



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 AM UTC

PDB ID : 5UOE / pdb_00005ue
Title : Crystal Structure Analysis of Elbow-Engineered-Fab-Bound Human Insulin
Degrading Enzyme (IDE)
Authors : Liang, W.G.; Bailey, L.; Kossiakoff, T.; Tang, W.J.
Deposited on : 2017-01-31
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

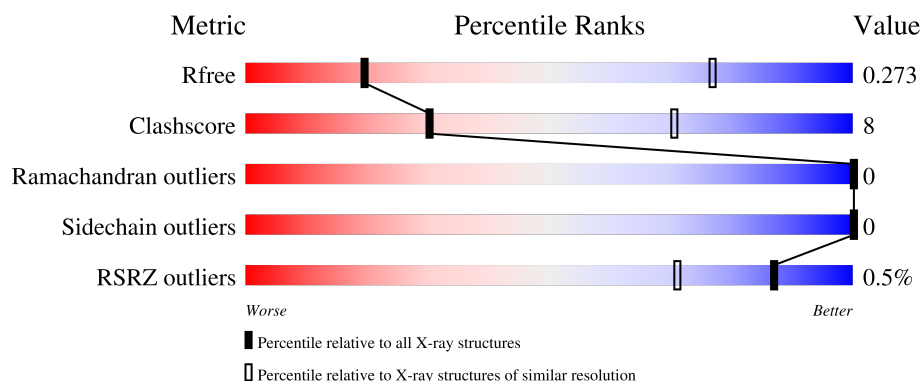
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



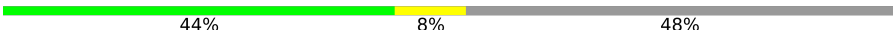
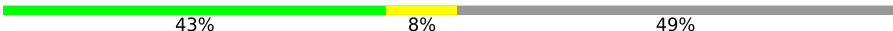
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	990	 78% 18% .
1	B	990	 79% 17% .
1	C	990	 75% 21% .
1	D	990	 76% 20% .
1	E	990	 77% 20% .

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Mol	Chain	Length	Quality of chain
2	H	229	
2	M	229	
2	P	229	
2	S	229	
2	V	229	
3	L	215	
3	N	215	
3	Q	215	
3	T	215	
3	W	215	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 47331 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 Insulin-degrading enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	953	Total	C	N	O	S	0	0	0
			7762	5003	1302	1435	22			
1	B	952	Total	C	N	O	S	0	0	0
			7752	4997	1303	1430	22			
1	C	953	Total	C	N	O	S	0	0	0
			7770	5009	1308	1431	22			
1	D	953	Total	C	N	O	S	0	0	0
			7764	5006	1307	1429	22			
1	E	953	Total	C	N	O	S	0	0	0
			7764	5006	1307	1429	22			

There are 125 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	expression tag	UNP P14735
A	31	HIS	-	expression tag	UNP P14735
A	32	HIS	-	expression tag	UNP P14735
A	33	HIS	-	expression tag	UNP P14735
A	34	HIS	-	expression tag	UNP P14735
A	35	HIS	-	expression tag	UNP P14735
A	36	HIS	-	expression tag	UNP P14735
A	37	ALA	-	expression tag	UNP P14735
A	38	ALA	-	expression tag	UNP P14735
A	39	GLY	-	expression tag	UNP P14735
A	40	ILE	-	expression tag	UNP P14735
A	41	PRO	-	expression tag	UNP P14735
A	110	LEU	CYS	engineered mutation	UNP P14735
A	171	SER	CYS	engineered mutation	UNP P14735
A	178	ALA	CYS	engineered mutation	UNP P14735
A	257	VAL	CYS	engineered mutation	UNP P14735
A	414	LEU	CYS	engineered mutation	UNP P14735
A	573	ASN	CYS	engineered mutation	UNP P14735
A	590	SER	CYS	engineered mutation	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
A	789	SER	CYS	engineered mutation	UNP P14735
A	812	ALA	CYS	engineered mutation	UNP P14735
A	819	ALA	CYS	engineered mutation	UNP P14735
A	904	SER	CYS	engineered mutation	UNP P14735
A	966	ASN	CYS	engineered mutation	UNP P14735
A	974	ALA	CYS	engineered mutation	UNP P14735
B	30	MET	-	expression tag	UNP P14735
B	31	HIS	-	expression tag	UNP P14735
B	32	HIS	-	expression tag	UNP P14735
B	33	HIS	-	expression tag	UNP P14735
B	34	HIS	-	expression tag	UNP P14735
B	35	HIS	-	expression tag	UNP P14735
B	36	HIS	-	expression tag	UNP P14735
B	37	ALA	-	expression tag	UNP P14735
B	38	ALA	-	expression tag	UNP P14735
B	39	GLY	-	expression tag	UNP P14735
B	40	ILE	-	expression tag	UNP P14735
B	41	PRO	-	expression tag	UNP P14735
B	110	LEU	CYS	engineered mutation	UNP P14735
B	171	SER	CYS	engineered mutation	UNP P14735
B	178	ALA	CYS	engineered mutation	UNP P14735
B	257	VAL	CYS	engineered mutation	UNP P14735
B	414	LEU	CYS	engineered mutation	UNP P14735
B	573	ASN	CYS	engineered mutation	UNP P14735
B	590	SER	CYS	engineered mutation	UNP P14735
B	789	SER	CYS	engineered mutation	UNP P14735
B	812	ALA	CYS	engineered mutation	UNP P14735
B	819	ALA	CYS	engineered mutation	UNP P14735
B	904	SER	CYS	engineered mutation	UNP P14735
B	966	ASN	CYS	engineered mutation	UNP P14735
B	974	ALA	CYS	engineered mutation	UNP P14735
C	30	MET	-	expression tag	UNP P14735
C	31	HIS	-	expression tag	UNP P14735
C	32	HIS	-	expression tag	UNP P14735
C	33	HIS	-	expression tag	UNP P14735
C	34	HIS	-	expression tag	UNP P14735
C	35	HIS	-	expression tag	UNP P14735
C	36	HIS	-	expression tag	UNP P14735
C	37	ALA	-	expression tag	UNP P14735
C	38	ALA	-	expression tag	UNP P14735
C	39	GLY	-	expression tag	UNP P14735
C	40	ILE	-	expression tag	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
C	41	PRO	-	expression tag	UNP P14735
C	110	LEU	CYS	engineered mutation	UNP P14735
C	171	SER	CYS	engineered mutation	UNP P14735
C	178	ALA	CYS	engineered mutation	UNP P14735
C	257	VAL	CYS	engineered mutation	UNP P14735
C	414	LEU	CYS	engineered mutation	UNP P14735
C	573	ASN	CYS	engineered mutation	UNP P14735
C	590	SER	CYS	engineered mutation	UNP P14735
C	789	SER	CYS	engineered mutation	UNP P14735
C	812	ALA	CYS	engineered mutation	UNP P14735
C	819	ALA	CYS	engineered mutation	UNP P14735
C	904	SER	CYS	engineered mutation	UNP P14735
C	966	ASN	CYS	engineered mutation	UNP P14735
C	974	ALA	CYS	engineered mutation	UNP P14735
D	30	MET	-	expression tag	UNP P14735
D	31	HIS	-	expression tag	UNP P14735
D	32	HIS	-	expression tag	UNP P14735
D	33	HIS	-	expression tag	UNP P14735
D	34	HIS	-	expression tag	UNP P14735
D	35	HIS	-	expression tag	UNP P14735
D	36	HIS	-	expression tag	UNP P14735
D	37	ALA	-	expression tag	UNP P14735
D	38	ALA	-	expression tag	UNP P14735
D	39	GLY	-	expression tag	UNP P14735
D	40	ILE	-	expression tag	UNP P14735
D	41	PRO	-	expression tag	UNP P14735
D	110	LEU	CYS	engineered mutation	UNP P14735
D	171	SER	CYS	engineered mutation	UNP P14735
D	178	ALA	CYS	engineered mutation	UNP P14735
D	257	VAL	CYS	engineered mutation	UNP P14735
D	414	LEU	CYS	engineered mutation	UNP P14735
D	573	ASN	CYS	engineered mutation	UNP P14735
D	590	SER	CYS	engineered mutation	UNP P14735
D	789	SER	CYS	engineered mutation	UNP P14735
D	812	ALA	CYS	engineered mutation	UNP P14735
D	819	ALA	CYS	engineered mutation	UNP P14735
D	904	SER	CYS	engineered mutation	UNP P14735
D	966	ASN	CYS	engineered mutation	UNP P14735
D	974	ALA	CYS	engineered mutation	UNP P14735
E	30	MET	-	expression tag	UNP P14735
E	31	HIS	-	expression tag	UNP P14735
E	32	HIS	-	expression tag	UNP P14735

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Chain	Residue	Modelled	Actual	Comment	Reference
E	33	HIS	-	expression tag	UNP P14735
E	34	HIS	-	expression tag	UNP P14735
E	35	HIS	-	expression tag	UNP P14735
E	36	HIS	-	expression tag	UNP P14735
E	37	ALA	-	expression tag	UNP P14735
E	38	ALA	-	expression tag	UNP P14735
E	39	GLY	-	expression tag	UNP P14735
E	40	ILE	-	expression tag	UNP P14735
E	41	PRO	-	expression tag	UNP P14735
E	110	LEU	CYS	engineered mutation	UNP P14735
E	171	SER	CYS	engineered mutation	UNP P14735
E	178	ALA	CYS	engineered mutation	UNP P14735
E	257	VAL	CYS	engineered mutation	UNP P14735
E	414	LEU	CYS	engineered mutation	UNP P14735
E	573	ASN	CYS	engineered mutation	UNP P14735
E	590	SER	CYS	engineered mutation	UNP P14735
E	789	SER	CYS	engineered mutation	UNP P14735
E	812	ALA	CYS	engineered mutation	UNP P14735
E	819	ALA	CYS	engineered mutation	UNP P14735
E	904	SER	CYS	engineered mutation	UNP P14735
E	966	ASN	CYS	engineered mutation	UNP P14735
E	974	ALA	CYS	engineered mutation	UNP P14735

- Molecule 2 is a protein called FAB Heavy chain with engineered elbow.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	119	Total	C	N	O	S	0	0	0
			901	568	153	177	3			
2	M	117	Total	C	N	O	S	0	0	0
			882	555	150	174	3			
2	P	118	Total	C	N	O	S	0	0	0
			893	564	151	175	3			
2	S	117	Total	C	N	O	S	0	0	0
			882	555	150	174	3			
2	V	117	Total	C	N	O	S	0	0	0
			881	555	150	173	3			

- Molecule 3 is a protein called FAB light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	108	Total	C	N	O	S	0	0	0
			820	516	136	165	3			

