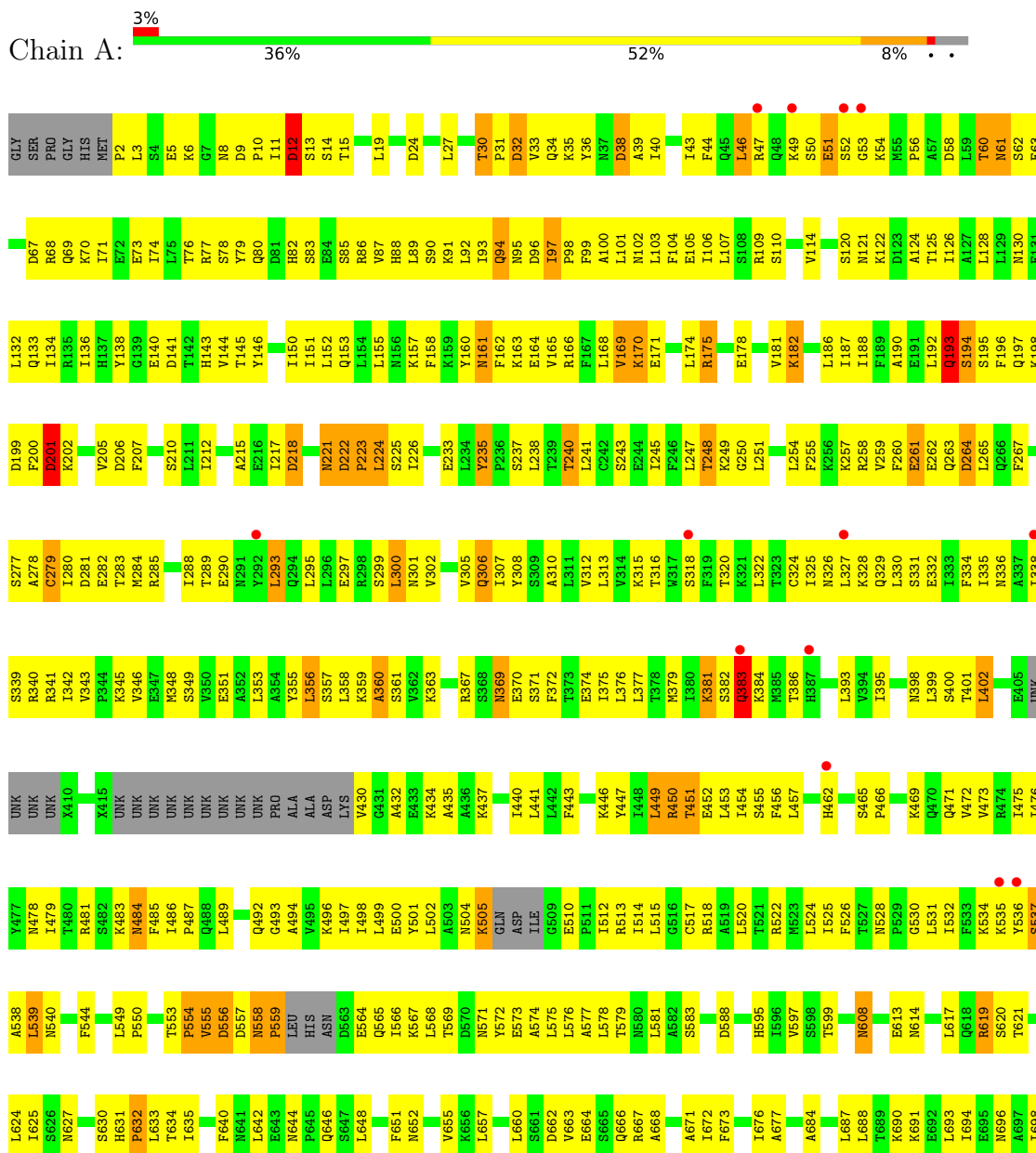
- Molecule 2 is water.

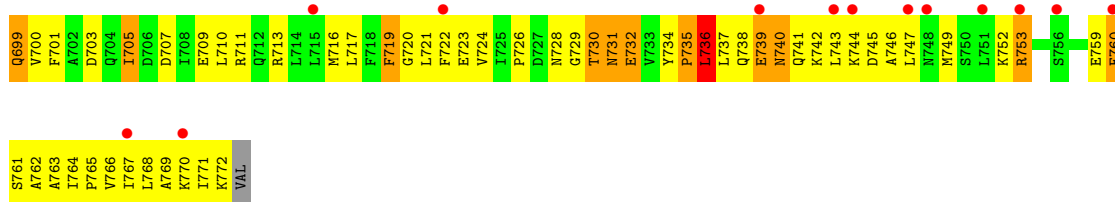
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	66	Total O 66 66	0	0
2	B	75	Total O 75 75	0	0

### 3 Residue-property plots

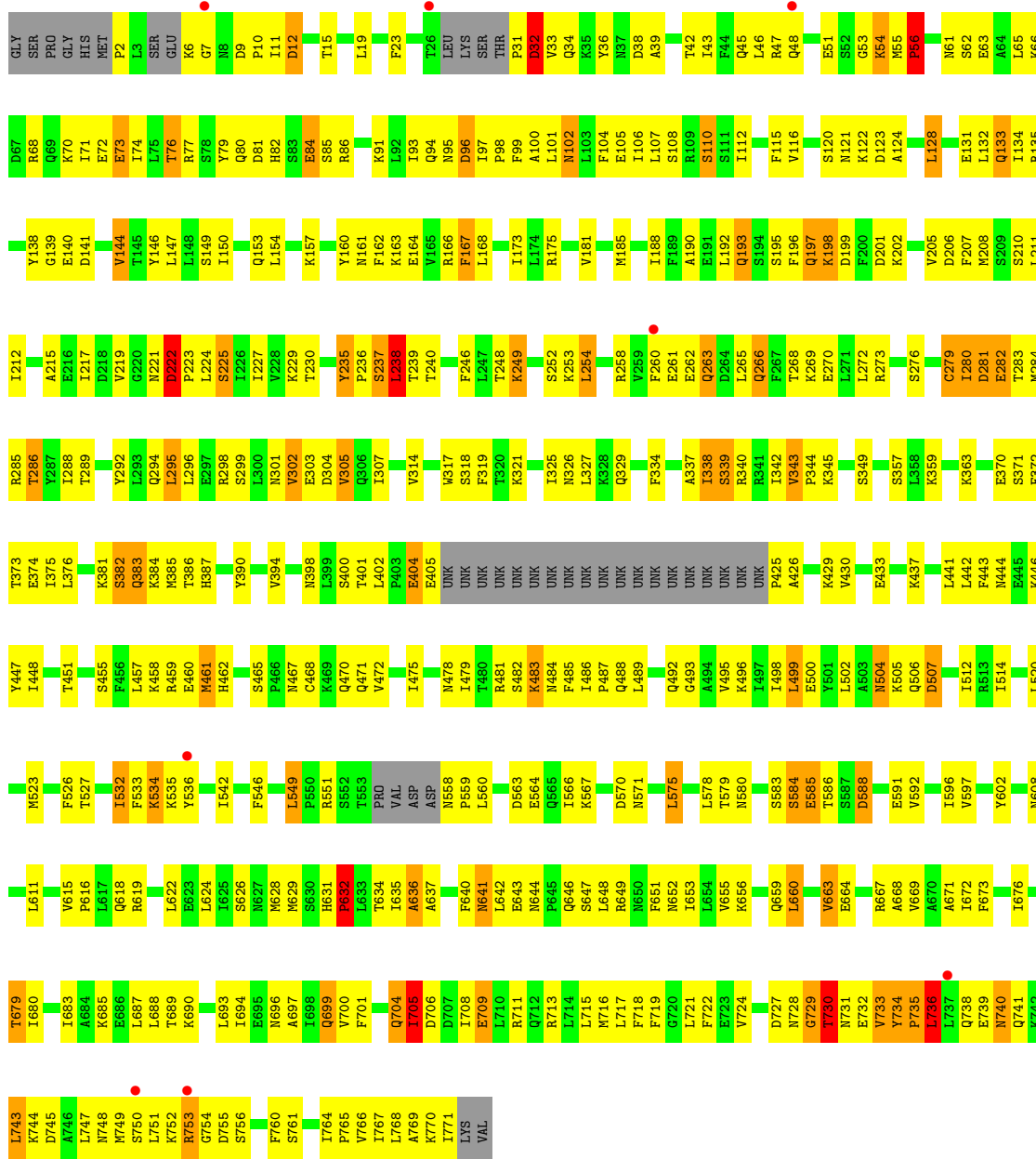
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: SWI5-dependent HO expression protein 4





● Molecule 1: SWI5-dependent HO expression protein 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.02Å 149.94Å 158.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.00 – 2.90 42.95 – 2.83	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.00-2.90) 83.0 (42.95-2.83)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.37 (at 2.81Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.231 , 0.296 0.246 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	75.8	Xtrriage
Anisotropy	0.683	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 74.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12015	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1003e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.40	0/6012	0.65	0/8121
1	B	0.42	0/6006	0.67	2/8109 (0.0%)
All	All	0.41	0/12018	0.66	2/16230 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	PRO	N-CA-CB	5.67	110.10	103.30
1	B	222	ASP	N-CA-C	-5.21	96.93	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5954	0	6152	471	0
1	B	5920	0	6132	436	0
2	A	66	0	0	22	0
2	B	75	0	0	21	0
All	All	12015	0	12284	890	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 37.

