



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:59 AM UTC

PDB ID : 5CFY / pdb_00005cfy
Title : CRYSTAL STRUCTURE OF GLTPH R397A IN COMPLEX WITH NA⁺ AND L-ASP
Authors : Boudker, O.; Oh, S.
Deposited on : 2015-07-08
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

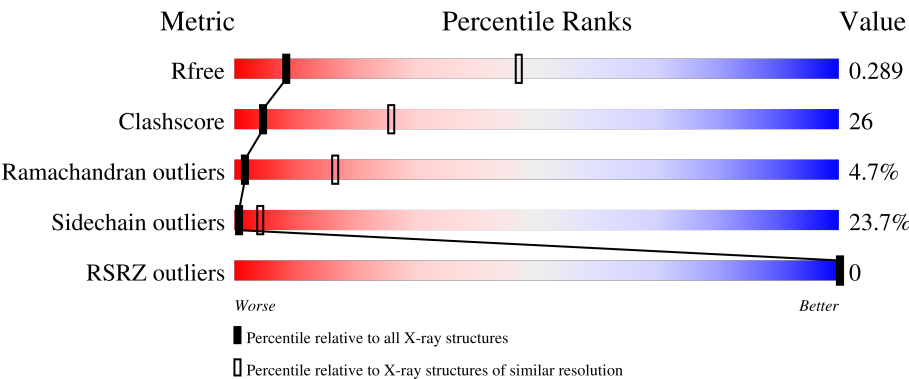
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	425	42%43%12%.
1	B	425	41%42%12%..
1	C	425	44%41%12%..
1	D	425	43%40%12%..
1	E	425	44%42%10%..

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Mol	Chain	Length	Quality of chain
1	F	425	38% 45% 12% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18240 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 425aa long hypothetical proton glutamate symport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	B	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	C	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	D	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	E	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			
1	F	411	Total	C	N	O	S	0	0	0
			3028	1994	486	531	17			

There are 42 discrepancies between the modelled and reference sequences:

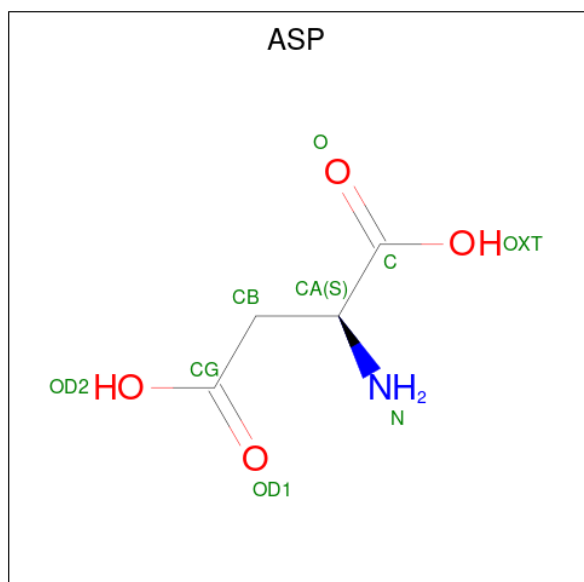
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	HIS	ASP	engineered mutation	UNP O59010
A	40	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	397	ALA	ARG	engineered mutation	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	397	ALA	ARG	engineered mutation	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	397	ALA	ARG	engineered mutation	UNP O59010
D	37	HIS	ASP	engineered mutation	UNP O59010
D	40	HIS	LYS	engineered mutation	UNP O59010
D	132	HIS	LYS	engineered mutation	UNP O59010
D	223	HIS	LYS	engineered mutation	UNP O59010
D	264	HIS	LYS	engineered mutation	UNP O59010
D	368	HIS	GLU	engineered mutation	UNP O59010
D	397	ALA	ARG	engineered mutation	UNP O59010
E	37	HIS	ASP	engineered mutation	UNP O59010
E	40	HIS	LYS	engineered mutation	UNP O59010
E	132	HIS	LYS	engineered mutation	UNP O59010
E	223	HIS	LYS	engineered mutation	UNP O59010
E	264	HIS	LYS	engineered mutation	UNP O59010
E	368	HIS	GLU	engineered mutation	UNP O59010
E	397	ALA	ARG	engineered mutation	UNP O59010
F	37	HIS	ASP	engineered mutation	UNP O59010
F	40	HIS	LYS	engineered mutation	UNP O59010
F	132	HIS	LYS	engineered mutation	UNP O59010
F	223	HIS	LYS	engineered mutation	UNP O59010
F	264	HIS	LYS	engineered mutation	UNP O59010
F	368	HIS	GLU	engineered mutation	UNP O59010
F	397	ALA	ARG	engineered mutation	UNP O59010