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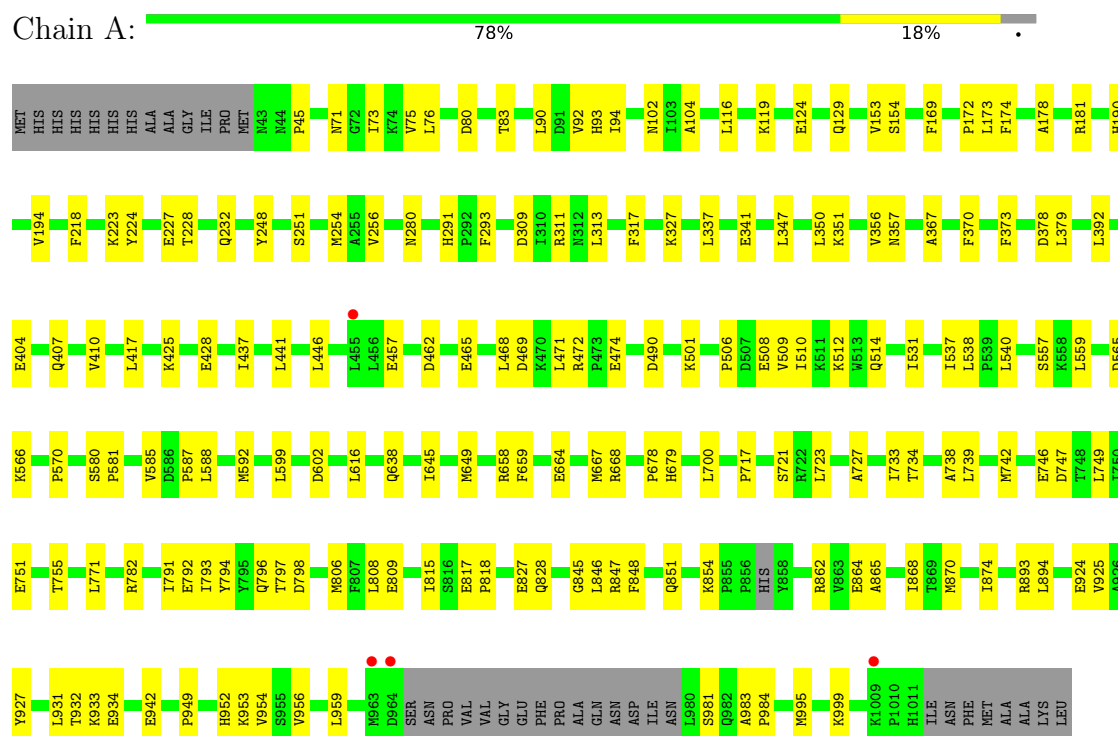
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	109	Total	C	N	O	S	0	0	0
			827	520	137	167	3			
3	Q	108	Total	C	N	O	S	0	0	0
			820	516	136	165	3			
3	T	107	Total	C	N	O	S	0	0	0
			815	513	135	164	3			
3	W	105	Total	C	N	O	S	0	0	0
			798	501	132	162	3			

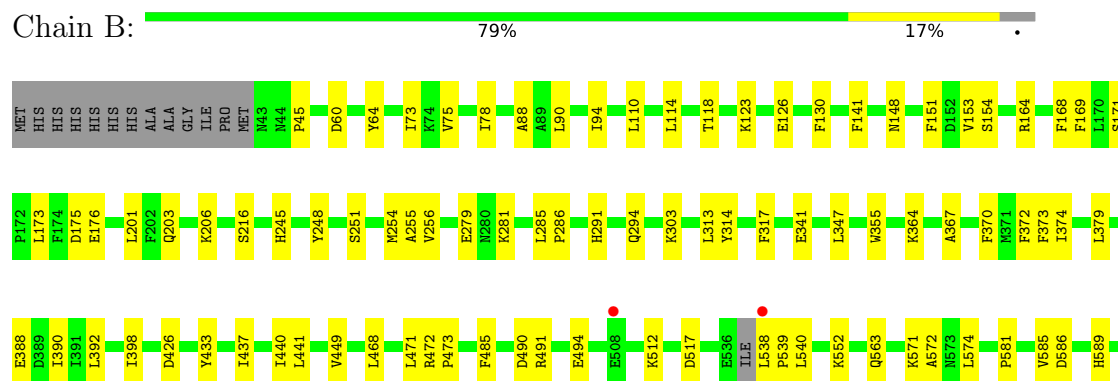
3 Residue-property plots

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: Insulin-degrading enzyme

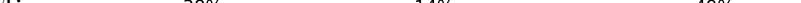


• Molecule 1: Insulin-degrading enzyme



CYS ASN VAL ASN HIS LYS PRO SER ASN THR LYS VAL ASP LYS LYS VAL GLU PRO LYS SER CYS ASP LYS THR HIS THR

- Molecule 2: FAB Heavy chain with engineered elbow

Chain M: 

Residue	Category
T119	GLU
V120	ILE
PHE	SER
ASN	E4
GLN	V6
ILE	E9
LYS	L14
PRO	L15
GLY	R22
VAL	A26
PHE	G29
LEU	F30
ALA	S36
PRO	Q42
SER	L48
SER	S53
GLY	G59
THR	S60
ALA	T61
LEU	Y62
GLY	R70
CYS	D76
LEU	K79
LYS	R80
VAL	T81
ASP	A82
TRR	Y83
PHE	L84
PHE	Q85
GLU	R86
GLU	L89
PRO	R90
ASN	A91
SER	E92
GLY	D93
ALA	T94
THR	C99
SER	A100
GLY	R101
VAL	HIS
THR	V106
SER	L109
PRO	D110
ALA	Y111
THR	

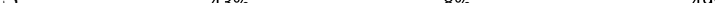
LEU	GLN	SER	SER	GLY	LEU	TYR	SER	SER	SER	SER	VAL	VAL	THR	THR	VAL	VAL	PRO	SER	SER	SER	SER	LEU	LEU	GLY	THR	THR	THR	THR	ILE	CYS	ASN	ASN	VAL	VAL	ASN	HIS	LYS	PRO	SER	SER	ASN	THR	THR	LYS	VAL	VAL	GLU	PRO	LYS	SER	SER	CYS	ASP	ASP	LYS	THR	THR	HIS	THR	THR
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- Molecule 2: FAB Heavy chain with engineered elbow

Chain P: 32% 20% 48%

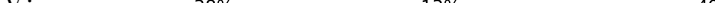
ASP	GLY	D83	GLU
LYS	ALA	T94	ILE
THR	LEU	Y97	SER
HIS	SER	Y98	E4
THR	GLY	C99	Q6
	VAL	A100	
	HIS	H101	E9
	THR	H102	
	PHE	Y103	V15
	PRO		Q16
	ALA	A107	
	VAL	G108	R22
	LEU	L109	A26
	GLN		A27
	SER	V120	S28
	SER	F121	G29
	GLY	ASN	N31
	LEU	GLN	I32
	TYR	ILE	S33
	SER	LYS	S34
	LEU	GLY	S35
	SER	PRO	S36
	SER	SER	I37
	VAL	PHE	H38
	VAL	THR	
	VAL	LEU	R41
	PRO	ALA	
	SER	PRO	W50
	HIS	SER	
	SER	SER	S53
	LEU	LYS	I54
	GLY	SER	Y55
	THR	THR	S56
	GLN	SER	Y57
	THR	GLY	S58
	THR	GLY	S59
	ILE	THR	S60
	CYS	ALA	T61
	ASN	ALA	Y62
	VAL	LEU	T63
	ASN	GLY	A64
	HIS	CYS	
	LYS	LEU	R70
	PRO	VAL	F71
	SER	LYS	
	ASN	ASP	
	THR	TYR	N80
	LYS	PHE	T81
	VAL	PRO	A82
	ASP	GLY	Y83
	LYS	PRO	L84
	LYS	VAL	Q85
	VAL	THR	R86
	GLU	VAL	
	PRO	SER	L89
	LYS	THR	R90
	SER	ASN	A91
	CYS	SER	S92

- Molecule 2: FAB Heavy chain with engineered elbow

Chain S:  43% 8% 49%

TYR	THR	GLY	GLU
ILE	THR	THR	ILE
CYS	ALA	ALA	SER
ASN	ALA	ALA	E4
VAL	LEU	LEU	
ASN	GLY		V15
HIS	CYS	CYS	Q16
LYS	LEU	LEU	P17
PRO	VAL	VAL	
SER	LYS	LYS	F30
ASN	ASP		
THR	THR	THR	S33
LYS	PHE	PHE	S34
VAL	PRO	PRO	
ASP	GLU	GLU	S36
LYS	VAL	VAL	
LYS	VAL	THR	Q42
VAL	THR		
GLU	VAL	VAL	G47
PRO	SER	SER	
LYS	THR	THR	W50
SER	ASN	ASN	
CYS	SER	SER	S53
ASP	GLY	GLY	
LYS	ALA	ALA	S56
THR	LEU	LEU	
HIS	THR	THR	Y62
THR	SER	SER	
	GLY	GLY	M86
	VAL	VAL	
	HIS	HIS	L89
	THR	THR	
	PHE	PHE	A100
	PRO	PRO	R101
	ALA	ALA	
	VAL	VAL	L109
	LEU	LEU	D110
	GLN	GLN	
	SER	SER	V120
	SER	SER	PHE
	GLY	GLY	ASN
	LEU	LEU	GLN
	THR	THR	ILE
	SER	SER	LYS
	LEU	LEU	GLY
	SER	SER	PRO
	VAL	VAL	SER
	VAL	VAL	VAL
	VAL	VAL	PHE
	THR	THR	PRO
	VAL	VAL	LEU
	THR	THR	ALA
	PRO	PRO	PRO
	SER	SER	SER
	SER	SER	SER
	LEU	LEU	LYS
	GLY	GLY	SER
	THR	THR	THR
	GLN	GLN	SER
	THR	THR	GLY

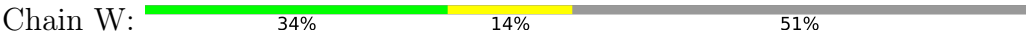
- Molecule 2: FAB Heavy chain with engineered elbow

Chain V:  %

[illegible]

SER	THR	TYR	SER	LEU	SER	SER	SER	THR	THR	LEU	LEU	LEU	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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● Molecule 3: FAB light chain



SER	D2	I3	S8	P9	L12	S15	D18	R19	I22	R25	A26	S27	Q28	A33	Y37	Q38	Q39	K40	P45	K46	S51	A52	D71	T75	L79	Q90	Q91	S92	Y93	F94	I97	T98	T103	K104	V105	E106	I107	LYS	ARG	THR	VAL	ALA	ALA
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PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO	SER	ASP	SER	GLN	LEU	LYS	SER	THR	ALA	SER	VAL	VAL	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	S51	A52	LYS	VAL	GLN	TRP	LYS	VAL	ASP	ASN	ALA	LEU	GLN	SER	GLY	ASN	GLN	GLU	SER	VAL	THR	GLU	GLN	ASP	SER	LYS	ASP	SER	THR	ALA	THR
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TYR	SER	LEU	SER	SER	THR	LEU	THR	LEU	SER	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	LYS	VAL	TYR	ALA	CYS	GLU	VAL	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	ASN	ARG	GLY	GLU	CYS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	131.32Å 242.05Å 310.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 3.80 49.24 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.24-3.80) 91.6 (49.24-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.77Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.220 , 0.270 0.225 , 0.273	Depositor DCC
R_{free} test set	2000 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å ²)	69.1	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	47331	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.13	0/7955	0.32	0/10764
1	B	0.12	0/7946	0.32	0/10752
1	C	0.15	0/7965	0.34	0/10777
1	D	0.13	0/7959	0.33	0/10771
1	E	0.13	0/7959	0.33	0/10771
2	H	0.14	0/922	0.39	0/1253
2	M	0.13	0/902	0.38	0/1226
2	P	0.13	0/914	0.39	0/1242
2	S	0.12	0/902	0.34	0/1226
2	V	0.16	0/901	0.42	0/1224
3	L	0.23	0/838	0.50	0/1137
3	N	0.16	0/845	0.43	0/1147
3	Q	0.26	0/838	0.47	0/1137
3	T	0.15	0/833	0.42	0/1130
3	W	0.21	0/816	0.44	0/1108
All	All	0.14	0/48495	0.35	0/65665

There are no bond length outliers.

There are no bond angle outliers.

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	7762	0	7681	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7752	0	7669	104	0
1	C	7770	0	7703	138	0
1	D	7764	0	7695	122	0
1	E	7764	0	7695	121	0
2	H	901	0	856	16	0
2	M	882	0	841	28	0
2	P	893	0	850	40	0
2	S	882	0	841	14	0
2	V	881	0	840	23	0
3	L	820	0	797	19	0
3	N	827	0	804	18	0
3	Q	820	0	797	27	0
3	T	815	0	795	30	0
3	W	798	0	771	24	0
All	All	47331	0	46635	790	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 8.