All (890) 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:A:61:ASN:CG	1:A:62:SER:H	1.65	0.99
1:B:655:VAL:HG12	1:B:693:LEU:HD13	1.44	0.98
1:B:667:ARG:HD2	1:B:709:GLU:HB3	1.45	0.98
1:B:99:PHE:HA	1:B:102:ASN:HD21	1.28	0.97
1:A:363:LYS:HE3	1:A:398:ASN:O	1.65	0.96
1:A:101:LEU:O	1:A:105:GLU:HG3	1.67	0.94
1:A:555:VAL:HG22	1:A:556:ASP:H	1.31	0.94
1:A:734:TYR:O	1:A:738:GLN:HB2	1.67	0.93
1:A:528:ASN:HD22	1:A:531:LEU:H	1.14	0.92
1:B:629:MET:HG3	1:B:672:ILE:HG23	1.49	0.92
1:B:72:GLU:HB2	1:B:107:LEU:HD22	1.50	0.92
1:B:738:GLN:HG3	1:B:739:GLU:HG3	1.47	0.92
1:B:705:ILE:HG12	1:B:711:ARG:HD3	1.53	0.91
1:B:426:ALA:HB3	2:B:800:HOH:O	1.69	0.91
1:A:198:LYS:HA	1:A:201:ASP:HB2	1.53	0.90
1:B:235:TYR:O	1:B:239:THR:HG22	1.72	0.90
1:A:5:GLU:HG2	1:A:12:ASP:HA	1.52	0.90
1:A:109:ARG:HE	1:B:80:GLN:HE22	1.19	0.89
1:A:549:LEU:HD23	1:A:571:ASN:HD22	1.35	0.89
1:B:342:ILE:HG21	1:B:345:LYS:HB2	1.55	0.88
1:B:461:MET:HE3	1:B:472:VAL:HG11	1.56	0.87
1:B:481:ARG:HG2	1:B:481:ARG:HH11	1.39	0.87
1:B:741:GLN:NE2	1:B:745:ASP:HB2	1.89	0.87
1:B:343:VAL:HB	1:B:344:PRO:HD3	1.56	0.85
1:A:360:ALA:HA	1:A:363:LYS:HB2	1.57	0.84
1:B:542:ILE:HD11	1:B:592:VAL:HG13	1.58	0.84
1:A:619:ARG:HG3	1:A:620:SER:N	1.93	0.84
1:B:268:THR:HG22	1:B:305:VAL:HG21	1.60	0.83
1:A:505:LYS:H	1:A:505:LYS:HD2	1.41	0.83
1:A:328:LYS:NZ	1:A:361:SER:HB3	1.93	0.83
1:A:535:LYS:HD3	2:A:775:HOH:O	1.78	0.82
1:B:736:LEU:HD12	1:B:736:LEU:H	1.43	0.82
1:A:24:ASP:OD2	1:B:280:ILE:HG23	1.78	0.82
1:B:583:SER:O	1:B:585:GLU:N	2.11	0.82
1:A:663:VAL:HA	1:A:666:GLN:HE21	1.42	0.81
1:A:264:ASP:HB3	1:A:267:PHE:HB3	1.61	0.81
1:B:735:PRO:HA	1:B:738:GLN:HG2	1.62	0.79
1:A:632:PRO:O	1:A:634:THR:N	2.15	0.79
1:A:740:ASN:ND2	1:A:743:LEU:H	1.79	0.79
1:B:404:GLU:O	1:B:405:GLU:HG3	1.82	0.79
1:B:72:GLU:O	1:B:76:THR:HG22	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:LEU:HD23	1:A:690:LYS:NZ	1.97	0.78
1:B:749:MET:HA	1:B:752:LYS:HD3	1.66	0.78
1:A:484:ASN:O	1:A:487:PRO:HD2	1.85	0.77
1:B:734:TYR:O	1:B:738:GLN:HB3	1.85	0.77
1:B:7:GLY:N	1:B:10:PRO:HG3	1.99	0.77
1:B:342:ILE:CG2	1:B:343:VAL:N	2.48	0.77
1:A:61:ASN:CG	1:A:62:SER:N	2.36	0.76
1:A:619:ARG:HE	1:A:664:GLU:HB3	1.49	0.76
1:B:326:ASN:OD1	1:B:329:GLN:HB2	1.85	0.76
1:A:514:ILE:HG22	1:A:518:ARG:HH12	1.52	0.75
1:B:611:LEU:HD11	1:B:653:ILE:HD13	1.69	0.75
1:A:395:ILE:O	1:A:399:LEU:HD23	1.87	0.75
1:A:332:GLU:O	1:A:336:ASN:HB2	1.87	0.75
1:B:385:MET:HA	1:B:387:HIS:CE1	2.22	0.75
1:B:526:PHE:O	1:B:527:THR:HG23	1.87	0.74
1:A:450:ARG:C	1:A:452:GLU:H	1.89	0.74
1:B:102:ASN:H	1:B:102:ASN:ND2	1.85	0.74
1:B:31:PRO:O	1:B:33:VAL:HG23	1.87	0.74
1:A:676:ILE:HD12	1:A:677:ALA:H	1.53	0.74
1:A:212:ILE:HD11	1:A:251:LEU:HD22	1.69	0.73
1:B:6:LYS:N	1:B:10:PRO:HB3	2.04	0.73
1:B:238:LEU:HD23	1:B:238:LEU:H	1.51	0.73
1:B:173:ILE:HA	1:B:185:MET:HE1	1.70	0.73
1:A:565:GLN:HG2	1:A:566:ILE:N	2.04	0.72
1:A:558:ASN:OD1	1:A:559:PRO:HD2	1.89	0.72
1:B:161:ASN:HB3	1:B:164:GLU:HG3	1.71	0.72
1:B:102:ASN:HD22	1:B:102:ASN:N	1.87	0.72
1:A:567:LYS:HG2	1:A:569:THR:H	1.53	0.72
1:A:729:GLY:O	1:A:731:ASN:N	2.21	0.72
1:B:43:ILE:HD12	1:B:71:ILE:HD12	1.71	0.72
1:B:99:PHE:CA	1:B:102:ASN:HD21	2.03	0.72
1:A:2:PRO:HG2	1:A:5:GLU:OE1	1.90	0.71
1:B:370:GLU:O	1:B:374:GLU:HG2	1.91	0.71
1:A:520:LEU:O	1:A:524:LEU:HD13	1.90	0.71
1:A:514:ILE:HG22	1:A:518:ARG:NH1	2.06	0.71
1:B:457:LEU:HD13	1:B:472:VAL:HG22	1.71	0.71
1:B:444:ASN:O	1:B:448:ILE:HB	1.89	0.71
1:A:568:LEU:HD11	1:A:617:LEU:HD11	1.73	0.70
1:A:69:GLN:HB2	2:B:832:HOH:O	1.91	0.70
1:B:736:LEU:HD12	1:B:736:LEU:N	2.07	0.70
1:B:47:ARG:HG3	1:B:53:GLY:HA2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:ARG:HG2	1:A:267:PHE:CD2	2.27	0.70
1:B:104:PHE:HA	1:B:107:LEU:HD12	1.72	0.70
1:A:198:LYS:HB3	1:A:202:LYS:HE3	1.72	0.70
1:B:752:LYS:NZ	1:B:752:LYS:HB3	2.07	0.70
1:A:334:PHE:O	1:A:338:ILE:HG13	1.92	0.69
1:A:676:ILE:HD12	1:A:677:ALA:N	2.06	0.69
1:B:101:LEU:HD21	1:B:132:LEU:HD23	1.74	0.69
1:A:83:SER:O	1:A:87:VAL:HG23	1.91	0.69
1:A:109:ARG:HE	1:B:80:GLN:NE2	1.90	0.69
1:B:68:ARG:HD2	1:B:106:ILE:HG22	1.75	0.69
1:A:705:ILE:HG22	1:A:711:ARG:HD3	1.75	0.69
1:A:762:ALA:O	1:A:766:VAL:HG23	1.92	0.69
1:B:753:ARG:C	1:B:755:ASP:H	1.93	0.69
1:A:36:TYR:HE1	1:A:77:ARG:HD3	1.58	0.69
1:A:99:PHE:HA	1:A:102:ASN:HD22	1.58	0.69
1:B:549:LEU:HD11	1:B:575:LEU:HD22	1.73	0.69
1:B:42:THR:O	1:B:45:GLN:HB2	1.93	0.69
1:B:688:LEU:HD11	1:B:724:VAL:HG23	1.75	0.68
1:A:687:LEU:HD23	1:A:690:LYS:HZ2	1.56	0.68
1:B:70:LYS:O	1:B:74:ILE:HD13	1.93	0.68
1:A:528:ASN:ND2	1:A:531:LEU:H	1.89	0.68
1:A:73:GLU:OE1	1:B:108:SER:HB2	1.93	0.68
1:A:263:GLN:HA	2:A:801:HOH:O	1.94	0.68
1:A:572:TYR:CE1	1:A:576:LEU:HD11	2.29	0.68
1:B:161:ASN:HD21	1:B:163:LYS:HD2	1.58	0.68
1:A:486:ILE:HD11	1:A:522:ARG:HG3	1.75	0.68
1:B:481:ARG:HG2	1:B:481:ARG:NH1	2.09	0.67
1:B:342:ILE:HG23	1:B:343:VAL:H	1.58	0.67
1:B:465:SER:HB2	2:B:844:HOH:O	1.94	0.67
1:A:369:ASN:ND2	1:A:372:PHE:HB2	2.09	0.67
1:A:630:SER:C	1:A:632:PRO:HD3	2.15	0.67
1:B:302:VAL:HB	1:B:305:VAL:HG12	1.76	0.67
1:A:736:LEU:H	1:A:736:LEU:HD12	1.57	0.67
1:A:338:ILE:HG22	1:A:338:ILE:O	1.95	0.67
1:A:207:PHE:O	1:A:210:SER:HB3	1.95	0.67
1:A:557:ASP:O	1:A:558:ASN:HB3	1.95	0.67
1:B:667:ARG:CD	1:B:709:GLU:HB3	2.23	0.67
1:A:471:GLN:O	1:A:475:ILE:HG13	1.95	0.66
1:A:673:PHE:HA	1:A:676:ILE:HD11	1.76	0.66
1:B:738:GLN:HG3	1:B:739:GLU:N	2.10	0.66
1:A:326:ASN:ND2	1:A:328:LYS:HG2	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:HG2	1:A:443:PHE:CD1	2.31	0.66
1:B:729:GLY:O	1:B:731:ASN:N	2.28	0.66
1:B:735:PRO:O	1:B:738:GLN:HG2	1.96	0.66
1:A:736:LEU:HD12	1:A:736:LEU:N	2.10	0.66
1:A:338:ILE:HD11	1:A:349:SER:CB	2.26	0.66
1:A:12:ASP:O	1:A:14:SER:N	2.29	0.66
1:A:217:ILE:O	1:A:218:ASP:HB2	1.94	0.66
1:A:102:ASN:HA	1:A:105:GLU:OE2	1.96	0.66
1:B:102:ASN:ND2	1:B:102:ASN:N	2.43	0.66
1:A:157:LYS:HG2	1:A:157:LYS:O	1.96	0.65
1:A:525:ILE:HG13	1:A:577:ALA:HB2	1.78	0.65
1:A:640:PHE:CE2	1:A:676:ILE:HG12	2.31	0.65
1:B:149:SER:O	1:B:153:GLN:HG2	1.96	0.65
1:B:644:ASN:HB3	1:B:647:SER:HB3	1.77	0.65
1:A:313:LEU:HD23	1:A:318:SER:HB2	1.78	0.65
1:B:635:ILE:O	1:B:637:ALA:N	2.30	0.65
1:A:212:ILE:CD1	1:A:251:LEU:HD22	2.26	0.65
1:A:377:LEU:HD11	1:A:447:TYR:HB3	1.78	0.65
1:A:300:LEU:HD13	1:A:325:ILE:CD1	2.27	0.65
1:A:550:PRO:HD3	1:A:571:ASN:ND2	2.12	0.65
1:A:740:ASN:HD22	1:A:743:LEU:CB	2.10	0.65
1:B:162:PHE:HB2	1:B:196:PHE:CD2	2.32	0.65
1:B:282:GLU:HA	1:B:285:ARG:HB2	1.79	0.65
1:A:11:ILE:HG22	1:A:11:ILE:O	1.96	0.64