- Molecule 2 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 9 4 1 4	0	0
2	B	1	Total C N O 9 4 1 4	0	0
2	C	1	Total C N O 9 4 1 4	0	0
2	D	1	Total C N O 9 4 1 4	0	0
2	E	1	Total C N O 9 4 1 4	0	0
2	F	1	Total C N O 9 4 1 4	0	0

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	B	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0
3	D	2	Total Na 2 2	0	0
3	E	2	Total Na 2 2	0	0
3	F	2	Total Na 2 2	0	0

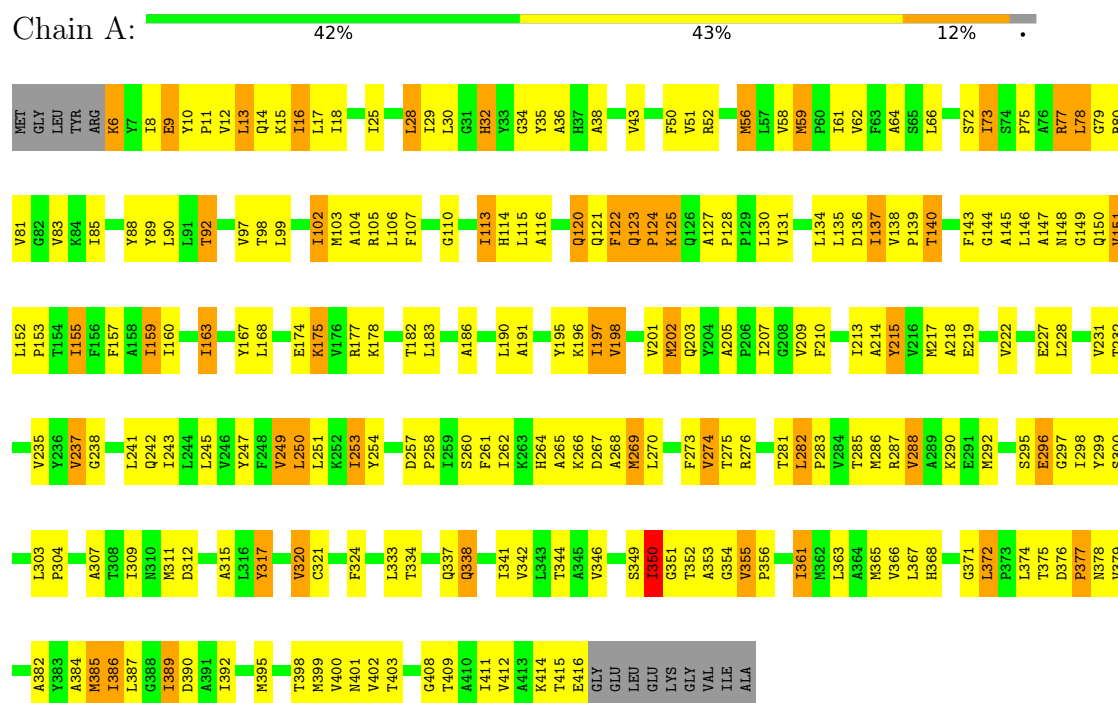
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	1	Total O 1 1	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	F	1	Total O 1 1	0	0