All (790) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:402:ARG:HG3	1:C:468:LEU:HD21	1.46	0.97
1:E:716:ILE:HB	1:E:717:PRO:HD3	1.58	0.86
3:W:3:ILE:HG13	3:W:27:SER:HB3	1.60	0.84
1:C:599:LEU:HD23	1:C:662:ILE:HD12	1.61	0.83
1:C:893:ARG:HG3	1:C:893:ARG:HH11	1.42	0.82
1:E:838:ARG:HB2	1:E:847:ARG:HD3	1.66	0.78
1:B:94:ILE:HG13	1:B:248:TYR:HB3	1.65	0.77
1:C:94:ILE:HG13	1:C:248:TYR:HB3	1.66	0.77
2:M:86:MET:HB3	2:M:89:LEU:HD21	1.69	0.74
3:L:8:SER:HB3	3:L:9:PRO:HD3	1.71	0.73
1:C:596:TYR:OH	1:C:649:MET:O	2.08	0.72
1:E:574:LEU:HG	1:E:729:LEU:HD22	1.72	0.71
1:E:489:THR:HA	1:E:501:LYS:HB2	1.74	0.70
2:H:109:LEU:HB2	3:L:37:TYR:OH	1.93	0.69
3:L:8:SER:HB2	3:L:23:THR:HB	1.74	0.68
2:S:101:ARG:O	2:S:109:LEU:HA	1.94	0.67
1:B:809:GLU:HG3	1:B:839:ARG:HH22	1.60	0.67
2:S:86:MET:HB3	2:S:89:LEU:HD21	1.75	0.67
1:B:538:LEU:N	1:B:539:PRO:CD	2.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:W:9:PRO:O	3:W:103:THR:HG22	1.95	0.66
1:E:203:GLN:HB3	1:E:494:GLU:OE2	1.95	0.66
3:T:8:SER:HB3	3:T:9:PRO:HD3	1.78	0.66
1:C:596:TYR:CD1	1:C:716:ILE:HG12	2.30	0.66
1:A:508:GLU:O	1:A:512:LYS:HG3	1.96	0.65
1:B:123:LYS:HB2	1:B:126:GLU:HB2	1.77	0.65
1:C:893:ARG:HG3	1:C:893:ARG:NH1	2.10	0.65
1:A:124:GLU:OE2	1:A:181:ARG:NH2	2.30	0.65
2:V:50:TRP:HZ2	2:V:53:SER:HB3	1.61	0.65
2:V:51:VAL:HG12	2:V:52:ALA:H	1.59	0.65
1:D:822:THR:O	1:D:827:GLU:HG2	1.96	0.65
3:W:8:SER:HB3	3:W:9:PRO:HD3	1.78	0.65
1:A:678:PRO:HD2	1:A:851:GLN:NE2	2.13	0.64
1:A:73:ILE:HG12	1:A:254:MET:HB2	1.78	0.64
1:D:796:GLN:HB3	1:D:952:HIS:HB2	1.81	0.63
1:E:262:GLU:HB2	1:E:267:LEU:HG	1.80	0.63
1:E:129:GLN:HA	1:E:817:GLU:HG3	1.80	0.63
1:E:114:LEU:HD13	1:E:168:PHE:HB3	1.81	0.63
2:P:70:ARG:NH1	2:P:93:ASP:OD2	2.31	0.62
2:P:86:MET:HB3	2:P:89:LEU:HD21	1.79	0.62
1:B:789:SER:HB3	1:B:856:PRO:HG3	1.81	0.62
1:A:45:PRO:HG3	1:B:176:GLU:HB3	1.82	0.62
1:E:512:LYS:HE2	3:W:94:PHE:CE2	2.35	0.62
2:M:101:ARG:O	2:M:109:LEU:HA	1.99	0.62
3:T:90:GLN:HG2	3:T:91:GLN:H	1.65	0.61
1:C:337:LEU:HD21	1:C:410:VAL:HG11	1.82	0.61
1:E:94:ILE:HG13	1:E:248:TYR:HB3	1.81	0.61
1:C:92:VAL:HG22	1:C:254:MET:HG2	1.83	0.60
2:V:9:GLU:OE2	2:V:99:CYS:HB3	2.01	0.60
2:M:110:ASP:OD1	2:M:111:TYR:N	2.33	0.60
1:C:942:GLU:HA	1:C:949:PRO:HD2	1.82	0.59
1:D:771:LEU:HB2	1:D:952:HIS:HB3	1.85	0.59
3:N:90:GLN:HG2	3:N:91:GLN:N	2.17	0.59
1:A:392:LEU:HD22	3:L:94:PHE:HD2	1.67	0.59
1:B:839:ARG:HG2	1:B:844:GLN:HB3	1.85	0.59
2:V:32:ILE:HB	2:V:37:ILE:HD11	1.85	0.59
1:D:809:GLU:OE1	1:D:893:ARG:NH1	2.36	0.58
1:D:806:MET:HE2	1:D:928:LEU:HB2	1.85	0.58
1:B:114:LEU:HD13	1:B:168:PHE:HB3	1.85	0.58
1:C:806:MET:HE2	1:C:928:LEU:HB2	1.85	0.58
1:E:727:ALA:HB3	1:E:742:MET:HE1	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:944:LEU:O	1:E:951:ARG:NH1	2.36	0.58
1:E:546:PRO:C	1:E:562:LYS:HE3	2.28	0.58
1:A:679:HIS:ND1	1:A:851:GLN:OE1	2.37	0.57
3:Q:3:ILE:HB	3:Q:91:GLN:OE1	2.03	0.57
1:B:538:LEU:N	1:B:539:PRO:HD3	2.19	0.57
1:A:727:ALA:HB3	1:A:742:MET:HE1	1.86	0.57
1:D:574:LEU:HD22	1:D:729:LEU:HD22	1.86	0.57
2:S:109:LEU:HB2	3:T:37:TYR:OH	2.05	0.57
1:A:350:LEU:HD13	1:A:356:VAL:HG21	1.86	0.57
3:T:30:VAL:HG12	3:T:32:SER:O	2.05	0.57
1:E:224:TYR:HA	1:E:228:THR:HB	1.85	0.57
1:E:490:ASP:OD2	1:E:501:LYS:HG3	2.04	0.57
1:D:77:LEU:HD21	1:D:271:VAL:HG21	1.87	0.57
2:P:50:TRP:CD2	3:Q:97:ILE:HB	2.38	0.57
3:Q:30:VAL:HG23	3:Q:93:TYR:CE2	2.40	0.57
1:B:809:GLU:OE1	1:B:893:ARG:NH1	2.37	0.57
1:C:413:GLU:OE2	1:C:528:ASN:HB2	2.05	0.57
1:B:727:ALA:HB3	1:B:742:MET:HE1	1.87	0.56
1:C:581:PRO:HD3	1:C:758:LEU:HD21	1.85	0.56
1:E:76:LEU:HD23	1:E:437:ILE:HG21	1.85	0.56
1:D:73:ILE:HG13	1:D:251:SER:HB2	1.87	0.56
1:D:678:PRO:HD2	1:D:851:GLN:HE21	1.69	0.56
1:B:341:GLU:HB2	1:B:609:TYR:CD1	2.41	0.56
1:D:400:LYS:HZ3	1:D:523:LYS:HA	1.69	0.56
1:A:942:GLU:HA	1:A:949:PRO:HD2	1.87	0.56
1:C:441:LEU:HD11	1:C:446:LEU:HD23	1.86	0.56
1:C:572:ALA:HA	1:C:731:GLY:HA3	1.87	0.56
1:D:400:LYS:NZ	1:D:523:LYS:HA	2.21	0.56
1:B:616:LEU:HD11	1:B:638:GLN:HG3	1.88	0.56
1:D:767:ARG:HD3	1:D:1005:PHE:O	2.05	0.56
1:A:864:GLU:OE2	1:A:953:LYS:NZ	2.30	0.56
1:C:75:VAL:HG22	1:C:256:VAL:HB	1.88	0.56
1:C:599:LEU:HD13	1:C:654:ILE:HG23	1.86	0.56
1:D:92:VAL:HG12	1:D:94:ILE:H	1.71	0.56
3:L:33:ALA:HB1	3:L:92:SER:O	2.05	0.56
1:B:572:ALA:HA	1:B:731:GLY:HA3	1.87	0.55
1:C:116:LEU:HD22	1:C:124:GLU:HG2	1.88	0.55
1:C:116:LEU:HD13	1:C:178:ALA:HB1	1.88	0.55
3:N:5:MET:HE2	3:N:91:GLN:HG3	1.87	0.55
1:C:56:LYS:NZ	1:C:60:ASP:O	2.26	0.55
1:B:45:PRO:HB3	1:E:120:LYS:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:ALA:HA	1:E:892:ARG:HH11	1.72	0.55
1:B:596:TYR:OH	1:B:649:MET:O	2.23	0.55
1:C:73:ILE:HG13	1:C:251:SER:HB2	1.87	0.55
2:H:108:GLY:O	3:L:37:TYR:OH	2.25	0.55
1:C:556:MET:HA	1:C:757:PRO:HB3	1.88	0.55
1:E:123:LYS:HB2	1:E:126:GLU:HB2	1.87	0.55
1:E:815:ILE:HG22	1:E:870:MET:HE2	1.88	0.55
1:E:832:ILE:HB	1:E:851:GLN:HB3	1.88	0.55
1:B:599:LEU:HD21	1:B:659:PHE:HA	1.87	0.55
2:P:50:TRP:HD1	2:P:64:ALA:HB2	1.72	0.55
1:A:782:ARG:HD2	1:A:959:LEU:HB2	1.89	0.55
1:B:960:ALA:HB3	1:B:963:MET:HG3	1.89	0.55
1:D:65:ARG:HB2	1:D:264:LEU:HD13	1.88	0.55
3:W:3:ILE:HD12	3:W:28:GLN:HB2	1.88	0.55
1:C:679:HIS:HB3	1:C:851:GLN:HB2	1.89	0.54
3:Q:3:ILE:HG23	3:Q:27:SER:HB2	1.89	0.54
1:A:616:LEU:HD11	1:A:638:GLN:HG3	1.89	0.54
2:H:61:THR:HB	2:H:63:TYR:CE2	2.42	0.54
1:C:272:VAL:O	1:C:276:SER:OG	2.22	0.54
1:C:678:PRO:HD2	1:C:851:GLN:NE2	2.22	0.54
1:E:793:ILE:O	1:E:847:ARG:HA	2.07	0.54
2:H:5:VAL:HG13	2:H:30:PHE:CE2	2.41	0.54
2:V:101:ARG:O	2:V:109:LEU:HA	2.07	0.54
1:E:441:LEU:HD11	1:E:446:LEU:HD23	1.90	0.54
1:E:501:LYS:HE2	1:E:503:GLU:OE2	2.08	0.54
2:H:102:HIS:HA	2:H:109:LEU:H	1.71	0.54
1:D:809:GLU:OE2	1:D:839:ARG:NH2	2.38	0.54
1:A:75:VAL:HG22	1:A:256:VAL:HB	1.90	0.54
1:B:813:GLN:OE1	1:B:892:ARG:NH2	2.40	0.54
1:E:123:LYS:CB	1:E:126:GLU:HB2	2.38	0.54
2:M:70:ARG:NH1	2:M:93:ASP:OD2	2.40	0.54
1:B:767:ARG:NH1	1:B:1006:PRO:HA	2.23	0.54
1:C:552:LYS:HZ2	1:C:743:GLN:HG3	1.73	0.54
2:S:100:ALA:HB3	2:S:109:LEU:HD22	1.89	0.53
1:D:794:TYR:HB3	1:D:954:VAL:HG13	1.90	0.53
1:D:827:GLU:CD	1:D:862:ARG:HH22	2.16	0.53
1:D:304:ILE:HB	1:D:481:VAL:HG22	1.90	0.53
1:D:402:ARG:NH1	1:D:468:LEU:O	2.40	0.53
1:D:716:ILE:HB	1:D:717:PRO:HD3	1.90	0.53
3:T:32:SER:H	3:T:67:ARG:NH1	2.07	0.53
2:V:52:ALA:HB2	2:V:63:TYR:HD1	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:ALA:HB2	1:A:983:ALA:HA	1.90	0.53
1:C:402:ARG:HG3	1:C:468:LEU:CD2	2.28	0.53
1:E:771:LEU:HB2	1:E:952:HIS:HB3	1.91	0.53
1:E:913:SER:O	1:E:915:GLN:HG3	2.08	0.53
3:Q:32:SER:HB3	3:Q:67:ARG:NH1	2.23	0.53
1:C:552:LYS:NZ	1:C:743:GLN:HG3	2.23	0.53
1:D:309:ASP:N	1:D:672:ASN:OD1	2.38	0.53
1:D:945:ALA:O	1:D:951:ARG:NH1	2.41	0.53
2:P:101:ARG:O	2:P:109:LEU:HA	2.09	0.53
1:A:441:LEU:HD11	1:A:446:LEU:HD23	1.89	0.53
1:B:512:LYS:HD3	2:M:106:VAL:HG13	1.90	0.53
1:E:92:VAL:HG12	1:E:94:ILE:H	1.74	0.53
1:D:94:ILE:HG13	1:D:248:TYR:HB3	1.91	0.53
3:N:90:GLN:HG2	3:N:91:GLN:H	1.73	0.53
1:B:90:LEU:HD13	1:B:169:PHE:CE2	2.44	0.52
1:B:618:TYR:HB2	1:B:631:VAL:HG22	1.89	0.52
1:C:559:LEU:HD11	1:C:729:LEU:HG	1.92	0.52
1:C:850:ILE:HG21	1:C:859:LEU:HD22	1.91	0.52
1:E:119:LYS:HD2	1:E:171:SER:HB2	1.91	0.52
1:E:722:ARG:HG2	1:E:756:LYS:HB2	1.90	0.52
2:M:9:GLU:OE2	2:M:9:GLU:N	2.42	0.52
1:B:552:LYS:NZ	1:B:743:GLN:HG2	2.25	0.52