1:A:572:TYR:O	1:A:576:LEU:HD13	1.97	0.64
1:B:690:LYS:O	1:B:694:ILE:HG12	1.97	0.64
1:A:355:TYR:CD2	1:B:19:LEU:HD23	2.32	0.64
1:B:38:ASP:O	1:B:42:THR:HG23	1.98	0.64
1:B:97:ILE:HB	1:B:98:PRO:HD3	1.77	0.64
1:B:371:SER:O	1:B:374:GLU:HB2	1.96	0.64
1:B:162:PHE:HB2	1:B:196:PHE:CE2	2.32	0.64
1:A:367:ARG:HG3	1:A:399:LEU:HD12	1.78	0.64
1:A:687:LEU:HD22	1:A:693:LEU:CD2	2.27	0.64
1:B:338:ILE:HG22	1:B:339:SER:N	2.13	0.64
1:A:768:LEU:HD23	1:A:771:ILE:HD12	1.79	0.64
1:B:668:ALA:O	1:B:671:ALA:HB3	1.98	0.63
1:A:328:LYS:HZ3	1:A:361:SER:HB3	1.62	0.63
1:A:565:GLN:HG2	1:A:566:ILE:H	1.63	0.63
1:A:6:LYS:HB2	1:A:6:LYS:NZ	2.12	0.63
1:A:716:MET:HB3	2:A:784:HOH:O	1.99	0.63
1:B:739:GLU:O	1:B:740:ASN:C	2.36	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:ASN:HB3	1:A:617:LEU:HD12	1.80	0.63
1:B:383:GLN:O	1:B:385:MET:N	2.31	0.63
1:A:161:ASN:HD22	1:A:163:LYS:HE3	1.64	0.63
1:A:698:ILE:HD13	1:A:740:ASN:ND2	2.14	0.63
1:A:300:LEU:HD13	1:A:325:ILE:HD11	1.80	0.62
1:A:49:LYS:HD3	2:A:828:HOH:O	1.98	0.62
1:B:470:GLN:HB3	1:B:512:ILE:HD13	1.80	0.62
1:A:126:ILE:HD13	1:A:164:GLU:OE2	1.99	0.62
1:B:43:ILE:O	1:B:46:LEU:HD13	1.99	0.62
1:B:102:ASN:HA	1:B:105:GLU:OE2	1.99	0.62
1:B:266:GLN:O	1:B:270:GLU:HG2	2.00	0.62
1:B:437:LYS:HE2	2:B:825:HOH:O	1.98	0.62
1:A:667:ARG:HD3	1:A:709:GLU:OE1	2.00	0.62
1:A:152:LEU:HD22	1:A:187:ILE:HG21	1.82	0.62
1:B:65:LEU:HA	1:B:68:ARG:HH21	1.64	0.62
1:A:518:ARG:HG3	1:A:518:ARG:HH11	1.64	0.62
1:B:567:LYS:O	1:B:570:ASP:HB2	2.00	0.62
1:B:47:ARG:HD3	1:B:99:PHE:CB	2.29	0.62
1:B:84:GLU:CD	1:B:84:GLU:H	2.02	0.62
1:B:135:ARG:NH1	1:B:141:ASP:OD1	2.32	0.62
1:B:597:VAL:HG11	1:B:634:THR:O	1.99	0.62
1:A:549:LEU:HA	1:A:571:ASN:ND2	2.15	0.61
1:B:641:ASN:HD21	1:B:643:GLU:HB2	1.64	0.61
1:B:190:ALA:O	1:B:193:GLN:HB3	1.99	0.61
1:B:289:THR:HG23	1:B:318:SER:OG	2.00	0.61
1:A:698:ILE:HG21	1:A:740:ASN:HD21	1.65	0.61
1:A:530:GLY:O	1:A:534:LYS:HB2	2.00	0.61
1:A:297:GLU:OE2	1:A:322:LEU:HD22	2.00	0.61
1:A:479:ILE:CG2	1:A:489:LEU:HD22	2.31	0.61
1:A:247:LEU:O	1:A:248:THR:O	2.19	0.61
1:A:326:ASN:OD1	1:A:329:GLN:HG3	2.00	0.61
1:B:715:LEU:HD23	1:B:760:PHE:HB3	1.83	0.61
1:B:696:ASN:O	1:B:700:VAL:HG23	2.01	0.61
1:B:754:GLY:HA3	2:B:826:HOH:O	1.99	0.61
1:B:99:PHE:O	1:B:102:ASN:ND2	2.34	0.60
1:B:743:LEU:HD22	1:B:747:LEU:HD11	1.83	0.60
1:A:434:LYS:HD2	2:A:800:HOH:O	2.00	0.60
1:A:437:LYS:HE2	1:A:441:LEU:HD11	1.83	0.60
1:A:90:SER:O	1:A:94:GLN:HG3	2.01	0.60
1:B:258:ARG:HA	1:B:262:GLU:HG2	1.82	0.60
1:B:79:TYR:CD1	1:B:86:ARG:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:CG2	1:B:305:VAL:HG21	2.29	0.60
1:B:385:MET:HA	1:B:387:HIS:HE1	1.65	0.60
1:A:320:THR:HA	2:A:816:HOH:O	2.01	0.60
1:A:402:LEU:HB3	1:A:440:ILE:HG21	1.82	0.60
1:B:157:LYS:O	1:B:157:LYS:HG2	2.00	0.60
1:B:728:ASN:O	1:B:730:THR:N	2.35	0.60
1:A:450:ARG:O	1:A:452:GLU:N	2.35	0.60
1:A:493:GLY:O	1:A:496:LYS:HB2	2.01	0.60
1:B:7:GLY:H	1:B:10:PRO:HG3	1.66	0.60
1:A:367:ARG:HG3	1:A:399:LEU:CD1	2.32	0.60
1:A:375:ILE:O	1:A:379:MET:HG3	2.00	0.60
1:A:284:MET:O	1:A:288:ILE:HG13	2.01	0.60
1:B:141:ASP:OD1	1:B:147:LEU:HD11	2.02	0.60
1:B:651:PHE:CZ	1:B:690:LYS:HG2	2.37	0.59
1:B:680:ILE:HG22	1:B:680:ILE:O	2.01	0.59
1:A:504:ASN:HB3	1:A:505:LYS:HD2	1.82	0.59
1:A:740:ASN:HD22	1:A:743:LEU:HB3	1.67	0.59
1:B:751:LEU:HD11	1:B:761:SER:HB3	1.83	0.59
1:A:51:GLU:HG2	2:A:809:HOH:O	2.01	0.59
1:A:238:LEU:HD13	1:A:241:LEU:HD13	1.85	0.59
1:A:498:ILE:HG21	1:A:520:LEU:HB2	1.83	0.59
1:B:583:SER:O	1:B:585:GLU:HG3	2.02	0.59
1:B:618:GLN:OE1	1:B:660:LEU:HD21	2.02	0.59
1:A:151:ILE:HG21	1:A:188:ILE:HD13	1.84	0.59
1:A:77:ARG:HB2	1:A:77:ARG:NH1	2.18	0.59
1:A:93:ILE:HG23	1:A:100:ALA:HB1	1.84	0.59
1:A:434:LYS:HE3	2:A:832:HOH:O	2.03	0.59
1:B:161:ASN:ND2	1:B:163:LYS:HD2	2.17	0.59
1:B:735:PRO:HA	1:B:738:GLN:CG	2.30	0.59
1:B:735:PRO:O	1:B:738:GLN:N	2.34	0.59
1:A:343:VAL:HA	1:A:346:VAL:HG23	1.85	0.59
1:B:535:LYS:HG3	2:B:782:HOH:O	2.02	0.59
1:A:257:LYS:O	1:A:261:GLU:HG2	2.03	0.58
1:B:495:VAL:O	1:B:499:LEU:HB2	2.02	0.58
1:A:144:VAL:HG23	1:A:145:THR:N	2.18	0.58
1:A:539:LEU:HD12	1:A:539:LEU:H	1.67	0.58
1:A:705:ILE:HG22	1:A:711:ARG:CD	2.33	0.58
1:A:87:VAL:O	1:A:91:LYS:HG2	2.03	0.58
1:B:93:ILE:HG23	1:B:100:ALA:CB	2.33	0.58
1:A:565:GLN:NE2	1:A:567:LYS:HA	2.19	0.58
1:B:741:GLN:HE21	1:B:745:ASP:HB2	1.64	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:CYS:SG	1:A:316:THR:HG22	2.44	0.58
1:A:355:TYR:O	1:A:358:LEU:HB2	2.03	0.58
1:B:253:LYS:HE2	2:B:775:HOH:O	2.03	0.58
1:B:383:GLN:HG3	1:B:386:THR:OG1	2.03	0.58
1:A:359:LYS:O	1:A:361:SER:N	2.33	0.58
1:A:450:ARG:C	1:A:452:GLU:N	2.53	0.58
1:B:768:LEU:O	1:B:771:ILE:HG22	2.03	0.58
1:A:259:VAL:HG11	1:A:295:LEU:HD11	1.85	0.58
1:B:302:VAL:O	1:B:304:ASP:N	2.36	0.58
1:B:32:ASP:O	1:B:34:GLN:N	2.35	0.58
1:B:752:LYS:NZ	1:B:752:LYS:CB	2.67	0.58
1:A:68:ARG:O	1:A:71:ILE:N	2.37	0.57
1:A:455:SER:HB2	1:A:492:GLN:HG2	1.85	0.57
1:A:47:ARG:HG2	2:A:774:HOH:O	2.04	0.57
1:A:505:LYS:HG2	2:A:780:HOH:O	2.04	0.57
1:A:720:GLY:O	1:A:723:GLU:HB3	2.05	0.57
1:B:47:ARG:HD3	1:B:99:PHE:CG	2.39	0.57
1:B:47:ARG:HD3	1:B:99:PHE:HB2	1.86	0.57
1:B:51:GLU:HB3	2:B:831:HOH:O	2.03	0.57
1:B:197:GLN:HG3	1:B:198:LYS:H	1.70	0.57
1:B:340:ARG:CZ	1:B:375:ILE:HG12	2.34	0.57
1:A:677:ALA:O	1:A:684:ALA:HB2	2.05	0.57
1:A:47:ARG:HD2	1:A:96:ASP:OD2	2.05	0.57
1:A:205:VAL:HG22	1:A:241:LEU:HD21	1.87	0.57
1:A:285:ARG:HG3	1:A:316:THR:HA	1.87	0.57
1:A:198:LYS:HB3	1:A:202:LYS:CE	2.35	0.57
1:A:381:LYS:HE3	1:A:451:THR:HG22	1.87	0.57
1:B:36:TYR:HE1	1:B:81:ASP:HB2	1.70	0.57
1:B:46:LEU:HD23	1:B:56:PRO:HG2	1.87	0.57
1:B:632:PRO:HG2	1:B:679:THR:HG21	1.86	0.57
1:A:215:ALA:HB2	1:A:223:PRO:HB2	1.87	0.56
1:B:338:ILE:O	1:B:339:SER:C	2.43	0.56
1:A:483:LYS:HG2	2:A:785:HOH:O	2.04	0.56
1:B:372:PHE:CE2	1:B:376:LEU:HD11	2.39	0.56
1:A:61:ASN:ND2	1:A:62:SER:H	2.03	0.56
1:A:454:ILE:HG21	1:A:489:LEU:HD12	1.86	0.56
1:B:217:ILE:HG22	1:B:217:ILE:O	2.04	0.56
1:B:495:VAL:HG11	1:B:532:ILE:HG13	1.88	0.56
1:A:555:VAL:HG22	1:A:556:ASP:N	2.11	0.56
1:B:342:ILE:HG22	1:B:343:VAL:N	2.20	0.56
1:A:726:PRO:HG3	1:A:732:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:741:GLN:HE22	1:B:745:ASP:HB2	1.66	0.56
1:A:343:VAL:HA	1:A:346:VAL:CG2	2.35	0.56
1:B:237:SER:O	1:B:239:THR:HG23	2.06	0.56
1:B:260:PHE:CZ	1:B:295:LEU:HA	2.41	0.56
1:B:738:GLN:HA	2:B:814:HOH:O	2.05	0.56
1:A:322:LEU:HB3	1:A:324:CYS:SG	2.46	0.55
1:A:401:THR:HA	1:A:478:ASN:ND2	2.20	0.55