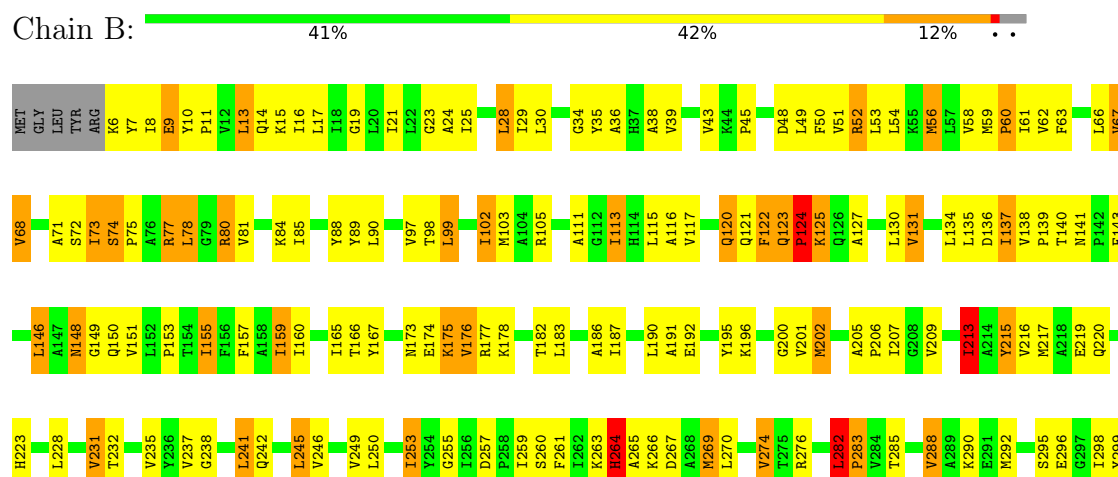
3 Residue-property plots [i](#)

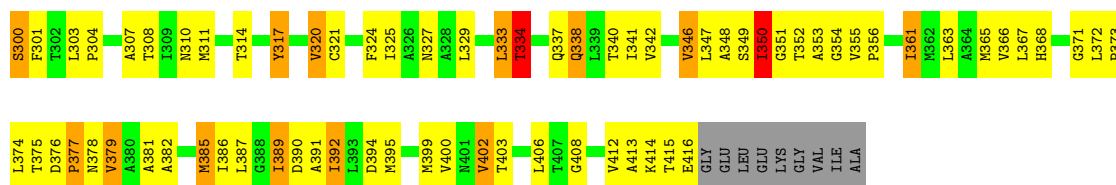
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 425aa long hypothetical proton glutamate symport protein



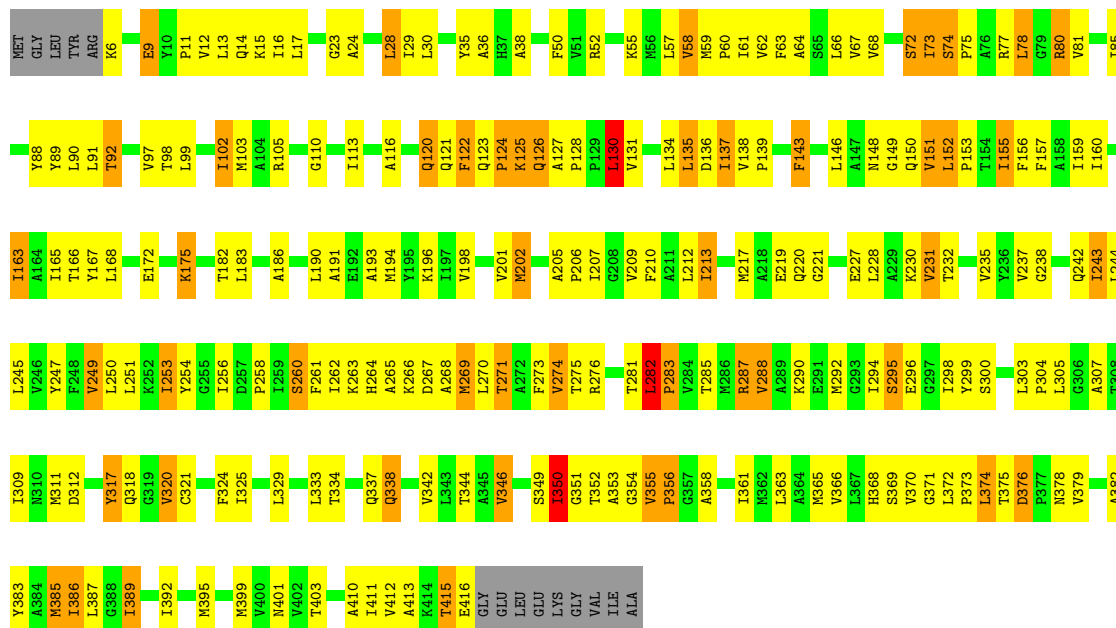
- Molecule 1: 425aa long hypothetical proton glutamate symport protein