1:E:341:GLU:HG2	1:E:347:LEU:HD23	1.91	0.52
1:E:679:HIS:HB3	1:E:851:GLN:HB2	1.90	0.52
2:M:30:PHE:CE2	2:M:101:ARG:HD2	2.44	0.52
3:L:13:SER:HA	3:L:106:GLU:O	2.09	0.52
1:B:864:GLU:CD	1:B:951:ARG:HH12	2.15	0.52
2:P:107:ALA:HB1	3:Q:35:ALA:HB2	1.91	0.52
2:V:50:TRP:CG	3:W:97:ILE:HB	2.45	0.52
1:C:586:ASP:OD1	1:C:589:HIS:ND1	2.42	0.52
1:D:150:TYR:HE1	1:D:431:ARG:HE	1.58	0.52
1:B:771:LEU:HB2	1:B:952:HIS:HB3	1.92	0.52
1:B:806:MET:HE2	1:B:928:LEU:HB2	1.92	0.52
1:C:679:HIS:ND1	1:C:851:GLN:OE1	2.37	0.52
1:D:441:LEU:HD11	1:D:446:LEU:HD23	1.90	0.52
1:B:291:HIS:O	1:B:294:GLN:NE2	2.42	0.52
1:C:793:ILE:O	1:C:847:ARG:HA	2.10	0.52
1:D:580:SER:HB2	1:D:723:LEU:HD23	1.92	0.52
3:Q:38:GLN:HB2	3:Q:48:LEU:HD11	1.92	0.52
1:A:827:GLU:OE2	1:A:862:ARG:HD2	2.10	0.52
1:D:114:LEU:HD13	1:D:168:PHE:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:678:PRO:HD2	1:D:851:GLN:NE2	2.24	0.52
2:M:22:ARG:HA	2:M:85:GLN:HA	1.91	0.52
1:B:279:GLU:HG2	1:B:281:LYS:HE3	1.92	0.51
1:C:490:ASP:HB2	1:C:501:LYS:HD3	1.92	0.51
1:C:655:ASP:HB3	1:C:658:ARG:HB2	1.91	0.51
1:A:679:HIS:HB3	1:A:851:GLN:HB2	1.90	0.51
2:H:22:ARG:HA	2:H:85:GLN:HA	1.92	0.51
2:M:91:ALA:HA	2:M:120:VAL:HG21	1.90	0.51
3:Q:32:SER:N	3:Q:67:ARG:HH11	2.08	0.51
3:T:12:LEU:HD11	3:T:105:VAL:HG13	1.92	0.51
1:A:510:ILE:O	1:A:514:GLN:HG2	2.10	0.51
1:B:392:LEU:HD22	3:N:94:PHE:HD2	1.75	0.51
1:B:942:GLU:HA	1:B:949:PRO:HD2	1.92	0.51
1:D:121:TYR:CD2	1:D:164:ARG:HG3	2.45	0.51
2:V:94:THR:OG1	2:V:120:VAL:HG22	2.11	0.51
1:C:865:ALA:HB2	1:C:983:ALA:HA	1.91	0.51
1:D:864:GLU:OE2	1:D:951:ARG:NH2	2.44	0.51
1:E:875:GLU:HG2	1:E:937:ILE:HD13	1.93	0.51
2:M:109:LEU:HB2	3:N:37:TYR:OH	2.10	0.51
1:C:92:VAL:HG12	1:C:94:ILE:H	1.75	0.51
1:C:804:GLU:C	1:C:844:GLN:HE22	2.19	0.51
1:D:343:PRO:HA	1:D:606:GLU:OE2	2.10	0.51
2:H:101:ARG:O	2:H:109:LEU:HA	2.10	0.51
2:M:86:MET:CB	2:M:89:LEU:HD21	2.40	0.51
1:A:538:LEU:HD13	1:A:734:THR:HG23	1.93	0.51
1:A:116:LEU:HD13	1:A:178:ALA:HB1	1.93	0.51
3:Q:5:MET:HE1	3:Q:30:VAL:HG11	1.93	0.51
1:B:437:ILE:HA	1:B:440:ILE:HG12	1.93	0.51
1:C:806:MET:SD	1:C:924:GLU:HB3	2.51	0.51
1:D:76:LEU:HD23	1:D:437:ILE:HG21	1.93	0.51
3:N:38:GLN:HB3	3:N:48:LEU:HD21	1.93	0.51
1:D:490:ASP:HB2	1:D:501:LYS:HD3	1.92	0.50
1:B:881:ALA:O	1:B:885:HIS:ND1	2.40	0.50
1:C:469:ASP:OD1	1:C:472:ARG:NH2	2.39	0.50
2:V:50:TRP:CD2	3:W:97:ILE:HB	2.47	0.50
1:A:797:THR:HG23	1:A:845:GLY:HA2	1.92	0.50
1:D:121:TYR:HB3	1:D:126:GLU:HG2	1.93	0.50
2:M:8:VAL:HG23	2:M:26:ALA:HB3	1.92	0.50
1:B:920:ARG:O	1:B:924:GLU:HG3	2.11	0.50
1:C:224:TYR:HA	1:C:228:THR:OG1	2.11	0.50
1:E:84:ASP:OD2	1:E:896:LYS:NZ	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:5:VAL:HG13	2:H:30:PHE:CD2	2.47	0.50
1:C:603:SER:CB	1:C:648:LYS:HZ1	2.23	0.50
1:D:54:ILE:HD11	1:D:66:GLY:H	1.77	0.50
1:E:308:LYS:HD3	1:E:672:ASN:HB3	1.94	0.50
2:M:26:ALA:HA	2:M:81:THR:HG22	1.93	0.50
1:A:224:TYR:HA	1:A:228:THR:HB	1.93	0.50
1:A:599:LEU:HD21	1:A:659:PHE:HA	1.93	0.50
1:C:228:THR:O	1:C:232:GLN:HG3	2.12	0.50
1:C:545:THR:OG1	1:C:547:TYR:O	2.28	0.50
1:D:722:ARG:HE	1:D:756:LYS:HB2	1.76	0.50
3:W:19:ARG:HH11	3:W:75:THR:HG21	1.76	0.50
3:T:5:MET:HE3	3:T:91:GLN:HB2	1.93	0.50
1:A:472:ARG:HD2	1:A:474:GLU:OE2	2.12	0.50
1:B:674:ARG:HD2	1:B:784:GLU:OE1	2.11	0.50
1:C:588:LEU:HG	1:C:592:MET:HE2	1.92	0.50
2:S:50:TRP:HZ2	2:S:53:SER:HB3	1.77	0.50
1:A:351:LYS:HE2	1:A:357:ASN:HA	1.92	0.49
1:B:203:GLN:HG3	1:B:494:GLU:OE2	2.11	0.49
1:B:206:LYS:HB3	1:B:216:SER:HA	1.94	0.49
1:B:796:GLN:HB3	1:B:952:HIS:HB2	1.94	0.49
1:E:716:ILE:HB	1:E:717:PRO:CD	2.38	0.49
3:L:90:GLN:HG2	3:L:91:GLN:N	2.26	0.49
3:L:90:GLN:HE21	3:L:97:ILE:HD13	1.77	0.49
3:W:38:GLN:OE1	3:W:40:LYS:NZ	2.40	0.49
1:A:80:ASP:O	1:A:83:THR:HG22	2.12	0.49
1:C:255:ALA:HB1	1:C:441:LEU:HD23	1.93	0.49
1:D:684:TYR:O	1:D:687:ARG:HG2	2.11	0.49
3:L:3:ILE:HG12	3:L:28:GLN:HG2	1.94	0.49
1:A:508:GLU:HG3	1:A:509:VAL:N	2.27	0.49
1:A:717:PRO:O	1:A:721:SER:OG	2.26	0.49
1:E:73:ILE:HG13	1:E:251:SER:HB2	1.94	0.49
1:A:817:GLU:HB3	1:A:818:PRO:HD3	1.94	0.49
1:B:341:GLU:HG2	1:B:347:LEU:HD23	1.92	0.49
1:B:686:LEU:HB2	1:B:956:VAL:HG21	1.94	0.49
1:C:519:ASN:HB3	1:C:522:PHE:HD2	1.76	0.49
1:C:809:GLU:HB3	1:C:889:LEU:HD21	1.95	0.49
1:D:337:LEU:HD21	1:D:410:VAL:HG11	1.93	0.49
1:A:874:ILE:O	1:A:933:LYS:HD3	2.13	0.49
1:C:155:HIS:NE2	1:C:261:ARG:HG2	2.27	0.49
1:B:679:HIS:HB3	1:B:851:GLN:HB2	1.95	0.49
1:C:175:ASP:OD2	1:C:177:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:HIS:CD2	1:C:370:PHE:HB2	2.48	0.49
1:C:908:TRP:NE1	1:C:912:ILE:HD11	2.27	0.49
1:E:317:PHE:HB2	1:E:373:PHE:HB3	1.94	0.49
1:B:865:ALA:HB2	1:B:983:ALA:HA	1.94	0.49
1:D:874:ILE:O	1:D:933:LYS:HD3	2.13	0.49
2:P:32:ILE:HG22	2:P:37:ILE:HD11	1.95	0.49
2:P:50:TRP:CD1	2:P:64:ALA:HB2	2.48	0.49
1:B:110:LEU:HD11	1:B:245:HIS:HB2	1.94	0.49
1:E:492:THR:O	1:E:492:THR:HG22	2.13	0.49
1:A:559:LEU:HB2	1:A:742:MET:HE3	1.94	0.49
2:M:76:ASP:HB2	2:M:83:TYR:HE2	1.78	0.49
3:T:38:GLN:HB3	3:T:48:LEU:HD11	1.94	0.49
1:C:93:HIS:O	1:C:93:HIS:ND1	2.44	0.49
2:P:6:GLN:HB2	2:P:28:SER:HB2	1.95	0.49
1:C:581:PRO:O	1:C:585:VAL:HG23	2.13	0.48
1:C:792:GLU:HA	1:C:848:PHE:O	2.12	0.48
2:V:50:TRP:NE1	3:W:97:ILE:HD12	2.28	0.48
1:A:90:LEU:HD13	1:A:169:PHE:CE2	2.48	0.48
1:A:588:LEU:HG	1:A:592:MET:HE2	1.94	0.48
2:H:30:PHE:CE1	2:H:101:ARG:HD2	2.48	0.48
3:T:3:ILE:HG23	3:T:27:SER:HB2	1.95	0.48
1:A:747:ASP:O	1:A:751:GLU:HG2	2.13	0.48
1:C:387:VAL:HG11	1:C:480:ILE:HD11	1.96	0.48
1:C:716:ILE:HB	1:C:717:PRO:HD3	1.94	0.48
1:C:721:SER:O	1:C:722:ARG:NH1	2.40	0.48
2:S:110:ASP:OD1	2:S:110:ASP:N	2.42	0.48
2:V:37:ILE:HB	2:V:54:ILE:HG23	1.96	0.48
1:A:602:ASP:OD1	1:A:658:ARG:NH2	2.45	0.48
1:D:85:LYS:NZ	1:D:135:ALA:O	2.46	0.48
1:E:125:ASN:HB3	1:E:821:ASN:ND2	2.29	0.48
1:E:320:PRO:HD3	1:E:470:LYS:HD2	1.94	0.48
2:P:91:ALA:HA	2:P:120:VAL:HG21	1.94	0.48
2:P:109:LEU:HB2	3:Q:37:TYR:OH	2.13	0.48
2:V:67:VAL:HG12	2:V:70:ARG:NH2	2.29	0.48
3:W:12:LEU:HD11	3:W:105:VAL:HG22	1.95	0.48
3:W:90:GLN:HG2	3:W:91:GLN:N	2.28	0.48
1:D:313:LEU:HB2	1:D:379:LEU:HD11	1.95	0.48
1:B:388:GLU:HB2	2:M:62:TYR:OH	2.14	0.48
1:B:908:TRP:NE1	1:B:912:ILE:HD11	2.28	0.48
1:C:794:TYR:HB3	1:C:954:VAL:HG13	1.95	0.48
1:E:125:ASN:HD22	1:E:821:ASN:HD22	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:38:HIS:HB3	2:P:50:TRP:CH2	2.49	0.48
1:C:305:VAL:HB	1:C:499:GLN:HB2	1.95	0.48
1:C:915:GLN:HG2	1:C:1008:VAL:HG11	1.94	0.48
1:D:76:LEU:HD22	1:D:449:VAL:HG21	1.96	0.48
1:D:603:SER:OG	1:D:648:LYS:NZ	2.33	0.48
2:H:38:HIS:HD1	2:H:50:TRP:HE1	1.60	0.48
3:T:22:ILE:HG21	3:T:103:THR:HG21	1.95	0.48
1:A:291:HIS:HD2	1:A:293:PHE:O	1.97	0.48
1:A:357:ASN:HB2	1:A:378:ASP:OD2	2.13	0.48
1:A:392:LEU:HD22	3:L:94:PHE:CD2	2.48	0.48
1:B:517:ASP:OD2	3:N:93:TYR:OH	2.26	0.48
1:B:793:ILE:O	1:B:847:ARG:HA	2.13	0.48
1:D:172:PRO:HG2	1:D:174:PHE:CE2	2.49	0.48
3:Q:90:GLN:HG2	3:Q:91:GLN:N	2.29	0.48
1:A:796:GLN:HB3	1:A:952:HIS:HB2	1.96	0.48
1:E:580:SER:HB2	1:E:723:LEU:HD23	1.96	0.48
2:V:86:MET:HE2	2:V:89:LEU:HD21	1.96	0.48
1:B:791:ILE:HD11	1:B:860:GLU:OE2	2.13	0.48
1:D:90:LEU:HD13	1:D:169:PHE:CE2	2.48	0.48
1:D:506:PRO:HB3	2:S:34:SER:O	2.14	0.48
1:E:870:MET:O	1:E:874:ILE:HG13	2.14	0.48
2:M:15:VAL:HG11	2:M:89:LEU:HD13	1.96	0.48
1:B:255:ALA:HB1	1:B:441:LEU:HD23	1.96	0.47
1:D:950:ARG:HG2	1:D:952:HIS:CE1	2.50	0.47