1:B:325:ILE:HD12	1:B:325:ILE:O	2.06	0.55
1:B:649:ARG:O	1:B:653:ILE:HG13	2.06	0.55
1:A:8:ASN:C	1:A:10:PRO:HD3	2.26	0.55
1:A:162:PHE:C	1:A:164:GLU:N	2.58	0.55
1:B:93:ILE:HG23	1:B:100:ALA:HB1	1.88	0.55
1:B:102:ASN:H	1:B:102:ASN:HD22	1.49	0.55
1:A:694:ILE:HD12	1:A:736:LEU:HD22	1.89	0.55
1:B:2:PRO:HB3	1:B:6:LYS:NZ	2.21	0.55
1:B:597:VAL:HG21	1:B:635:ILE:HD13	1.89	0.55
1:B:237:SER:O	1:B:239:THR:N	2.40	0.55
1:B:363:LYS:HD2	2:B:802:HOH:O	2.07	0.55
1:B:619:ARG:HE	1:B:664:GLU:HB2	1.71	0.55
1:A:109:ARG:NH2	1:B:81:ASP:OD2	2.39	0.55
1:A:651:PHE:CZ	1:A:690:LYS:HD3	2.41	0.55
1:A:46:LEU:HD11	1:A:56:PRO:HD2	1.87	0.55
1:A:328:LYS:HZ2	1:A:361:SER:HB3	1.71	0.55
1:A:535:LYS:HG2	2:A:804:HOH:O	2.05	0.55
1:B:429:LYS:HE2	1:B:433:GLU:OE2	2.06	0.55
1:B:640:PHE:HB3	1:B:683:ILE:HD13	1.89	0.55
1:A:402:LEU:HD11	1:A:481:ARG:CB	2.37	0.55
1:A:759:GLU:O	1:A:761:SER:N	2.39	0.55
1:B:546:PHE:CZ	1:B:602:TYR:HB3	2.41	0.55
1:B:579:THR:HA	1:B:624:LEU:HD13	1.88	0.55
1:A:157:LYS:HD3	1:A:158:PHE:HE2	1.72	0.55
1:A:166:ARG:O	1:A:169:VAL:HG23	2.07	0.55
1:A:457:LEU:HD13	1:A:472:VAL:HG22	1.89	0.55
1:B:732:GLU:O	1:B:733:VAL:HG22	2.07	0.55
1:A:144:VAL:CG2	1:A:145:THR:N	2.70	0.54
1:A:162:PHE:HD1	1:A:196:PHE:CG	2.24	0.54
1:B:458:LYS:HD2	1:B:493:GLY:HA3	1.89	0.54
1:B:679:THR:C	1:B:680:ILE:HD12	2.27	0.54
1:B:131:GLU:O	1:B:135:ARG:HG2	2.07	0.54
1:B:713:ARG:HG2	1:B:713:ARG:HH11	1.71	0.54
1:B:262:GLU:O	1:B:263:GLN:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:OG	1:B:110:SER:HB2	2.07	0.54
1:A:367:ARG:CG	1:A:399:LEU:HD12	2.38	0.54
1:A:538:ALA:O	1:A:540:ASN:N	2.40	0.54
1:B:45:GLN:HA	1:B:48:GLN:OE1	2.08	0.54
1:B:266:GLN:O	1:B:266:GLN:NE2	2.41	0.54
1:B:671:ALA:HA	1:B:713:ARG:HD3	1.90	0.54
1:B:514:ILE:HD12	1:B:514:ILE:H	1.72	0.54
1:A:168:LEU:HD23	1:A:188:ILE:CG2	2.38	0.54
1:A:707:ASP:HB3	1:A:710:LEU:HB3	1.90	0.54
1:B:15:THR:HA	2:B:836:HOH:O	2.08	0.54
1:B:663:VAL:O	1:B:667:ARG:HB2	2.08	0.54
1:A:300:LEU:HD23	1:A:306:GLN:HG2	1.90	0.54
1:B:584:SER:O	1:B:586:THR:N	2.40	0.54
1:B:738:GLN:CG	1:B:739:GLU:HG3	2.30	0.54
1:A:400:SER:O	1:A:478:ASN:HB3	2.07	0.54
1:A:479:ILE:HG21	1:A:489:LEU:HD22	1.90	0.54
1:B:551:ARG:O	1:B:560:LEU:HD23	2.08	0.54
1:A:331:SER:O	1:A:335:ILE:HG13	2.07	0.53
1:B:106:ILE:HG22	1:B:106:ILE:O	2.08	0.53
1:B:222:ASP:N	1:B:223:PRO:HD3	2.23	0.53
1:B:284:MET:O	1:B:288:ILE:HG13	2.08	0.53
1:B:383:GLN:O	1:B:386:THR:N	2.41	0.53
1:A:104:PHE:HA	1:A:107:LEU:HD22	1.90	0.53
1:A:579:THR:HA	1:A:624:LEU:HD13	1.89	0.53
1:A:315:LYS:HA	1:A:355:TYR:HE1	1.73	0.53
1:B:222:ASP:CG	1:B:225:SER:HB2	2.28	0.53
1:A:671:ALA:HA	1:A:713:ARG:HD2	1.91	0.53
1:B:401:THR:HA	1:B:478:ASN:ND2	2.24	0.53
1:B:144:VAL:HG21	1:B:175:ARG:NH2	2.23	0.53
1:A:175:ARG:HD2	1:A:178:GLU:OE2	2.08	0.53
1:A:223:PRO:O	1:A:225:SER:N	2.42	0.53
1:A:481:ARG:HA	1:A:481:ARG:NE	2.24	0.53
1:A:655:VAL:HG13	1:A:693:LEU:HA	1.91	0.53
1:A:730:THR:O	1:A:731:ASN:C	2.46	0.53
1:A:771:ILE:HG22	1:A:772:LYS:N	2.23	0.53
1:B:455:SER:O	1:B:459:ARG:HG3	2.08	0.53
1:B:705:ILE:HG12	1:B:711:ARG:CD	2.33	0.53
1:A:538:ALA:C	1:A:540:ASN:H	2.11	0.53
1:B:222:ASP:H	1:B:223:PRO:HD3	1.74	0.53
1:A:302:VAL:HB	1:A:305:VAL:HG22	1.90	0.53
1:B:307:ILE:HG21	1:B:345:LYS:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:C	1:A:164:GLU:H	2.11	0.52
1:A:351:GLU:HG3	1:B:23:PHE:CE1	2.44	0.52
1:A:499:LEU:HD23	1:A:499:LEU:O	2.09	0.52
1:B:752:LYS:CB	1:B:752:LYS:HZ2	2.21	0.52
1:A:476:ILE:HD12	1:A:498:ILE:HD13	1.92	0.52
1:A:701:PHE:O	1:A:705:ILE:HG23	2.09	0.52
1:A:696:ASN:O	1:A:700:VAL:HG22	2.09	0.52
1:B:738:GLN:CG	1:B:739:GLU:N	2.71	0.52
1:A:52:SER:O	1:A:53:GLY:C	2.48	0.52
1:A:60:THR:OG1	1:A:61:ASN:N	2.42	0.52
1:A:632:PRO:C	1:A:634:THR:H	2.13	0.52
1:A:738:GLN:O	1:A:771:ILE:HA	2.09	0.52
1:B:202:LYS:HA	1:B:205:VAL:HG12	1.91	0.52
1:B:307:ILE:HD13	1:B:345:LYS:HB3	1.90	0.52
1:B:390:TYR:O	1:B:394:VAL:HG23	2.10	0.52
1:B:673:PHE:O	1:B:676:ILE:HG22	2.10	0.52
1:A:640:PHE:CZ	1:A:676:ILE:HG12	2.45	0.52
1:A:164:GLU:OE1	1:A:164:GLU:HA	2.10	0.52
1:A:258:ARG:O	1:A:262:GLU:HB2	2.10	0.52
1:A:688:LEU:HD23	1:A:721:LEU:HD22	1.92	0.52
1:B:131:GLU:OE1	1:B:135:ARG:NE	2.43	0.52
1:B:622:LEU:HD13	1:B:669:VAL:HG22	1.90	0.52
1:B:749:MET:HE2	2:B:780:HOH:O	2.10	0.52
1:A:97:ILE:CD1	1:A:98:PRO:HD3	2.40	0.52
1:B:188:ILE:O	1:B:192:LEU:HG	2.10	0.52
1:A:54:LYS:O	1:A:56:PRO:HD3	2.09	0.51
1:A:722:PHE:CD2	1:A:767:ILE:HG23	2.45	0.51
1:B:239:THR:OG1	1:B:240:THR:N	2.44	0.51
1:B:498:ILE:HG22	1:B:502:LEU:HD12	1.93	0.51
1:B:504:ASN:O	1:B:506:GLN:HG3	2.10	0.51
1:B:597:VAL:HB	1:B:635:ILE:CD1	2.40	0.51
1:B:766:VAL:O	1:B:769:ALA:HB3	2.09	0.51
1:B:215:ALA:HB2	1:B:223:PRO:HB2	1.93	0.51
1:B:475:ILE:O	1:B:479:ILE:HG12	2.10	0.51
1:A:358:LEU:HD23	1:B:11:ILE:HD13	1.92	0.51
1:A:358:LEU:HD23	1:B:11:ILE:HG21	1.91	0.51
1:B:84:GLU:OE2	1:B:84:GLU:N	2.43	0.51
1:B:749:MET:HE3	1:B:752:LYS:HZ2	1.74	0.51
1:A:109:ARG:HH21	1:B:80:GLN:HE21	1.58	0.51
1:A:247:LEU:O	1:A:248:THR:C	2.49	0.51
1:A:307:ILE:HG22	1:A:348:MET:SD	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ILE:HD13	1:B:208:MET:HE3	1.92	0.51
1:A:505:LYS:NZ	1:A:505:LYS:HB3	2.26	0.51
1:A:106:ILE:HG13	1:A:107:LEU:CD1	2.41	0.51
1:A:473:VAL:HG21	1:A:501:TYR:CE2	2.45	0.51
1:A:614:ASN:ND2	1:A:617:LEU:H	2.08	0.51
1:B:260:PHE:HZ	1:B:295:LEU:HA	1.75	0.51
1:A:687:LEU:HD23	1:A:690:LYS:HZ3	1.74	0.51
1:B:96:ASP:OD1	1:B:99:PHE:HB3	2.11	0.51
1:B:430:VAL:HG12	1:B:430:VAL:O	2.11	0.51
1:B:655:VAL:HG23	1:B:656:LYS:N	2.26	0.51
1:A:109:ARG:NE	1:B:80:GLN:HE22	1.99	0.51
1:A:260:PHE:C	1:A:262:GLU:H	2.14	0.51
1:A:574:ALA:O	1:A:578:LEU:HB2	2.11	0.50
1:B:272:LEU:HD12	1:B:305:VAL:HG22	1.93	0.50
1:B:615:VAL:HB	1:B:616:PRO:HD3	1.92	0.50
1:B:687:LEU:HD13	1:B:693:LEU:HD21	1.92	0.50
1:B:713:ARG:C	1:B:715:LEU:H	2.14	0.50
1:A:50:SER:O	1:A:52:SER:N	2.44	0.50
1:A:157:LYS:HD3	1:A:158:PHE:CE2	2.46	0.50
1:A:308:TYR:O	1:A:312:VAL:HG23	2.10	0.50
1:A:315:LYS:HA	1:A:355:TYR:CE1	2.46	0.50
1:A:532:ILE:C	1:A:534:LYS:H	2.13	0.50
1:A:667:ARG:NH1	1:A:709:GLU:OE1	2.43	0.50
1:A:766:VAL:O	1:A:769:ALA:HB3	2.11	0.50
1:B:730:THR:O	1:B:731:ASN:HB2	2.11	0.50
1:B:747:LEU:O	1:B:750:SER:HB2	2.11	0.50
1:A:162:PHE:CZ	1:A:200:PHE:HA	2.46	0.50
1:B:302:VAL:C	1:B:304:ASP:H	2.15	0.50
1:B:499:LEU:HD13	1:B:520:LEU:HD13	1.93	0.50
1:A:536:TYR:O	1:A:537:SER:O	2.28	0.50
1:A:761:SER:O	1:A:764:ILE:HG13	2.11	0.50
1:B:12:ASP:HB2	1:B:15:THR:OG1	2.12	0.50
1:A:307:ILE:HG13	1:A:345:LYS:HG2	1.92	0.50