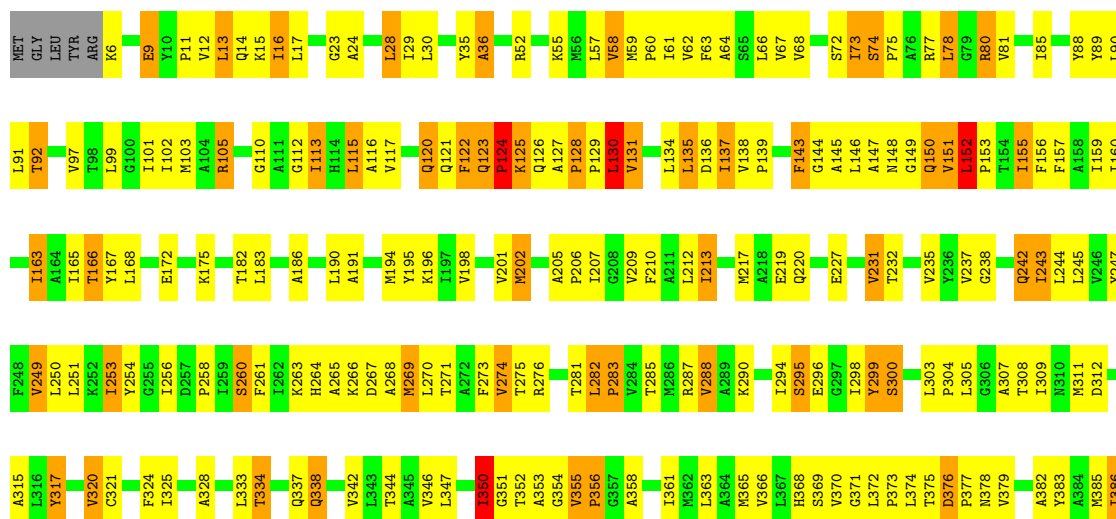
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain C: 44% 41% 12% ..