2:P:26:ALA:HA	2:P:81:THR:HG23	1.96	0.47
2:P:86:MET:HE2	2:P:89:LEU:HD21	1.96	0.47
3:T:90:GLN:HG2	3:T:91:GLN:N	2.29	0.47
1:A:472:ARG:HB3	1:A:474:GLU:HG2	1.95	0.47
1:D:426:ASP:HB3	1:D:899:LYS:HB3	1.96	0.47
2:H:50:TRP:CD1	3:L:97:ILE:HB	2.50	0.47
3:Q:4:GLN:O	3:Q:27:SER:OG	2.28	0.47
1:C:309:ASP:N	1:C:672:ASN:OD1	2.42	0.47
1:D:137:SER:N	1:D:152:ASP:OD1	2.43	0.47
1:D:190:HIS:O	1:D:194:VAL:HG23	2.14	0.47
1:D:944:LEU:O	1:D:951:ARG:NH1	2.47	0.47
3:N:39:GLN:O	3:N:85:ALA:HB1	2.14	0.47
1:A:794:TYR:HB3	1:A:954:VAL:HG13	1.95	0.47
1:A:894:LEU:HG	1:A:925:VAL:HG21	1.96	0.47
1:C:304:ILE:HB	1:C:481:VAL:HG22	1.95	0.47
1:C:579:PHE:HZ	1:C:765:ARG:CZ	2.28	0.47
1:C:862:ARG:NH1	1:C:981:SER:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:SER:HB2	1:D:281:LYS:HB3	1.97	0.47
1:E:678:PRO:HD2	1:E:851:GLN:NE2	2.29	0.47
2:M:42:GLN:HB2	2:M:48:LEU:HD23	1.96	0.47
1:B:468:LEU:HD12	1:B:471:LEU:HD12	1.96	0.47
1:C:119:LYS:HD3	1:D:236:ASP:HB2	1.95	0.47
2:P:30:PHE:CE2	2:P:101:ARG:HD2	2.50	0.47
1:A:417:LEU:HD21	1:A:531:ILE:HG22	1.97	0.47
2:P:54:ILE:HA	2:P:60:SER:O	2.14	0.47
2:P:102:HIS:HA	2:P:109:LEU:H	1.78	0.47
1:A:119:LYS:HA	1:A:173:LEU:HD21	1.96	0.47
1:A:425:LYS:HD2	1:A:428:GLU:OE2	2.15	0.47
1:B:285:LEU:HD12	1:B:286:PRO:HD2	1.95	0.47
1:B:586:ASP:OD1	1:B:589:HIS:ND1	2.48	0.47
1:B:870:MET:O	1:B:874:ILE:HG13	2.15	0.47
1:C:348:SER:HB2	1:C:606:GLU:OE2	2.15	0.47
1:C:367:ALA:HB3	1:C:370:PHE:CE1	2.49	0.47
1:C:689:LEU:HD23	1:C:995:MET:HE3	1.97	0.47
1:E:581:PRO:O	1:E:585:VAL:HG23	2.15	0.47
3:L:62:ARG:NE	3:L:83:ASP:OD2	2.46	0.47
1:B:388:GLU:OE1	2:M:62:TYR:OH	2.26	0.47
1:C:778:VAL:HG22	1:C:955:SER:HB2	1.97	0.47
1:C:995:MET:HE2	1:C:995:MET:HB3	1.76	0.47
1:D:441:LEU:HD13	1:D:449:VAL:HG11	1.96	0.47
1:E:569:LEU:O	1:E:571:LYS:N	2.44	0.47
1:E:663:LYS:HG3	1:E:704:LEU:HD21	1.96	0.47
3:T:50:TYR:O	3:T:54:SER:OG	2.30	0.47
1:D:572:ALA:HA	1:D:731:GLY:HA3	1.97	0.47
1:E:163:ASP:O	1:E:167:GLN:HG2	2.15	0.47
1:E:559:LEU:HB2	1:E:742:MET:HE3	1.97	0.47
1:E:809:GLU:OE1	1:E:893:ARG:NH1	2.48	0.47
2:M:9:GLU:OE1	2:M:99:CYS:HB3	2.14	0.47
2:V:44:PRO:HD3	2:V:95:ALA:HA	1.97	0.47
1:A:367:ALA:HB3	1:A:370:PHE:CE1	2.50	0.46
1:B:864:GLU:OE2	1:B:951:ARG:NH1	2.32	0.46
1:E:657:LYS:HA	1:E:657:LYS:HD2	1.70	0.46
1:E:777:PHE:HB3	1:E:992:ILE:HD11	1.97	0.46
2:P:91:ALA:O	2:P:94:THR:HG22	2.15	0.46
3:T:32:SER:OG	3:T:33:ALA:N	2.48	0.46
1:A:311:ARG:HH22	1:A:664:GLU:CD	2.24	0.46
1:B:881:ALA:HA	1:B:884:LYS:HE2	1.97	0.46
1:C:90:LEU:HD13	1:C:169:PHE:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:LEU:HD13	2:P:57:TYR:HE1	1.80	0.46
1:E:943:MET:HE1	1:E:950:ARG:NH1	2.30	0.46
2:H:100:ALA:HB3	2:H:109:LEU:HD22	1.96	0.46
2:P:53:SER:OG	2:P:62:TYR:HB2	2.15	0.46
3:T:8:SER:N	3:T:23:THR:O	2.38	0.46
1:C:341:GLU:HG2	1:C:347:LEU:HD23	1.98	0.46
1:C:791:ILE:HA	1:C:956:VAL:O	2.16	0.46
1:A:809:GLU:OE1	1:A:893:ARG:NH1	2.48	0.46
1:B:643:LYS:HD2	1:B:744:MET:HG2	1.97	0.46
1:B:817:GLU:HB3	1:B:818:PRO:HD3	1.97	0.46
1:C:722:ARG:NE	1:C:756:LYS:HB2	2.30	0.46
1:C:856:PRO:HA	1:C:859:LEU:HD12	1.98	0.46
1:D:691:THR:O	1:D:999:LYS:NZ	2.35	0.46
1:D:794:TYR:CE1	1:D:845:GLY:HA3	2.50	0.46
2:P:15:VAL:HG22	2:P:16:GLN:H	1.81	0.46
3:T:83:ASP:O	3:T:87:TYR:OH	2.27	0.46
1:A:749:LEU:HB3	1:A:755:THR:OG1	2.16	0.46
1:B:75:VAL:HA	1:B:256:VAL:O	2.15	0.46
1:C:994:ASN:HB3	1:C:997:GLU:HB3	1.97	0.46
1:D:153:VAL:HG22	1:D:154:SER:H	1.81	0.46
1:D:596:TYR:OH	1:D:649:MET:O	2.32	0.46
3:T:9:PRO:HG2	3:T:22:ILE:HA	1.98	0.46
1:B:540:LEU:HA	1:B:563:GLN:HE22	1.81	0.46
1:D:218:PHE:HB2	1:D:495:TRP:NE1	2.31	0.46
1:D:628:TYR:CZ	1:D:630:SER:HB2	2.50	0.46
1:D:776:TRP:CD2	1:D:989:PRO:HB3	2.51	0.46
1:D:927:TYR:CE2	1:D:931:LEU:HD21	2.51	0.46
3:W:25:ARG:NE	3:W:71:ASP:OD1	2.44	0.46
1:C:797:THR:OG1	1:C:798:ASP:N	2.49	0.46
2:M:53:SER:OG	2:M:62:TYR:HB2	2.16	0.46
1:A:223:LYS:HE3	1:A:227:GLU:OE2	2.16	0.46
1:E:796:GLN:HB3	1:E:952:HIS:HB2	1.98	0.46
2:M:101:ARG:NH1	2:M:110:ASP:OD2	2.49	0.46
3:Q:7:GLN:NE2	3:Q:103:THR:OG1	2.49	0.46
1:A:815:ILE:HG22	1:A:870:MET:HE2	1.98	0.46
1:B:688:LEU:HD22	1:B:694:ALA:HB1	1.97	0.46
1:C:387:VAL:HG21	1:C:480:ILE:HD13	1.97	0.46
1:D:102:ASN:OD1	1:D:102:ASN:N	2.47	0.46
1:D:664:GLU:OE2	1:D:668:ARG:NE	2.46	0.46
1:D:856:PRO:O	1:D:860:GLU:N	2.40	0.46
1:D:871:GLU:OE2	1:D:941:LYS:NZ	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:LYS:HD3	1:E:831:TYR:HD2	1.80	0.46
1:E:791:ILE:HA	1:E:956:VAL:O	2.15	0.46
2:V:16:GLN:HB3	2:V:17:PRO:CD	2.46	0.46
1:C:75:VAL:HA	1:C:256:VAL:O	2.15	0.45
1:E:547:TYR:CD1	1:E:918:PHE:HB3	2.50	0.45
2:P:30:PHE:CZ	2:P:101:ARG:HD2	2.51	0.45
1:B:73:ILE:HG13	1:B:251:SER:HB2	1.98	0.45
1:B:201:LEU:HD13	1:B:314:TYR:HE2	1.81	0.45
1:C:88:ALA:HB3	1:C:151:PHE:CE1	2.51	0.45
1:C:311:ARG:HH22	1:C:664:GLU:CD	2.25	0.45
1:D:91:ASP:OD1	1:D:146:HIS:ND1	2.43	0.45
1:D:777:PHE:HB3	1:D:992:ILE:HD11	1.98	0.45
1:E:223:LYS:HE3	1:E:227:GLU:OE2	2.15	0.45
1:E:838:ARG:HB2	1:E:847:ARG:CD	2.42	0.45
1:A:868:ILE:HD11	1:A:984:PRO:HB3	1.98	0.45
1:B:64:TYR:CD2	1:B:78:ILE:HG12	2.51	0.45
1:B:291:HIS:CD2	1:B:370:PHE:HB2	2.51	0.45
1:B:317:PHE:HB2	1:B:373:PHE:HB3	1.97	0.45
1:C:944:LEU:O	1:C:951:ARG:NH2	2.47	0.45
1:E:311:ARG:HH22	1:E:664:GLU:CD	2.22	0.45
1:E:441:LEU:HD13	1:E:449:VAL:HG11	1.97	0.45
1:B:141:PHE:CE1	1:B:148:ASN:HB3	2.52	0.45
1:C:155:HIS:CD2	1:C:261:ARG:HG2	2.51	0.45
1:D:768:GLU:HB3	1:D:843:ILE:HG13	1.98	0.45
1:E:291:HIS:CD2	1:E:370:PHE:HB2	2.51	0.45
1:E:596:TYR:OH	1:E:649:MET:O	2.31	0.45
1:B:574:LEU:HD22	1:B:729:LEU:HD22	1.99	0.45
1:B:913:SER:O	1:B:915:GLN:HG3	2.17	0.45
1:C:99:ASP:O	1:C:217:LYS:HE3	2.17	0.45
1:C:441:LEU:HD13	1:C:449:VAL:HG11	1.98	0.45
1:C:855:PRO:HA	1:C:963:MET:HE1	1.99	0.45
1:D:388:GLU:HB3	3:T:94:PHE:CE2	2.51	0.45
2:P:71:PHE:HB3	2:P:84:LEU:HD11	1.99	0.45
1:D:569:LEU:O	1:D:571:LYS:N	2.48	0.45
1:E:704:LEU:HA	1:E:707:VAL:HG12	1.99	0.45
3:W:33:ALA:HB1	3:W:92:SER:O	2.16	0.45
1:A:104:ALA:HB1	1:A:218:PHE:HB3	1.98	0.45
1:B:910:GLU:OE1	1:B:920:ARG:NH2	2.33	0.45
1:C:579:PHE:HZ	1:C:765:ARG:NH1	2.14	0.45
1:D:116:LEU:HD13	1:D:178:ALA:HB1	1.98	0.45
1:D:559:LEU:HD13	1:D:742:MET:HE3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:80:GLN:H	3:L:83:ASP:HB2	1.80	0.45
2:P:107:ALA:HA	3:Q:92:SER:OG	2.15	0.45
1:A:791:ILE:HA	1:A:956:VAL:O	2.15	0.45
1:B:303:LYS:HB3	1:B:485:PHE:CD2	2.52	0.45
1:C:643:LYS:HD2	1:C:744:MET:HG2	1.98	0.45
1:C:822:THR:HG21	1:C:866:PHE:CD1	2.52	0.45
1:E:573:ASN:ND2	1:E:900:LEU:HG	2.32	0.45
1:E:597:LEU:HD11	1:E:627:MET:HG2	1.98	0.45
3:Q:5:MET:CE	3:Q:91:GLN:HB2	2.47	0.45
1:A:792:GLU:HA	1:A:848:PHE:O	2.17	0.45
1:A:797:THR:OG1	1:A:798:ASP:N	2.49	0.45
1:C:489:THR:HA	1:C:501:LYS:HB2	1.99	0.45
1:E:597:LEU:HD12	1:E:622:ASN:HB3	1.99	0.45
1:A:645:ILE:O	1:A:649:MET:HB2	2.17	0.45
1:C:117:GLY:O	1:C:173:LEU:HB2	2.17	0.45
1:D:582:PHE:O	1:D:589:HIS:HB3	2.17	0.45
1:E:102:ASN:OD1	1:E:102:ASN:N	2.50	0.45
1:E:556:MET:HE3	1:E:750:ILE:HD11	1.99	0.45
2:M:30:PHE:CZ	2:M:101:ARG:HD2	2.52	0.45
3:T:25:ARG:HG3	3:T:71:ASP:OD2	2.17	0.45
1:A:71:ASN:O	1:A:280:ASN:ND2	2.50	0.44
1:C:722:ARG:CD	1:C:756:LYS:HB2	2.47	0.44
1:D:863:VAL:O	1:D:867:LEU:HG	2.17	0.44
1:E:192:LYS:HB3	1:E:192:LYS:HE2	1.71	0.44
1:E:699:GLU:O	1:E:702:GLU:HG2	2.17	0.44
2:P:41:ARG:NH1	2:P:93:ASP:HA	2.32	0.44