1:A:36:TYR:CE1	1:A:77:ARG:HD3	2.44	0.50
1:A:79:TYR:CD1	1:A:86:ARG:HG3	2.47	0.50
1:A:138:TYR:N	1:A:138:TYR:CD2	2.80	0.50
1:A:182:LYS:HE3	1:A:233:GLU:OE1	2.12	0.50
1:B:157:LYS:O	1:B:157:LYS:CG	2.60	0.50
1:A:281:ASP:OD2	1:A:283:THR:HB	2.12	0.50
1:A:528:ASN:ND2	1:A:530:GLY:H	2.10	0.50
1:A:719:PHE:CD1	1:A:760:PHE:HE1	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:LYS:O	1:B:500:GLU:HG3	2.12	0.50
1:B:68:ARG:CD	1:B:106:ILE:HG22	2.40	0.49
1:A:138:TYR:N	1:A:138:TYR:HD2	2.10	0.49
1:A:250:GLY:O	1:A:254:LEU:HD13	2.13	0.49
1:A:512:ILE:HG23	1:A:513:ARG:N	2.27	0.49
1:B:483:LYS:HE3	1:B:526:PHE:CZ	2.47	0.49
1:B:629:MET:HE1	1:B:676:ILE:HD13	1.94	0.49
1:A:186:LEU:HD12	1:B:31:PRO:HG2	1.94	0.49
1:A:538:ALA:C	1:A:540:ASN:N	2.65	0.49
1:A:567:LYS:HE2	1:A:569:THR:HB	1.93	0.49
1:A:621:THR:O	1:A:625:ILE:HG13	2.13	0.49
1:A:745:ASP:OD2	1:A:746:ALA:N	2.46	0.49
1:B:205:VAL:HG13	1:B:206:ASP:N	2.27	0.49
1:B:236:PRO:O	1:B:237:SER:O	2.31	0.49
1:B:526:PHE:O	1:B:527:THR:CG2	2.58	0.49
1:A:104:PHE:O	1:A:107:LEU:HB2	2.13	0.49
1:A:122:LYS:N	1:A:158:PHE:HE1	2.10	0.49
1:B:381:LYS:O	1:B:382:SER:OG	2.28	0.49
1:B:764:ILE:N	1:B:765:PRO:HD2	2.28	0.49
1:B:470:GLN:HB3	1:B:512:ILE:HG21	1.94	0.49
1:A:47:ARG:CG	2:A:774:HOH:O	2.59	0.49
1:A:338:ILE:HD11	1:A:349:SER:HB2	1.94	0.49
1:A:39:ALA:O	1:A:43:ILE:HG13	2.13	0.49
1:B:482:SER:O	1:B:484:ASN:N	2.46	0.49
1:B:224:LEU:HD11	1:B:254:LEU:HD22	1.95	0.49
1:B:753:ARG:C	1:B:755:ASP:N	2.62	0.49
1:A:70:LYS:O	1:A:74:ILE:HG12	2.13	0.48
1:A:122:LYS:N	1:A:158:PHE:CE1	2.81	0.48
1:A:152:LEU:HD22	1:A:187:ILE:CG2	2.42	0.48
1:A:243:SER:HB3	1:A:284:MET:HE1	1.94	0.48
1:A:644:ASN:OD1	1:A:646:GLN:N	2.46	0.48
1:B:651:PHE:HZ	1:B:690:LYS:HG2	1.76	0.48
1:A:193:GLN:HG3	1:A:194:SER:N	2.28	0.48
1:A:258:ARG:HG2	1:A:267:PHE:CE2	2.48	0.48
1:A:539:LEU:HD12	1:A:539:LEU:N	2.28	0.48
1:B:738:GLN:HE21	1:B:739:GLU:HG3	1.78	0.48
1:A:465:SER:O	1:A:466:PRO:C	2.51	0.48
1:B:160:TYR:N	2:B:846:HOH:O	2.44	0.48
1:B:162:PHE:C	1:B:164:GLU:N	2.67	0.48
1:A:68:ARG:O	1:A:69:GLN:C	2.51	0.48
1:A:76:THR:O	1:A:80:GLN:HG2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ASN:O	1:A:730:THR:HG23	2.13	0.48
1:B:168:LEU:HD13	1:B:188:ILE:HG21	1.96	0.48
1:B:66:LYS:HE2	1:B:70:LYS:CE	2.44	0.48
1:B:533:PHE:O	1:B:536:TYR:O	2.31	0.48
1:B:592:VAL:O	1:B:596:ILE:HG13	2.14	0.48
1:B:624:LEU:O	1:B:628:MET:HG3	2.14	0.48
1:A:165:VAL:CG1	1:A:168:LEU:HD22	2.43	0.48
1:A:171:GLU:OE1	1:A:171:GLU:HA	2.12	0.48
1:B:47:ARG:CD	1:B:99:PHE:HB2	2.44	0.48
1:B:744:LYS:O	1:B:748:ASN:OD1	2.32	0.48
1:B:141:ASP:CG	1:B:147:LEU:HD11	2.34	0.48
1:A:483:LYS:HE2	1:A:526:PHE:CZ	2.48	0.48
1:A:555:VAL:CG2	1:A:556:ASP:H	2.13	0.48
1:A:768:LEU:C	1:A:770:LYS:H	2.16	0.48
1:B:629:MET:C	1:B:631:HIS:H	2.17	0.48
1:A:310:ALA:O	1:A:313:LEU:N	2.47	0.48
1:A:340:ARG:O	1:A:340:ARG:HG2	2.14	0.48
1:A:360:ALA:O	1:A:361:SER:C	2.52	0.48
1:B:588:ASP:O	1:B:591:GLU:HB2	2.13	0.48
1:B:729:GLY:C	1:B:731:ASN:H	2.13	0.48
1:A:264:ASP:HB3	1:A:267:PHE:CB	2.38	0.47
1:B:667:ARG:HG2	1:B:667:ARG:HH11	1.79	0.47
1:B:750:SER:C	1:B:752:LYS:H	2.17	0.47
1:A:11:ILE:O	1:A:11:ILE:CG2	2.61	0.47
1:B:72:GLU:O	1:B:76:THR:CG2	2.57	0.47
1:B:559:PRO:HB2	1:B:608:ASN:ND2	2.30	0.47
1:B:716:MET:HG2	1:B:760:PHE:HE1	1.79	0.47
1:A:15:THR:HG22	1:A:15:THR:O	2.14	0.47
1:B:96:ASP:OD1	1:B:99:PHE:CB	2.62	0.47
1:B:370:GLU:HG3	1:B:447:TYR:OH	2.14	0.47
1:A:351:GLU:HG3	1:B:23:PHE:CD1	2.49	0.47
1:A:432:ALA:HB2	2:A:791:HOH:O	2.13	0.47
1:A:454:ILE:HG21	1:A:489:LEU:CD1	2.44	0.47
1:A:505:LYS:HD2	1:A:505:LYS:N	2.18	0.47
1:B:146:TYR:HE2	1:B:150:ILE:HD11	1.80	0.47
1:A:476:ILE:HD12	1:A:498:ILE:CD1	2.44	0.47
1:A:500:GLU:HB3	2:A:834:HOH:O	2.14	0.47
1:B:112:ILE:HG12	1:B:146:TYR:CZ	2.50	0.47
1:A:94:GLN:HE22	1:A:124:ALA:HB1	1.79	0.47
1:A:97:ILE:HD12	1:A:98:PRO:HD3	1.95	0.47
1:A:103:LEU:O	1:A:107:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ASP:H	1:B:223:PRO:CD	2.27	0.47
1:B:338:ILE:O	1:B:339:SER:O	2.33	0.47
1:A:505:LYS:H	1:A:505:LYS:CD	2.21	0.47
1:A:632:PRO:C	1:A:634:THR:N	2.68	0.47
1:B:448:ILE:HG21	1:B:479:ILE:HD11	1.95	0.47
1:B:482:SER:OG	1:B:485:PHE:CD2	2.68	0.47
1:B:631:HIS:N	1:B:632:PRO:HD3	2.28	0.47
1:B:680:ILE:HD12	1:B:680:ILE:N	2.29	0.47
1:A:514:ILE:HD12	1:A:564:GLU:HB3	1.97	0.47
1:B:357:SER:O	1:B:363:LYS:HE3	2.15	0.47
1:B:644:ASN:HB3	1:B:647:SER:CB	2.43	0.47
1:B:751:LEU:CD1	1:B:761:SER:HB3	2.45	0.47
1:A:235:TYR:CE1	1:A:278:ALA:HA	2.50	0.47
1:A:528:ASN:HD22	1:A:531:LEU:HG	1.80	0.47
1:B:84:GLU:CD	1:B:84:GLU:N	2.67	0.47
1:B:299:SER:C	1:B:301:ASN:H	2.17	0.47
1:B:640:PHE:CB	1:B:683:ILE:HD13	2.45	0.47
1:A:88:HIS:NE2	1:A:92:LEU:HD11	2.30	0.47
1:A:27:LEU:O	1:B:236:PRO:HB3	2.14	0.46
1:A:34:GLN:O	1:A:38:ASP:HB2	2.15	0.46
1:A:327:LEU:HD11	1:A:359:LYS:HD3	1.97	0.46
1:A:528:ASN:HD22	1:A:531:LEU:N	1.96	0.46
1:B:146:TYR:CE2	1:B:150:ILE:HD11	2.50	0.46
1:A:339:SER:O	1:A:341:ARG:HG3	2.14	0.46
1:A:367:ARG:HD2	1:A:443:PHE:HB2	1.98	0.46
1:A:473:VAL:HG21	1:A:501:TYR:CD2	2.51	0.46
1:B:461:MET:HE3	1:B:472:VAL:HG21	1.97	0.46
1:A:349:SER:O	1:A:353:LEU:HB2	2.16	0.46
1:B:36:TYR:CE1	1:B:81:ASP:HB2	2.50	0.46
1:A:341:ARG:O	1:A:343:VAL:N	2.49	0.46
1:A:597:VAL:HG11	1:A:634:THR:O	2.15	0.46
1:B:202:LYS:O	1:B:205:VAL:HG12	2.15	0.46
1:B:597:VAL:HB	1:B:635:ILE:HD11	1.97	0.46
1:A:238:LEU:HD13	1:A:241:LEU:CD1	2.45	0.46
1:A:455:SER:HB2	1:A:492:GLN:CG	2.46	0.46
1:B:9:ASP:N	1:B:10:PRO:HD3	2.30	0.46
1:B:282:GLU:HG2	1:B:285:ARG:HD3	1.97	0.46
1:B:340:ARG:NH1	1:B:375:ILE:HG12	2.30	0.46
1:B:739:GLU:O	1:B:741:GLN:N	2.48	0.46
1:A:402:LEU:HD12	1:A:402:LEU:O	2.15	0.46
1:A:518:ARG:NH1	1:A:518:ARG:HG3	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:PRO:O	1:A:737:LEU:N	2.49	0.46
1:B:82:HIS:HB2	1:B:85:SER:OG	2.16	0.46
1:B:139:GLY:HA2	1:B:175:ARG:NH1	2.31	0.46
1:B:652:ASN:O	1:B:655:VAL:HG22	2.15	0.46
1:A:377:LEU:HD22	1:A:451:THR:HG21	1.97	0.46
1:B:207:PHE:O	1:B:210:SER:OG	2.33	0.46
1:A:555:VAL:HG13	1:A:556:ASP:N	2.30	0.46
1:A:741:GLN:HA	1:A:744:LYS:HB3	1.97	0.46
1:B:713:ARG:NH1	2:B:787:HOH:O	2.35	0.46
1:A:237:SER:O	1:A:238:LEU:HD23	2.15	0.46
1:B:36:TYR:HE1	1:B:81:ASP:CB	2.28	0.46
1:A:449:LEU:HD21	1:A:485:PHE:HB3	1.98	0.46
1:A:289:THR:HG23	1:A:318:SER:OG	2.16	0.45
1:B:468:CYS:O	1:B:472:VAL:HG23	2.16	0.45
1:B:701:PHE:O	1:B:705:ILE:HG13	2.16	0.45
1:B:752:LYS:HB3	1:B:752:LYS:HZ3	1.80	0.45
1:B:704:GLN:C	1:B:706:ASP:H	2.20	0.45
1:A:51:GLU:HB3	2:A:809:HOH:O	2.15	0.45
1:A:60:THR:O	1:A:61:ASN:C	2.55	0.45