3:W:79:LEU:HD23	3:W:79:LEU:HA	1.84	0.44
1:A:559:LEU:HD23	1:A:739:LEU:HD23	1.98	0.44
1:B:742:MET:HE2	1:B:742:MET:HB2	1.90	0.44
3:T:4:GLN:HG3	3:T:27:SER:OG	2.16	0.44
2:V:79:LYS:HE3	2:V:83:TYR:OH	2.18	0.44
2:V:91:ALA:HA	2:V:120:VAL:HG21	1.98	0.44
1:D:961:ARG:HD2	1:D:962:GLU:OE2	2.17	0.44
2:P:32:ILE:HG23	2:P:80:ASN:OD1	2.17	0.44
3:Q:13:SER:HA	3:Q:106:GLU:O	2.17	0.44
1:A:172:PRO:HG2	1:A:174:PHE:CE2	2.53	0.44
1:B:313:LEU:HB2	1:B:379:LEU:HD11	1.99	0.44
1:B:915:GLN:CD	1:B:920:ARG:HH22	2.26	0.44
1:C:90:LEU:HD13	1:C:169:PHE:CZ	2.52	0.44
1:E:252:ASN:ND2	1:E:283:VAL:O	2.50	0.44
1:E:699:GLU:HA	1:E:702:GLU:OE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:789:SER:HB3	1:E:963:MET:HE1	2.00	0.44
1:E:856:PRO:HA	1:E:859:LEU:HD12	1.99	0.44
2:M:79:LYS:O	2:M:81:THR:HG23	2.16	0.44
1:A:190:HIS:O	1:A:194:VAL:HG23	2.18	0.44
1:B:615:GLY:HA3	1:B:634:TYR:HE1	1.82	0.44
1:A:93:HIS:O	1:A:93:HIS:ND1	2.49	0.44
1:D:387:VAL:HG11	1:D:480:ILE:HD11	2.00	0.44
1:D:883:GLN:HA	1:D:886:ILE:HB	1.98	0.44
3:N:31:SER:HA	3:N:67:ARG:CZ	2.47	0.44
2:P:38:HIS:ND1	2:P:50:TRP:HH2	2.16	0.44
3:Q:43:LYS:HA	3:Q:43:LYS:HD2	1.64	0.44
1:A:854:LYS:HD2	1:A:854:LYS:HA	1.66	0.44
1:B:173:LEU:HD22	1:B:175:ASP:HB2	1.98	0.44
1:B:441:LEU:HD13	1:B:449:VAL:HG11	2.00	0.44
1:C:388:GLU:OE1	2:P:59:GLY:HA3	2.18	0.44
1:E:650:ALA:HB2	1:E:749:LEU:HD23	2.00	0.44
2:P:36:SER:OG	2:P:38:HIS:NE2	2.41	0.44
1:D:303:LYS:HB3	1:D:485:PHE:CD2	2.53	0.44
1:D:388:GLU:HB2	2:S:62:TYR:OH	2.18	0.44
1:D:652:PHE:CE2	1:D:654:ILE:HD13	2.53	0.44
1:E:314:TYR:HB2	1:E:479:ALA:HB3	1.99	0.44
2:P:9:GLU:OE2	2:P:99:CYS:HB3	2.17	0.44
3:Q:84:PHE:HD1	3:Q:105:VAL:O	1.99	0.44
2:S:16:GLN:HB3	2:S:17:PRO:HD2	1.99	0.44
2:V:97:TYR:O	2:V:116:THR:HG22	2.18	0.44
1:B:648:LYS:HE3	1:B:648:LYS:HB3	1.80	0.44
1:B:823:LEU:HB2	1:B:833:VAL:HG11	1.99	0.44
1:C:102:ASN:OD1	1:C:102:ASN:N	2.49	0.44
1:C:114:LEU:HD13	1:C:168:PHE:HB3	1.99	0.44
1:C:385:LEU:HD22	2:P:60:SER:HB3	2.00	0.44
1:D:541:GLU:OE2	1:D:734:THR:HB	2.17	0.44
1:D:814:ILE:HG12	1:D:885:HIS:ND1	2.32	0.44
1:A:129:GLN:HA	1:A:817:GLU:HG3	2.00	0.43
1:A:557:SER:OG	1:A:746:GLU:OE1	2.30	0.43
1:C:599:LEU:HD21	1:C:659:PHE:HA	2.00	0.43
1:D:492:THR:OG1	1:D:499:GLN:HG3	2.18	0.43
1:D:581:PRO:O	1:D:585:VAL:HG23	2.17	0.43
3:Q:90:GLN:HG2	3:Q:91:GLN:H	1.83	0.43
1:A:71:ASN:HB2	1:A:251:SER:OG	2.18	0.43
1:D:722:ARG:HA	1:D:756:LYS:O	2.17	0.43
1:A:537:ILE:HD11	1:A:570:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:TRP:HB3	1:B:390:ILE:HD11	2.01	0.43
1:D:791:ILE:HD11	1:D:860:GLU:OE2	2.19	0.43
1:E:379:LEU:HD13	1:E:384:LEU:HA	2.01	0.43
1:E:860:GLU:OE1	1:E:953:LYS:NZ	2.40	0.43
2:P:33:SER:HA	2:P:56:SER:HB2	1.99	0.43
2:S:42:GLN:HG3	2:S:47:GLY:O	2.18	0.43
1:A:153:VAL:HG22	1:A:154:SER:H	1.82	0.43
1:E:368:ARG:HH12	1:E:443:TYR:HD1	1.67	0.43
3:T:38:GLN:HE22	3:T:40:LYS:NZ	2.16	0.43
1:E:160:GLY:O	1:E:164:ARG:NH1	2.52	0.43
1:E:577:GLU:HB2	1:E:908:TRP:CZ2	2.54	0.43
1:C:860:GLU:OE2	1:C:955:SER:HB3	2.18	0.43
1:D:597:LEU:HD22	1:D:620:LEU:HD21	1.99	0.43
1:B:367:ALA:HB3	1:B:370:PHE:CE1	2.53	0.43
1:C:181:ARG:HB3	1:C:828:GLN:HG3	2.01	0.43
1:D:153:VAL:HG11	1:D:158:LEU:HA	1.99	0.43
1:D:550:LEU:HD11	1:D:558:LYS:CG	2.49	0.43
3:N:3:ILE:HD12	3:N:28:GLN:HB2	2.01	0.43
1:A:462:ASP:OD1	1:A:462:ASP:N	2.52	0.43
1:A:771:LEU:HB2	1:A:952:HIS:HB3	2.01	0.43
1:B:88:ALA:HB3	1:B:151:PHE:CE1	2.54	0.43
1:D:494:GLU:HB3	1:D:496:TYR:H	1.83	0.43
2:H:94:THR:HG23	2:H:94:THR:O	2.17	0.43
3:T:31:SER:HA	3:T:67:ARG:CZ	2.48	0.43
3:T:91:GLN:HE21	3:T:93:TYR:HB2	1.84	0.43
1:C:183:VAL:HG11	1:C:227:GLU:OE2	2.18	0.43
2:M:94:THR:OG1	2:M:120:VAL:HG22	2.19	0.43
3:N:3:ILE:HG13	3:N:27:SER:HB2	2.01	0.43
3:Q:104:LYS:HB2	3:Q:104:LYS:HE3	1.78	0.43
2:S:15:VAL:O	2:S:120:VAL:HA	2.19	0.43
3:W:15:SER:N	3:W:18:ASP:OD2	2.48	0.43
3:W:91:GLN:HB3	3:W:98:THR:H	1.83	0.43
1:A:581:PRO:O	1:A:585:VAL:HG23	2.19	0.43
1:A:793:ILE:O	1:A:847:ARG:HA	2.18	0.43
1:B:552:LYS:HZ1	1:B:743:GLN:HG2	1.83	0.43
1:C:153:VAL:HG22	1:C:154:SER:H	1.84	0.43
1:C:540:LEU:HA	1:C:563:GLN:OE1	2.19	0.43
1:D:82:THR:O	1:D:896:LYS:NZ	2.40	0.43
1:E:426:ASP:OD1	1:E:571:LYS:HE3	2.19	0.43
1:E:600:LEU:HD23	1:E:620:LEU:HD21	2.00	0.43
1:E:805:ASN:HA	1:E:844:GLN:HE22	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:39:GLN:HE21	3:N:88:TYR:HE2	1.65	0.43
3:W:90:GLN:HE21	3:W:97:ILE:HD13	1.84	0.43
1:A:806:MET:SD	1:A:924:GLU:HB3	2.59	0.42
1:D:865:ALA:HB2	1:D:983:ALA:HA	2.00	0.42
1:B:398:ILE:HD13	1:B:471:LEU:HB3	2.01	0.42
1:B:433:TYR:CZ	1:B:437:ILE:HD11	2.54	0.42
1:B:716:ILE:HB	1:B:717:PRO:HD3	2.01	0.42
1:C:437:ILE:HA	1:C:440:ILE:HG12	2.01	0.42
1:D:794:TYR:CE1	1:D:838:ARG:HD3	2.54	0.42
1:E:582:PHE:O	1:E:589:HIS:HB3	2.19	0.42
1:A:667:MET:HE3	1:A:667:MET:HB2	1.91	0.42
1:B:73:ILE:HG12	1:B:254:MET:HB2	2.00	0.42
1:B:777:PHE:HB3	1:B:992:ILE:HD11	2.01	0.42
1:C:472:ARG:HG2	1:C:473:PRO:HD2	2.01	0.42
1:D:599:LEU:HD13	1:D:654:ILE:HD12	2.01	0.42
1:E:81:PRO:HA	1:E:261:ARG:HG2	2.01	0.42
1:E:116:LEU:HD13	1:E:178:ALA:HB1	2.01	0.42
2:M:109:LEU:CD1	3:N:90:GLN:HE22	2.33	0.42
3:N:86:THR:C	3:N:87:TYR:HD1	2.26	0.42
1:B:75:VAL:HG22	1:B:256:VAL:HB	2.02	0.42
1:D:291:HIS:CD2	1:D:370:PHE:HB2	2.54	0.42
1:E:528:ASN:OD1	1:E:530:PHE:HB2	2.19	0.42
1:E:579:PHE:CE2	1:E:765:ARG:NH1	2.88	0.42
3:L:3:ILE:HG23	3:L:27:SER:HB2	2.01	0.42
2:P:93:ASP:O	2:P:97:TYR:OH	2.30	0.42
2:V:109:LEU:HB2	3:W:37:TYR:OH	2.19	0.42
1:B:915:GLN:HG2	1:B:1008:VAL:HG11	2.01	0.42
1:C:767:ARG:HG2	1:C:1007:LEU:HD21	2.01	0.42
1:D:743:GLN:HG3	1:D:747:ASP:OD2	2.20	0.42
1:E:90:LEU:HD13	1:E:169:PHE:CE2	2.54	0.42
1:E:652:PHE:CE2	1:E:654:ILE:HD13	2.54	0.42
2:P:15:VAL:HG11	2:P:89:LEU:HD13	2.00	0.42
3:Q:92:SER:HA	3:Q:97:ILE:CD1	2.50	0.42
3:W:22:ILE:CG2	3:W:103:THR:HG21	2.50	0.42
1:A:341:GLU:HG2	1:A:347:LEU:HD22	2.01	0.42
1:A:927:TYR:CE2	1:A:931:LEU:HD21	2.54	0.42
1:C:285:LEU:HD12	1:C:286:PRO:HD2	2.00	0.42
1:D:794:TYR:CD1	1:D:838:ARG:HD3	2.55	0.42
2:V:50:TRP:CZ2	2:V:53:SER:HB3	2.48	0.42
3:W:51:SER:O	3:W:52:ALA:HB3	2.19	0.42
1:B:794:TYR:HB3	1:B:954:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:MET:HE2	1:C:704:LEU:HD23	2.02	0.42
1:E:77:LEU:HD21	1:E:271:VAL:HG21	2.01	0.42
1:E:368:ARG:NH1	1:E:443:TYR:CD1	2.88	0.42
3:L:6:THR:HG22	3:L:25:ARG:O	2.20	0.42
2:M:76:ASP:HB2	2:M:83:TYR:CE2	2.54	0.42
1:A:317:PHE:HB2	1:A:373:PHE:HB3	2.02	0.42
1:A:580:SER:HB2	1:A:723:LEU:HD23	2.02	0.42
1:B:581:PRO:O	1:B:585:VAL:HG23	2.20	0.42
1:C:855:PRO:HA	1:C:856:PRO:HD3	1.95	0.42
1:D:802:THR:HG23	1:D:924:GLU:HG2	2.02	0.42
1:D:855:PRO:HA	1:D:856:PRO:HD3	1.92	0.42
1:E:855:PRO:HA	1:E:963:MET:CE	2.50	0.42
3:T:108:LYS:HB3	3:T:108:LYS:HE2	1.82	0.42
1:C:80:ASP:OD1	1:C:82:THR:HG22	2.19	0.42
1:C:586:ASP:OD2	1:C:588:LEU:HB3	2.20	0.42
1:D:791:ILE:HA	1:D:956:VAL:O	2.20	0.42
1:E:88:ALA:HB3	1:E:151:PHE:CE1	2.55	0.42
1:E:558:LYS:HE3	1:E:558:LYS:HB2	1.88	0.42
3:N:79:LEU:HD23	3:N:79:LEU:HA	1.88	0.42
1:A:75:VAL:HA	1:A:256:VAL:O	2.19	0.42
1:A:178:ALA:HA	1:A:181:ARG:HH21	1.84	0.42
1:A:404:GLU:HG2	1:A:407:GLN:NE2	2.35	0.42
1:A:733:ILE:HD13	1:A:738:ALA:HB2	2.02	0.42
1:B:130:PHE:CE1	1:B:164:ARG:NH1	2.88	0.42
1:B:426:ASP:OD1	1:B:571:LYS:NZ	2.44	0.42
1:D:599:LEU:HD23	1:D:662:ILE:HD12	2.02	0.42
1:D:793:ILE:O	1:D:847:ARG:HA	2.20	0.42
1:E:153:VAL:HG22	1:E:154:SER:H	1.85	0.42
2:M:14:LEU:HA	2:M:119:THR:O	2.20	0.42
2:P:103:TYR:H	2:P:108:GLY:HA3	1.84	0.42
3:T:40:LYS:HG2	3:T:85:ALA:HB2	2.02	0.42
1:A:337:LEU:HD21	1:A:410:VAL:HG11	2.01	0.41
1:C:141:PHE:CE1	1:C:148:ASN:HB3	2.55	0.41
1:C:510:ILE:O	1:C:514:GLN:HG3	2.19	0.41
1:D:550:LEU:HB2	1:D:560:TRP:CH2	2.55	0.41
1:D:820:PHE:CZ	1:D:824:ARG:HD3	2.54	0.41
1:E:565:ASP:OD1	1:E:565:ASP:N	2.53	0.41
3:N:36:TRP:HD1	3:N:49:ILE:HB	1.85	0.41
1:A:181:ARG:HB3	1:A:828:GLN:HG3	2.02	0.41
1:C:426:ASP:HB3	1:C:899:LYS:HB3	2.01	0.41
1:D:90:LEU:HD22	1:D:169:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:679:HIS:O	1:D:683:MET:HG3	2.20	0.41
1:D:724:HIS:CD2	1:D:763:LEU:HD21	2.55	0.41
2:H:101:ARG:NH1	2:H:111:TYR:HD2	2.19	0.41
2:P:100:ALA:HB3	2:P:109:LEU:HD22	2.02	0.41
2:S:30:PHE:CE2	2:S:101:ARG:HD2	2.54	0.41
1:A:862:ARG:NH2	1:A:981:SER:O	2.49	0.41
1:C:389:ASP:HA	3:Q:94:PHE:CD2	2.56	0.41
1:C:872:LYS:HE2	1:C:876:ASP:OD2	2.21	0.41
1:D:472:ARG:HD2	1:D:474:GLU:OE2	2.20	0.41
1:E:104:ALA:HB1	1:E:218:PHE:HB3	2.03	0.41
1:E:943:MET:HE1	1:E:950:ARG:CZ	2.50	0.41
1:B:60:ASP:OD2	1:B:64:TYR:OH	2.30	0.41
1:B:153:VAL:HG22	1:B:154:SER:H	1.86	0.41
1:D:576:PHE:HB2	1:D:629:LEU:HB3	2.02	0.41
1:E:385:LEU:HD22	2:V:60:SER:HB3	2.02	0.41
1:E:388:GLU:OE1	2:V:62:TYR:OH	2.26	0.41
3:L:6:THR:OG1	3:L:7:GLN:N	2.54	0.41
1:A:228:THR:O	1:A:232:GLN:HB2	2.21	0.41
1:B:388:GLU:OE1	2:M:59:GLY:HA3	2.21	0.41
1:C:796:GLN:O	1:C:952:HIS:HB2	2.20	0.41
1:B:118:THR:HB	1:B:171:SER:O	2.20	0.41
1:B:643:LYS:NZ	1:B:744:MET:HG2	2.36	0.41
1:B:907:TYR:O	1:B:911:ILE:HG13	2.20	0.41
1:C:80:ASP:O	1:C:83:THR:HG22	2.20	0.41
1:C:212:LYS:HA	1:C:212:LYS:HD2	1.81	0.41
1:C:506:PRO:HB3	2:P:34:SER:O	2.21	0.41
1:D:195:MET:HB2	1:D:786:HIS:CE1	2.55	0.41
3:Q:92:SER:HA	3:Q:97:ILE:HD12	2.03	0.41
2:S:33:SER:HA	2:S:56:SER:HB2	2.01	0.41
1:A:76:LEU:HD23	1:A:437:ILE:HG21	2.01	0.41
1:A:313:LEU:HB2	1:A:379:LEU:HD11	2.03	0.41
1:C:71:ASN:HB2	1:C:251:SER:OG	2.20	0.41
1:C:206:LYS:HG2	1:C:215:PHE:CE2	2.56	0.41
1:C:910:GLU:OE2	1:C:920:ARG:NE	2.39	0.41
1:D:550:LEU:HD12	1:D:559:LEU:O	2.20	0.41
1:D:817:GLU:HB3	1:D:818:PRO:HD3	2.02	0.41
1:D:822:THR:HG21	1:D:866:PHE:CD1	2.56	0.41
1:E:285:LEU:HD12	1:E:286:PRO:HD2	2.03	0.41
1:E:425:LYS:HD3	1:E:454:TYR:CE2	2.55	0.41
3:W:39:GLN:HB2	3:W:45:PRO:HG3	2.02	0.41
1:C:317:PHE:HB2	1:C:373:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:893:ARG:NH1	1:C:893:ARG:CG	2.80	0.41
1:E:399:GLN:O	1:E:402:ARG:HG2	2.20	0.41
3:L:90:GLN:NE2	3:L:97:ILE:HD13	2.35	0.41
3:T:38:GLN:HE22	3:T:40:LYS:HG3	1.86	0.41
1:A:92:VAL:HG12	1:A:94:ILE:H	1.86	0.41
1:A:94:ILE:HG13	1:A:248:TYR:HB3	2.02	0.41
1:A:124:GLU:CD	1:A:181:ARG:HH22	2.29	0.41
1:A:808:LEU:HD11	1:A:846:LEU:HD13	2.03	0.41
1:B:472:ARG:HG3	1:B:473:PRO:HD2	2.03	0.41
1:C:148:ASN:OD1	1:C:435:SER:OG	2.26	0.41
1:C:907:TYR:O	1:C:911:ILE:HG13	2.20	0.41
1:D:190:HIS:CE1	1:D:218:PHE:HZ	2.38	0.41
1:E:195:MET:HB2	1:E:786:HIS:CE1	2.56	0.41
1:E:317:PHE:O	1:E:373:PHE:N	2.53	0.41
1:E:572:ALA:HA	1:E:731:GLY:HA3	2.03	0.41
3:Q:5:MET:HE2	3:Q:91:GLN:HB2	2.01	0.41
1:A:870:MET:O	1:A:874:ILE:HG13	2.21	0.41
1:E:327:LYS:HD2	1:E:457:GLU:OE2	2.21	0.41
1:E:742:MET:HE2	1:E:742:MET:HB2	1.85	0.41
3:L:8:SER:N	3:L:23:THR:O	2.54	0.41
3:N:31:SER:HA	3:N:67:ARG:NH2	2.36	0.41
2:S:50:TRP:CZ3	3:T:96:PRO:HA	2.56	0.41
3:W:46:LYS:HD3	3:W:46:LYS:HA	1.89	0.41
1:A:468:LEU:HD12	1:A:471:LEU:HD12	2.03	0.40
1:A:506:PRO:HB3	2:H:34:SER:O	2.21	0.40
1:A:540:LEU:HD11	1:A:565:ASP:HB3	2.03	0.40
1:A:932:THR:HG22	1:A:934:GLU:H	1.85	0.40
1:A:995:MET:O	1:A:999:LYS:HG3	2.20	0.40
1:C:961:ARG:HD2	1:C:962:GLU:OE2	2.20	0.40
1:D:49:ARG:NH1	1:D:68:GLU:OE1	2.54	0.40
1:D:298:LEU:O	1:D:300:GLN:HG2	2.21	0.40
1:E:592:MET:SD	1:E:711:ARG:HG3	2.61	0.40
2:H:26:ALA:HA	2:H:81:THR:HG23	2.02	0.40
3:Q:79:LEU:HD23	3:Q:79:LEU:HA	1.82	0.40
1:A:309:ASP:O	1:A:668:ARG:NH1	2.48	0.40
1:A:490:ASP:OD1	1:A:501:LYS:HG3	2.22	0.40
1:B:364:LYS:HD2	1:B:374:ILE:CG2	2.52	0.40
1:E:117:GLY:O	1:E:173:LEU:HB2	2.21	0.40
1:E:874:ILE:O	1:E:933:LYS:HD3	2.21	0.40
2:P:50:TRP:CE3	2:P:50:TRP:HA	2.56	0.40
2:P:107:ALA:O	3:Q:50:TYR:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:62:ARG:HD2	3:Q:78:SER:O	2.20	0.40
3:T:31:SER:HA	3:T:67:ARG:NH1	2.36	0.40
2:V:107:ALA:HB2	3:W:33:ALA:C	2.45	0.40
1:A:465:GLU:O	1:A:469:ASP:HB2	2.21	0.40
1:B:364:LYS:HB3	1:B:372:PHE:HB2	2.03	0.40
1:C:319:ILE:HG13	1:C:371:MET:HB2	2.03	0.40
1:C:711:ARG:HA	1:C:711:ARG:HD2	1.88	0.40
1:D:75:VAL:HA	1:D:256:VAL:O	2.21	0.40
1:D:341:GLU:HG2	1:D:347:LEU:HD23	2.03	0.40
1:E:82:THR:HA	1:E:261:ARG:HH21	1.85	0.40
3:T:33:ALA:HB1	3:T:92:SER:O	2.21	0.40
1:A:102:ASN:OD1	1:A:102:ASN:N	2.53	0.40
1:A:565:ASP:CG	1:A:566:LYS:HZ2	2.29	0.40
1:A:587:PRO:HB3	1:A:700:LEU:HD23	2.02	0.40
1:B:490:ASP:OD1	1:B:491:ARG:N	2.50	0.40
1:C:74:LYS:HD2	1:C:74:LYS:H	1.87	0.40
1:C:302:TYR:CD2	1:C:502:GLN:HB3	2.57	0.40
1:C:311:ARG:HD2	1:C:384:LEU:HD22	2.03	0.40
1:C:838:ARG:HB2	1:C:847:ARG:HD3	2.04	0.40
1:E:73:ILE:HG12	1:E:254:MET:HB2	2.02	0.40
3:N:32:SER:N	3:N:67:ARG:NH1	2.69	0.40
2:P:22:ARG:NH1	2:P:83:TYR:CG	2.89	0.40
1:A:327:LYS:NZ	1:A:457:GLU:OE1	2.28	0.40
1:C:418:ASN:HB3	1:C:454:TYR:O	2.21	0.40
1:C:579:PHE:HZ	1:C:765:ARG:NH2	2.19	0.40
1:D:510:ILE:O	1:D:514:GLN:HG3	2.21	0.40
1:D:827:GLU:CG	1:D:862:ARG:HH22	2.35	0.40
1:E:296:GLU:HG3	1:E:297:HIS:CE1	2.57	0.40
1:E:743:GLN:HG3	1:E:747:ASP:OD2	2.21	0.40
1:E:792:GLU:HA	1:E:848:PHE:O	2.21	0.40
1:E:794:TYR:CD1	1:E:838:ARG:HD3	2.56	0.40
3:T:8:SER:HB3	3:T:23:THR:HB	2.04	0.40
3:T:32:SER:N	3:T:67:ARG:NH1	2.70	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	947/990 (96%)	924 (98%)	23 (2%)	0	100	100
1	B	946/990 (96%)	922 (98%)	24 (2%)	0	100	100
1	C	949/990 (96%)	923 (97%)	26 (3%)	0	100	100
1	D	949/990 (96%)	926 (98%)	23 (2%)	0	100	100
1	E	949/990 (96%)	919 (97%)	30 (3%)	0	100	100
2	H	117/229 (51%)	110 (94%)	7 (6%)	0	100	100
2	M	115/229 (50%)	109 (95%)	6 (5%)	0	100	100
2	P	116/229 (51%)	110 (95%)	6 (5%)	0	100	100
2	S	115/229 (50%)	109 (95%)	6 (5%)	0	100	100
2	V	115/229 (50%)	108 (94%)	7 (6%)	0	100	100
3	L	106/215 (49%)	97 (92%)	9 (8%)	0	100	100
3	N	107/215 (50%)	103 (96%)	4 (4%)	0	100	100
3	Q	106/215 (49%)	99 (93%)	7 (7%)	0	100	100
3	T	105/215 (49%)	99 (94%)	6 (6%)	0	100	100
3	W	103/215 (48%)	96 (93%)	7 (7%)	0	100	100
All	All	5845/7170 (82%)	5654 (97%)	191 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	840/879 (96%)	840 (100%)	0	100	100
1	B	838/879 (95%)	838 (100%)	0	100	100
1	C	841/879 (96%)	841 (100%)	0	100	100
1	D	840/879 (96%)	840 (100%)	0	100	100
1	E	840/879 (96%)	840 (100%)	0	100	100
2	H	94/191 (49%)	94 (100%)	0	100	100
2	M	92/191 (48%)	92 (100%)	0	100	100
2	P	93/191 (49%)	93 (100%)	0	100	100
2	S	92/191 (48%)	92 (100%)	0	100	100
2	V	92/191 (48%)	92 (100%)	0	100	100
3	L	93/190 (49%)	93 (100%)	0	100	100
3	N	94/190 (50%)	94 (100%)	0	100	100
3	Q	93/190 (49%)	93 (100%)	0	100	100
3	T	93/190 (49%)	93 (100%)	0	100	100
3	W	91/190 (48%)	91 (100%)	0	100	100
All	All	5126/6300 (81%)	5126 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	ASN
1	A	323	GLN
1	A	671	ASN
1	A	914	GLN
1	A	1011	HIS
1	B	184	ASN
1	B	312	ASN
1	B	376	ASN
1	B	515	ASN
1	B	519	ASN
1	B	563	GLN
1	B	573	ASN
1	B	821	ASN
1	B	914	GLN
1	C	125	ASN