1:A:91:LYS:O	1:A:95:ASN:HB2	2.16	0.45
1:A:369:ASN:HD21	1:A:372:PHE:HB2	1.79	0.45
1:B:219:VAL:HG23	1:B:219:VAL:O	2.17	0.45
1:B:735:PRO:CA	1:B:738:GLN:HG2	2.38	0.45
1:B:749:MET:HE3	1:B:749:MET:O	2.16	0.45
1:A:192:LEU:O	1:A:196:PHE:HD2	1.98	0.45
1:A:222:ASP:OD2	1:A:222:ASP:C	2.53	0.45
1:A:651:PHE:O	1:A:655:VAL:HG23	2.16	0.45
1:A:699:GLN:HA	1:A:742:LYS:CE	2.47	0.45
1:A:744:LYS:HB2	1:A:771:ILE:HG21	1.98	0.45
1:A:82:HIS:HB2	1:A:85:SER:OG	2.17	0.45
1:A:553:THR:O	1:A:555:VAL:N	2.50	0.45
1:A:763:ALA:O	1:A:767:ILE:HG13	2.17	0.45
1:B:32:ASP:HB2	1:B:33:VAL:H	1.64	0.45
1:B:36:TYR:CE1	1:B:82:HIS:CD2	3.05	0.45
1:A:24:ASP:HA	1:A:27:LEU:HB3	1.98	0.45
1:A:105:GLU:HA	1:A:146:TYR:CD2	2.52	0.45
1:A:240:THR:HG23	1:A:241:LEU:H	1.82	0.45
1:A:505:LYS:HG2	1:A:510:GLU:OE2	2.16	0.45
1:B:488:GLN:HG3	2:B:793:HOH:O	2.15	0.45
1:B:685:LYS:HA	1:B:688:LEU:HD12	1.99	0.45
1:B:19:LEU:HA	1:B:19:LEU:HD12	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLU:OE1	1:B:73:GLU:HA	2.17	0.45
1:B:116:VAL:HG13	1:B:154:LEU:HD23	1.98	0.45
1:B:533:PHE:O	1:B:534:LYS:C	2.54	0.45
1:B:687:LEU:HD22	1:B:693:LEU:CD2	2.46	0.45
1:A:278:ALA:O	1:A:280:ILE:N	2.47	0.45
1:A:761:SER:O	1:A:765:PRO:HD2	2.17	0.45
1:A:170:LYS:HG3	1:A:207:PHE:CE1	2.52	0.45
1:A:293:LEU:HD22	1:A:322:LEU:HD21	1.99	0.45
1:A:355:TYR:O	1:A:357:SER:N	2.50	0.45
1:A:379:MET:HA	1:A:383:GLN:CG	2.47	0.45
1:B:39:ALA:O	1:B:43:ILE:HG12	2.17	0.45
1:B:339:SER:HA	1:B:375:ILE:CD1	2.47	0.45
1:A:90:SER:HB2	1:A:91:LYS:HZ3	1.80	0.45
1:A:550:PRO:HD3	1:A:571:ASN:HD21	1.78	0.45
1:B:212:ILE:HG12	1:B:227:ILE:HD13	1.99	0.45
1:B:342:ILE:HG23	1:B:343:VAL:N	2.18	0.45
1:B:749:MET:CE	1:B:752:LYS:NZ	2.80	0.45
1:A:44:PHE:HE1	1:A:92:LEU:O	2.00	0.44
1:A:69:GLN:O	1:A:73:GLU:HG2	2.17	0.44
1:A:109:ARG:NE	1:B:80:GLN:NE2	2.61	0.44
1:A:130:ASN:O	1:A:134:ILE:HG13	2.17	0.44
1:B:626:SER:HA	1:B:672:ILE:HG12	1.98	0.44
1:A:93:ILE:HG23	1:A:100:ALA:CB	2.45	0.44
1:B:317:TRP:CE2	1:B:319:PHE:CZ	3.06	0.44
1:B:722:PHE:CD1	1:B:767:ILE:HG23	2.53	0.44
1:A:6:LYS:HB2	1:A:6:LYS:HZ2	1.79	0.44
1:A:338:ILE:HD11	1:A:349:SER:HB3	1.97	0.44
1:B:161:ASN:O	1:B:163:LYS:N	2.45	0.44
1:B:286:THR:O	1:B:289:THR:HB	2.17	0.44
1:A:90:SER:HB2	1:A:91:LYS:NZ	2.33	0.44
1:A:104:PHE:HB3	1:A:146:TYR:OH	2.18	0.44
1:A:381:LYS:HA	1:A:456:PHE:CE2	2.52	0.44
1:B:128:LEU:HD13	1:B:154:LEU:HD11	2.00	0.44
1:A:132:LEU:O	1:A:136:ILE:HG13	2.17	0.44
1:A:263:GLN:O	1:A:264:ASP:C	2.56	0.44
1:A:327:LEU:HD11	1:A:359:LYS:CD	2.47	0.44
1:A:327:LEU:CD2	1:A:356:LEU:HD22	2.47	0.44
1:B:7:GLY:O	1:B:10:PRO:HD3	2.18	0.44
1:B:196:PHE:HA	2:B:822:HOH:O	2.17	0.44
1:A:451:THR:HG22	1:A:451:THR:O	2.18	0.44
1:A:524:LEU:HD23	1:A:581:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLN:HE21	1:B:133:GLN:HB3	1.52	0.44
1:B:162:PHE:CE2	1:B:199:ASP:HB3	2.52	0.44
1:B:327:LEU:HD23	1:B:327:LEU:HA	1.82	0.44
1:A:221:ASN:O	1:A:222:ASP:CB	2.66	0.44
1:A:648:LEU:HD13	1:A:652:ASN:ND2	2.33	0.44
1:B:292:TYR:O	1:B:296:LEU:HG	2.18	0.44
1:A:740:ASN:ND2	1:A:743:LEU:N	2.57	0.44
1:B:558:ASN:N	1:B:559:PRO:HD3	2.33	0.44
1:B:659:GLN:HE22	1:B:699:GLN:NE2	2.15	0.44
1:A:196:PHE:O	1:A:199:ASP:HB2	2.18	0.44
1:A:631:HIS:N	1:A:632:PRO:HD3	2.33	0.44
1:A:705:ILE:HA	1:A:711:ARG:HD3	1.99	0.44
1:A:735:PRO:O	1:A:738:GLN:N	2.51	0.44
1:B:66:LYS:HG2	1:B:70:LYS:HE2	1.99	0.44
1:B:162:PHE:C	1:B:164:GLU:H	2.20	0.44
1:B:631:HIS:N	1:B:632:PRO:CD	2.81	0.44
1:A:301:ASN:OD1	1:A:301:ASN:N	2.51	0.43
1:A:668:ALA:O	1:A:671:ALA:HB3	2.17	0.43
1:B:101:LEU:HD21	1:B:132:LEU:CD2	2.46	0.43
1:B:646:GLN:O	1:B:649:ARG:HB2	2.17	0.43
1:B:687:LEU:C	1:B:689:THR:H	2.21	0.43
1:B:238:LEU:HD23	1:B:238:LEU:N	2.27	0.43
1:B:342:ILE:CG2	1:B:345:LYS:H	2.31	0.43
1:B:343:VAL:HB	1:B:344:PRO:CD	2.38	0.43
1:B:495:VAL:HG11	1:B:532:ILE:CG1	2.49	0.43
1:B:536:TYR:HB2	2:B:782:HOH:O	2.17	0.43
1:B:642:LEU:HD22	1:B:648:LEU:HD13	2.00	0.43
1:B:711:ARG:NH1	1:B:756:SER:OG	2.51	0.43
1:A:254:LEU:N	1:A:254:LEU:HD12	2.33	0.43
1:A:657:LEU:HA	1:A:660:LEU:HG	2.00	0.43
1:B:694:ILE:O	1:B:697:ALA:HB3	2.18	0.43
1:A:699:GLN:HE21	1:A:703:ASP:HB2	1.81	0.43
1:A:717:LEU:HG	1:A:721:LEU:HD12	2.01	0.43
1:B:144:VAL:HG11	1:B:181:VAL:HG22	2.01	0.43
1:B:486:ILE:HG21	1:B:523:MET:HA	2.00	0.43
1:A:5:GLU:CG	1:A:12:ASP:HA	2.37	0.43
1:A:30:THR:HA	1:A:31:PRO:HD3	1.74	0.43
1:A:61:ASN:ND2	1:A:63:GLU:H	2.17	0.43
1:A:67:ASP:O	1:A:71:ILE:HG13	2.18	0.43
1:A:223:PRO:O	1:A:226:ILE:N	2.51	0.43
1:A:722:PHE:CZ	1:A:737:LEU:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:PRO:HG3	1:B:131:GLU:HG3	1.99	0.43
1:B:400:SER:HB3	1:B:448:ILE:HD11	2.01	0.43
1:A:30:THR:HG22	1:A:33:VAL:CG2	2.48	0.43
1:A:243:SER:C	1:A:245:ILE:H	2.22	0.43
1:B:94:GLN:OE1	1:B:124:ALA:HB1	2.19	0.43
1:B:96:ASP:O	1:B:97:ILE:C	2.56	0.43
1:B:327:LEU:HD11	1:B:359:LYS:HG3	2.00	0.43
1:B:447:TYR:O	1:B:451:THR:OG1	2.35	0.43
1:B:489:LEU:O	1:B:492:GLN:N	2.48	0.43
1:B:571:ASN:O	1:B:575:LEU:HD22	2.18	0.43
1:A:68:ARG:O	1:A:70:LYS:N	2.52	0.43
1:A:330:LEU:CD1	1:A:356:LEU:HD11	2.49	0.43
1:B:559:PRO:HB2	1:B:608:ASN:HD22	1.83	0.43
1:A:198:LYS:HA	1:A:201:ASP:CB	2.37	0.43
1:A:282:GLU:OE1	1:A:285:ARG:NH1	2.52	0.43
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.87	0.43
1:A:614:ASN:HD22	1:A:617:LEU:H	1.65	0.43
1:A:771:ILE:CG2	1:A:772:LYS:N	2.82	0.43
1:B:196:PHE:O	1:B:197:GLN:C	2.57	0.43
1:B:717:LEU:O	1:B:721:LEU:HG	2.18	0.43
1:A:12:ASP:C	1:A:14:SER:H	2.21	0.43
1:A:224:LEU:HD22	1:A:255:PHE:CE1	2.53	0.43
1:A:381:LYS:HA	1:A:456:PHE:CZ	2.54	0.43
1:A:554:PRO:O	1:A:555:VAL:O	2.37	0.43
1:B:749:MET:O	1:B:752:LYS:HB2	2.19	0.43
1:A:34:GLN:O	1:A:35:LYS:C	2.56	0.43
1:A:170:LYS:HG2	1:A:174:LEU:HD12	2.01	0.43
1:A:370:GLU:O	1:A:374:GLU:HG2	2.18	0.43
1:A:379:MET:HG2	1:A:383:GLN:HE21	1.84	0.43
1:A:451:THR:O	1:A:452:GLU:C	2.56	0.43
1:A:502:LEU:HD13	1:A:544:PHE:CG	2.53	0.43
1:A:583:SER:HA	1:A:627:ASN:HD22	1.83	0.43
1:A:644:ASN:OD1	1:A:646:GLN:HB2	2.19	0.43
1:A:759:GLU:OE1	1:A:759:GLU:HA	2.19	0.43
1:B:2:PRO:HB3	1:B:6:LYS:CE	2.49	0.43
1:B:43:ILE:CD1	1:B:71:ILE:HD12	2.45	0.43
1:A:223:PRO:O	1:A:224:LEU:C	2.56	0.42
1:B:269:LYS:CD	1:B:273:ARG:NH2	2.82	0.42
1:B:334:PHE:HB3	1:B:349:SER:HB3	2.00	0.42
1:B:471:GLN:O	1:B:475:ILE:HG13	2.18	0.42
1:A:146:TYR:O	1:A:150:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LYS:NZ	1:B:447:TYR:OH	2.40	0.42
1:B:579:THR:HA	1:B:624:LEU:CD1	2.48	0.42
1:B:667:ARG:HD2	1:B:709:GLU:CB	2.32	0.42
1:A:486:ILE:HB	1:A:487:PRO:HD3	2.01	0.42