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Mol	Chain	Res	Type
1	C	184	ASN
1	C	190	HIS
1	C	563	GLN
1	C	841	ASN
1	C	885	HIS
1	D	43	ASN
1	D	53	HIS
1	D	167	GLN
1	D	190	HIS
1	D	239	GLN
1	D	376	ASN
1	D	718	GLN
1	D	841	ASN
1	D	851	GLN
1	E	184	ASN
1	E	294	GLN
1	E	724	HIS
2	H	42	GLN
3	L	7	GLN
3	L	28	GLN
3	L	80	GLN
2	P	114	GLN
2	S	87	ASN
3	T	91	GLN
2	V	114	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	953/990 (96%)	-0.04	4 (0%) 88 74	55, 72, 89, 121	0
1	B	952/990 (96%)	0.01	2 (0%) 91 81	56, 76, 92, 128	0
1	C	953/990 (96%)	-0.05	1 (0%) 92 87	55, 72, 90, 117	0
1	D	953/990 (96%)	-0.00	5 (0%) 87 71	54, 77, 93, 121	0
1	E	953/990 (96%)	-0.05	4 (0%) 88 74	51, 73, 90, 120	0
2	H	119/229 (51%)	0.16	1 (0%) 82 62	64, 78, 98, 106	0
2	M	117/229 (51%)	0.36	4 (3%) 48 33	73, 92, 106, 125	0
2	P	118/229 (51%)	0.27	1 (0%) 82 62	71, 88, 105, 112	0
2	S	117/229 (51%)	0.11	1 (0%) 81 60	71, 89, 105, 116	0
2	V	117/229 (51%)	0.27	2 (1%) 69 47	70, 89, 110, 119	0
3	L	108/215 (50%)	0.21	1 (0%) 81 60	64, 77, 96, 113	0
3	N	109/215 (50%)	0.22	2 (1%) 67 46	71, 89, 103, 109	0
3	Q	108/215 (50%)	0.07	0 100 100	63, 81, 96, 100	0
3	T	107/215 (49%)	0.11	0 100 100	64, 82, 95, 104	0
3	W	105/215 (48%)	0.28	0 100 100	70, 85, 99, 108	0
All	All	5889/7170 (82%)	0.02	28 (0%) 87 71	51, 76, 96, 128	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	93	TYR	3.5
1	C	494	GLU	3.3
1	D	1010	PRO	2.8
1	A	963	MET	2.8
2	P	36	SER	2.7
1	D	493	GLU	2.7
1	A	964	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	538	LEU	2.6
1	D	508	GLU	2.6
1	B	508	GLU	2.6
2	V	35	SER	2.5
1	E	702	GLU	2.4
2	M	120	VAL	2.3
2	M	60	SER	2.3
1	D	455	LEU	2.3
2	S	36	SER	2.2
1	E	508	GLU	2.2
2	V	36	SER	2.1
1	E	1011	HIS	2.1
1	A	455	LEU	2.1
1	A	1009	LYS	2.1
2	M	36	SER	2.1
2	M	29	GLY	2.1
2	H	60	SER	2.1
1	D	517	ASP	2.0
1	E	497	GLY	2.0
3	N	93	TYR	2.0
3	N	51	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.