1:B:55:MET:HG2	1:B:106:ILE:CD1	2.49	0.42
1:B:514:ILE:HD12	1:B:514:ILE:N	2.34	0.42
1:B:629:MET:CE	1:B:676:ILE:HD13	2.48	0.42
1:B:751:LEU:HD12	1:B:751:LEU:HA	1.81	0.42
1:A:747:LEU:HB3	1:A:768:LEU:HD21	2.02	0.42
1:B:133:GLN:HG3	1:B:167:PHE:CD1	2.54	0.42
1:B:205:VAL:CG1	1:B:206:ASP:N	2.81	0.42
1:B:735:PRO:O	1:B:736:LEU:C	2.57	0.42
1:A:257:LYS:O	1:A:261:GLU:CG	2.67	0.42
1:A:453:LEU:CD1	1:A:456:PHE:HD2	2.33	0.42
1:B:144:VAL:HG21	1:B:175:ARG:HH22	1.84	0.42
1:B:373:THR:HG21	1:B:443:PHE:HE1	1.83	0.42
1:A:36:TYR:CE1	1:A:77:ARG:HG2	2.55	0.42
1:A:79:TYR:CG	1:A:114:VAL:HG13	2.55	0.42
1:A:221:ASN:ND2	2:A:805:HOH:O	2.53	0.42
1:A:402:LEU:HD11	1:A:481:ARG:HB2	2.01	0.42
1:B:246:PHE:O	1:B:246:PHE:CD1	2.73	0.42
1:A:201:ASP:O	1:A:205:VAL:HG23	2.20	0.42
1:A:469:LYS:O	1:A:472:VAL:N	2.51	0.42
1:A:489:LEU:CD1	1:A:494:ALA:HB2	2.49	0.42
1:A:558:ASN:O	1:A:559:PRO:O	2.38	0.42
1:B:499:LEU:HD13	1:B:520:LEU:CD1	2.50	0.42
1:B:635:ILE:O	1:B:636:ALA:C	2.57	0.42
1:A:97:ILE:HD12	1:A:97:ILE:N	2.34	0.42
1:A:97:ILE:O	1:A:100:ALA:HB3	2.20	0.42
1:A:264:ASP:O	1:A:265:LEU:C	2.58	0.42
1:A:739:GLU:OE1	1:A:772:LYS:HD2	2.19	0.42
1:B:690:LYS:HD2	1:B:690:LYS:N	2.34	0.42
1:B:732:GLU:C	1:B:734:TYR:H	2.23	0.42
1:A:330:LEU:O	1:A:330:LEU:HD22	2.20	0.42
1:A:371:SER:O	1:A:375:ILE:HG13	2.19	0.42
1:B:47:ARG:HG2	1:B:47:ARG:O	2.19	0.42
1:B:663:VAL:HB	1:B:667:ARG:HH21	1.85	0.42
1:A:60:THR:O	1:A:61:ASN:O	2.38	0.42
1:A:128:LEU:O	1:A:132:LEU:HG	2.19	0.42
1:A:384:LYS:HE2	1:A:384:LYS:HB3	1.80	0.42
1:A:401:THR:CA	1:A:478:ASN:ND2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:ILE:HG21	1:A:740:ASN:ND2	2.33	0.42
1:B:98:PRO:O	1:B:102:ASN:ND2	2.53	0.42
1:B:138:TYR:O	1:B:140:GLU:N	2.53	0.42
1:B:261:GLU:OE1	1:B:262:GLU:OE2	2.38	0.42
1:A:258:ARG:O	1:A:258:ARG:HG3	2.20	0.41
1:B:115:PHE:HE2	1:B:128:LEU:HD11	1.85	0.41
1:B:248:THR:HG22	1:B:249:LYS:N	2.35	0.41
1:B:363:LYS:HE2	1:B:398:ASN:O	2.20	0.41
1:A:9:ASP:N	1:A:10:PRO:HD3	2.34	0.41
1:A:190:ALA:O	1:A:193:GLN:HB3	2.19	0.41
1:B:112:ILE:O	1:B:116:VAL:HG23	2.20	0.41
1:B:641:ASN:ND2	1:B:643:GLU:HB2	2.33	0.41
1:B:653:ILE:O	1:B:656:LYS:HG2	2.20	0.41
1:B:719:PHE:HB2	1:B:767:ILE:HD11	2.02	0.41
1:A:77:ARG:HB2	1:A:77:ARG:CZ	2.49	0.41
1:A:106:ILE:C	1:A:107:LEU:HD12	2.40	0.41
1:B:2:PRO:HB3	1:B:6:LYS:HE3	2.01	0.41
1:B:294:GLN:HE21	1:B:298:ARG:HH21	1.67	0.41
1:A:260:PHE:O	1:A:262:GLU:N	2.53	0.41
1:B:91:LYS:O	1:B:95:ASN:HB2	2.21	0.41
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.85	0.41
1:B:743:LEU:HD22	1:B:747:LEU:CD1	2.49	0.41
1:A:11:ILE:O	1:A:12:ASP:O	2.38	0.41
1:A:46:LEU:HD11	1:A:56:PRO:CD	2.51	0.41
1:A:193:GLN:C	1:A:195:SER:H	2.24	0.41
1:A:312:VAL:O	1:A:316:THR:HG23	2.20	0.41
1:A:481:ARG:NE	1:A:481:ARG:CA	2.82	0.41
1:A:752:LYS:O	1:A:753:ARG:O	2.37	0.41
1:B:208:MET:HE3	1:B:230:THR:HG21	2.02	0.41
1:B:499:LEU:HD12	1:B:499:LEU:HA	1.84	0.41
1:A:514:ILE:CG2	1:A:518:ARG:HH12	2.28	0.41
1:B:266:GLN:C	1:B:266:GLN:HE21	2.22	0.41
1:A:122:LYS:HA	1:A:158:PHE:CD1	2.55	0.41
1:A:157:LYS:CD	1:A:158:PHE:CE2	3.04	0.41
1:A:181:VAL:O	1:A:182:LYS:C	2.59	0.41
1:A:325:ILE:HG22	1:A:326:ASN:H	1.86	0.41
1:B:6:LYS:N	1:B:10:PRO:CB	2.78	0.41
1:B:7:GLY:H	1:B:10:PRO:CG	2.32	0.41
1:B:121:ASN:OD1	1:B:124:ALA:N	2.49	0.41
1:B:269:LYS:HD3	1:B:273:ARG:NH2	2.36	0.41
1:B:279:CYS:SG	1:B:288:ILE:HD12	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:C	1:B:304:ASP:N	2.73	0.41
1:B:460:GLU:O	1:B:462:HIS:N	2.54	0.41
1:B:536:TYR:N	2:B:782:HOH:O	2.52	0.41
1:B:122:LYS:HE2	1:B:164:GLU:OE1	2.20	0.41
1:B:337:ALA:O	1:B:342:ILE:HB	2.20	0.41
1:B:373:THR:HG21	1:B:443:PHE:CE1	2.55	0.41
1:B:699:GLN:OE1	1:B:700:VAL:HA	2.21	0.41
1:A:89:LEU:O	1:A:93:ILE:HG13	2.21	0.41
1:A:105:GLU:OE1	1:A:141:ASP:OD2	2.39	0.41
1:A:157:LYS:O	1:A:157:LYS:CG	2.66	0.41
1:A:299:SER:C	1:A:301:ASN:H	2.23	0.41
1:A:353:LEU:HB3	1:A:395:ILE:HD11	2.02	0.41
1:A:358:LEU:HB3	1:B:11:ILE:HD13	2.01	0.41
1:A:498:ILE:HG22	1:A:499:LEU:N	2.36	0.41
1:B:134:ILE:HG23	1:B:138:TYR:CE2	2.56	0.41
1:B:249:LYS:O	1:B:249:LYS:HG3	2.20	0.41
1:B:580:ASN:O	1:B:583:SER:OG	2.38	0.41
1:B:680:ILE:CG2	1:B:683:ILE:HG13	2.50	0.41
1:B:765:PRO:HG2	1:B:766:VAL:H	1.86	0.41
1:A:126:ILE:CD1	1:A:164:GLU:OE2	2.69	0.41
1:A:372:PHE:CZ	1:A:376:LEU:HD11	2.56	0.41
1:A:472:VAL:O	1:A:476:ILE:HG13	2.21	0.41
1:B:222:ASP:OD1	1:B:225:SER:HB2	2.21	0.41
1:B:229:LYS:HB2	1:B:229:LYS:HE3	1.81	0.41
1:B:276:SER:O	1:B:279:CYS:HB2	2.20	0.41
1:B:465:SER:C	1:B:467:ASN:H	2.24	0.41
1:B:486:ILE:N	1:B:487:PRO:CD	2.83	0.41
1:B:750:SER:C	1:B:752:LYS:N	2.74	0.41
1:A:121:ASN:O	1:A:122:LYS:C	2.60	0.40
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.85	0.40
1:A:382:SER:O	1:A:384:LYS:N	2.54	0.40
1:A:430:VAL:N	2:A:791:HOH:O	2.53	0.40
1:A:642:LEU:HD22	1:A:648:LEU:HA	2.03	0.40
1:A:694:ILE:O	1:A:698:ILE:HG13	2.21	0.40
1:B:198:LYS:HB2	1:B:198:LYS:HE3	1.72	0.40
1:B:505:LYS:HG2	2:B:778:HOH:O	2.20	0.40
1:A:68:ARG:C	1:A:70:LYS:N	2.74	0.40
1:A:144:VAL:CG2	1:A:145:THR:H	2.33	0.40
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.84	0.40
1:A:248:THR:HA	2:A:824:HOH:O	2.21	0.40
1:A:264:ASP:O	1:A:267:PHE:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LYS:NZ	1:A:398:ASN:HB3	2.36	0.40
1:A:476:ILE:CD1	1:A:498:ILE:HD13	2.52	0.40
1:B:269:LYS:O	1:B:273:ARG:HG3	2.20	0.40
1:A:158:PHE:HB2	1:A:160:TYR:CE2	2.57	0.40
1:A:307:ILE:CG2	1:A:348:MET:SD	3.10	0.40
1:A:496:LYS:NZ	2:A:813:HOH:O	2.52	0.40
1:A:588:ASP:HB3	2:A:831:HOH:O	2.21	0.40
1:A:608:ASN:HD22	1:A:608:ASN:HA	1.70	0.40
1:B:54:LYS:HB2	2:B:831:HOH:O	2.20	0.40
1:B:224:LEU:HB2	1:B:258:ARG:HH12	1.86	0.40
1:B:281:ASP:O	1:B:283:THR:N	2.55	0.40
1:B:563:ASP:O	1:B:564:GLU:C	2.60	0.40
1:B:752:LYS:O	1:B:754:GLY:N	2.53	0.40
1:A:125:THR:O	1:A:128:LEU:HB3	2.22	0.40
1:A:161:ASN:HD22	1:A:163:LYS:CE	2.32	0.40
1:A:293:LEU:CD2	1:A:322:LEU:HD21	2.51	0.40
1:A:356:LEU:C	1:A:358:LEU:H	2.24	0.40
1:A:595:HIS:HE1	2:A:808:HOH:O	2.05	0.40
1:A:597:VAL:HG21	1:A:635:ILE:HB	2.03	0.40
1:B:36:TYR:HD2	1:B:77:ARG:HH21	1.65	0.40
1:B:317:TRP:CE2	1:B:319:PHE:HZ	2.40	0.40
1:B:339:SER:HA	1:B:375:ILE:HD13	2.03	0.40
1:B:718:PHE:O	1:B:719:PHE:C	2.59	0.40
1:A:40:ILE:HD11	1:A:78:SER:HB3	2.04	0.40
1:A:768:LEU:C	1:A:770:LYS:N	2.75	0.40
1:B:197:GLN:O	1:B:198:LYS:C	2.59	0.40
1:B:321:LYS:HA	1:B:321:LYS:HD3	1.95	0.40
1:B:656:LYS:HD3	2:B:841:HOH:O	2.22	0.40
1:B:699:GLN:OE1	1:B:700:VAL:N	2.55	0.40

There are no symmetry-related clashes.

## 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	733/778 (94%)	562 (77%)	119 (16%)	52 (7%)	1	3
1	B	729/778 (94%)	570 (78%)	109 (15%)	50 (7%)	1	3
All	All	1462/1556 (94%)	1132 (77%)	228 (16%)	102 (7%)	1	3

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	13	SER
1	A	30	THR
1	A	32	ASP
1	A	51	GLU
1	A	61	ASN
1	A	222	ASP
1	A	224	LEU
1	A	248	THR
1	A	300	LEU
1	A	342	ILE
1	A	381	LYS
1	A	383	GLN
1	A	386	THR
1	A	537	SER
1	A	555	VAL
1	A	633	LEU
1	A	730	THR
1	A	736	LEU
1	A	753	ARG
1	A	760	PHE
1	B	61	ASN
1	B	144	VAL
1	B	197	GLN
1	B	222	ASP
1	B	237	SER
1	B	249	LYS
1	B	282	GLU
1	B	338	ILE
1	B	339	SER
1	B	384	LYS
1	B	507	ASP
1	B	534	LYS
1	B	584	SER
1	B	585	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	636	ALA
1	B	730	THR
1	B	733	VAL
1	A	223	PRO
1	A	249	LYS
1	A	261	GLU
1	A	356	LEU
1	A	369	ASN
1	A	451	THR
1	A	497	ILE
1	A	632	PRO
1	A	731	ASN
1	A	740	ASN
1	B	56	PRO
1	B	96	ASP
1	B	166	ARG
1	B	221	ASN
1	B	238	LEU
1	B	252	SER
1	B	303	GLU
1	B	461	MET
1	B	483	LYS
1	B	735	PRO
1	B	740	ASN
1	B	753	ARG
1	A	60	THR
1	A	197	GLN
1	A	218	ASP
1	A	279	CYS
1	A	539	LEU
1	A	554	PRO
1	A	691	LYS
1	A	735	PRO
1	B	32	ASP
1	B	62	SER
1	B	343	VAL
1	B	383	GLN
1	B	734	TYR
1	B	736	LEU
1	A	46	LEU
1	A	194	SER
1	A	360	ALA

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Mol	Chain	Res	Type
1	A	558	ASN
1	B	54	LYS
1	B	167	PHE
1	B	193	GLN
1	B	195	SER
1	B	382	SER
1	B	504	ASN
1	B	632	PRO
1	A	170	LYS
1	A	193	GLN
1	A	201	ASP
1	A	435	ALA
1	A	699	GLN
1	B	263	GLN
1	B	265	LEU
1	B	279	CYS
1	A	446	LYS
1	A	599	THR
1	A	662	ASP
1	B	566	ILE
1	B	280	ILE
1	B	305	VAL
1	B	705	ILE
1	A	672	ILE
1	B	729	GLY

### 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	680/694 (98%)	627 (92%)	53 (8%)	12	34
1	B	676/694 (97%)	625 (92%)	51 (8%)	13	37
All	All	1356/1388 (98%)	1252 (92%)	104 (8%)	13	35

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	ASP
1	A	19	LEU
1	A	32	ASP
1	A	38	ASP
1	A	58	ASP
1	A	94	GLN
1	A	97	ILE
1	A	120	SER
1	A	133	GLN
1	A	140	GLU
1	A	143	HIS
1	A	153	GLN
1	A	155	LEU
1	A	161	ASN
1	A	169	VAL
1	A	175	ARG
1	A	182	LYS
1	A	193	GLN
1	A	201	ASP
1	A	206	ASP
1	A	221	ASN
1	A	235	TYR
1	A	240	THR
1	A	264	ASP
1	A	277	SER
1	A	290	GLU
1	A	293	LEU
1	A	306	GLN
1	A	383	GLN
1	A	393	LEU
1	A	402	LEU
1	A	449	LEU
1	A	450	ARG
1	A	462	HIS
1	A	484	ASN
1	A	505	LYS
1	A	515	LEU
1	A	517	CYS
1	A	556	ASP
1	A	559	PRO
1	A	573	GLU
1	A	575	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	608	ASN
1	A	613	GLU
1	A	619	ARG
1	A	705	ILE
1	A	719	PHE
1	A	724	VAL
1	A	732	GLU
1	A	736	LEU
1	A	739	GLU
1	A	749	MET
1	B	12	ASP
1	B	32	ASP
1	B	56	PRO
1	B	63	GLU
1	B	73	GLU
1	B	76	THR
1	B	84	GLU
1	B	102	ASN
1	B	110	SER
1	B	120	SER
1	B	123	ASP
1	B	128	LEU
1	B	133	GLN
1	B	198	LYS
1	B	201	ASP
1	B	225	SER
1	B	235	TYR
1	B	238	LEU
1	B	254	LEU
1	B	266	GLN
1	B	281	ASP
1	B	286	THR
1	B	295	LEU
1	B	302	VAL
1	B	314	VAL
1	B	402	LEU
1	B	404	GLU
1	B	441	LEU
1	B	442	LEU
1	B	499	LEU
1	B	507	ASP
1	B	532	ILE

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Mol	Chain	Res	Type
1	B	549	LEU
1	B	575	LEU
1	B	578	LEU
1	B	588	ASP
1	B	632	PRO
1	B	641	ASN
1	B	660	LEU
1	B	663	VAL
1	B	679	THR
1	B	699	GLN
1	B	704	GLN
1	B	705	ILE
1	B	708	ILE
1	B	709	GLU
1	B	727	ASP
1	B	730	THR
1	B	736	LEU
1	B	743	LEU
1	B	770	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	ASN
1	A	80	GLN
1	A	94	GLN
1	A	102	ASN
1	A	113	HIS
1	A	153	GLN
1	A	161	ASN
1	A	193	GLN
1	A	291	ASN
1	A	306	GLN
1	A	467	ASN
1	A	478	ASN
1	A	528	ASN
1	A	565	GLN
1	A	571	ASN
1	A	608	ASN
1	A	614	ASN
1	A	627	ASN
1	A	652	ASN

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Mol	Chain	Res	Type
1	A	666	GLN
1	A	699	GLN
1	A	740	ASN
1	B	41	ASN
1	B	80	GLN
1	B	82	HIS
1	B	88	HIS
1	B	102	ASN
1	B	133	GLN
1	B	161	ASN
1	B	221	ASN
1	B	266	GLN
1	B	294	GLN
1	B	306	GLN
1	B	467	ASN
1	B	504	ASN
1	B	608	ASN
1	B	614	ASN
1	B	627	ASN
1	B	641	ASN
1	B	646	GLN
1	B	650	ASN
1	B	659	GLN
1	B	666	GLN
1	B	696	ASN
1	B	704	GLN
1	B	712	GLN
1	B	738	GLN
1	B	741	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	428:ASP	C	429:LYS	N	9.63

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	741/778 (95%)	0.16	26 (3%) 44 38	71, 97, 132, 155	0
1	B	741/778 (95%)	0.04	8 (1%) 80 80	31, 91, 125, 149	0
All	All	1482/1556 (95%)	0.10	34 (2%) 60 58	31, 94, 128, 155	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	760	PHE	8.1
1	A	47	ARG	5.9
1	A	338	ILE	4.5
1	B	536	TYR	4.4
1	B	26	THR	4.1
1	A	756	SER	4.1
1	A	52	SER	3.9
1	B	750	SER	3.5
1	B	753	ARG	3.5
1	A	536	TYR	3.4
1	A	292	TYR	3.3
1	B	48	GLN	3.3
1	A	387	HIS	3.0
1	A	748	ASN	2.9
1	A	722	PHE	2.9
1	A	770	LYS	2.7
1	B	737	LEU	2.6
1	A	744	LYS	2.6
1	B	7	GLY	2.5
1	A	739	GLU	2.4
1	A	751	LEU	2.4
1	A	743	LEU	2.4
1	A	327	LEU	2.3
1	A	318	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	462	HIS	2.2
1	A	53	GLY	2.2
1	A	383	GLN	2.2
1	A	715	LEU	2.1
1	B	260	PHE	2.1
1	A	767	ILE	2.1
1	A	49	LYS	2.1
1	A	535	LYS	2.1
1	A	753	ARG	2.0
1	A	747	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.