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

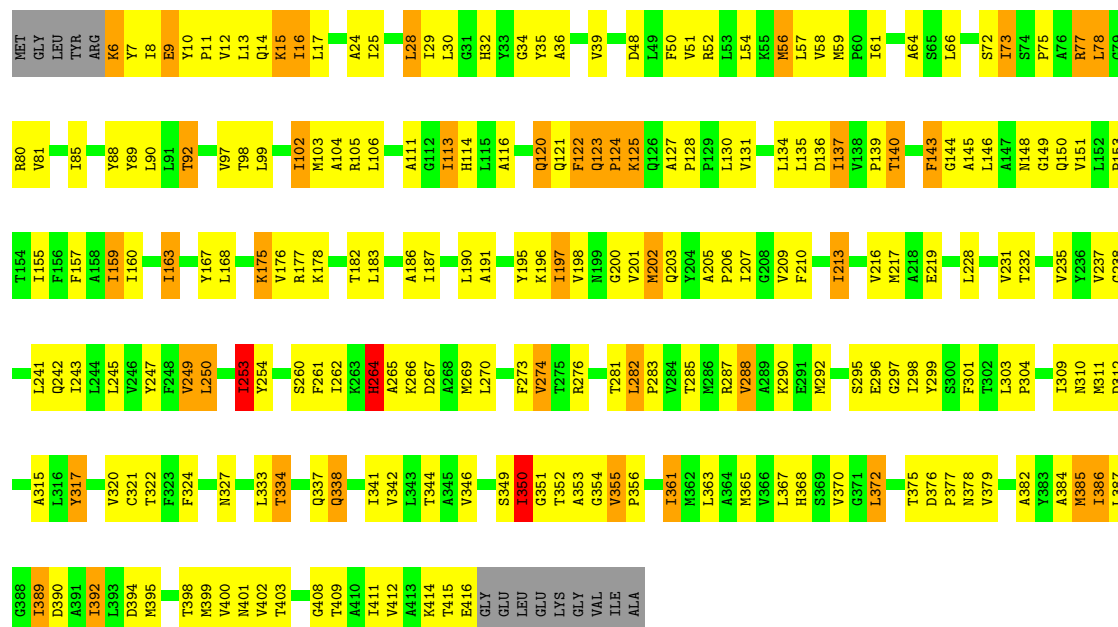
Chain D: 43% 40% 12% ..





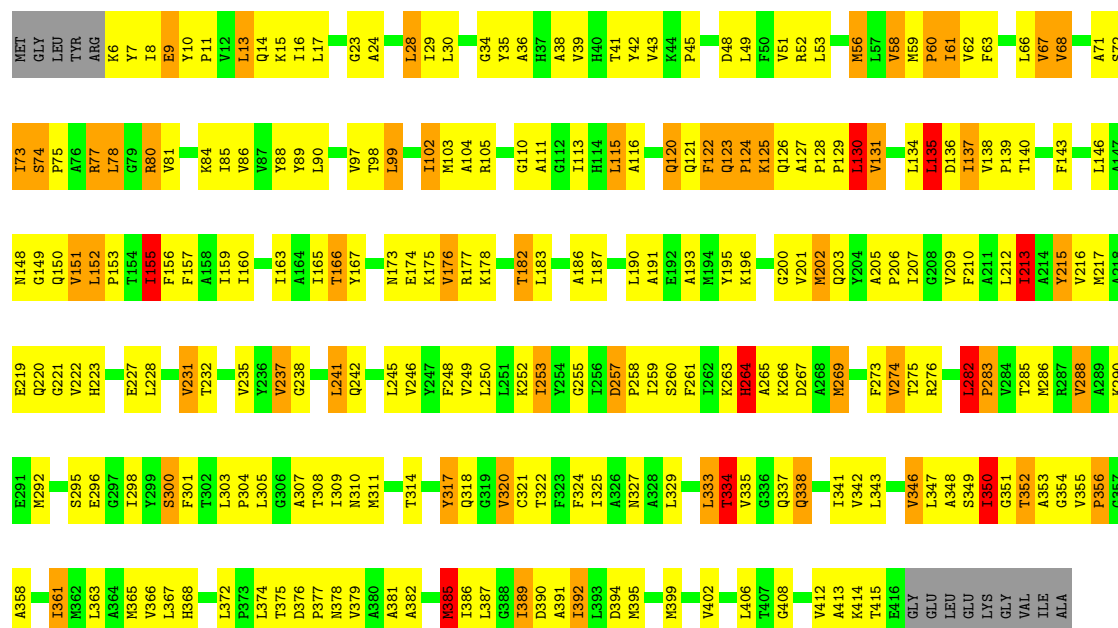
- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain E: 44% 42% 10% . .



- Molecule 1: 425aa long hypothetical proton glutamate symport protein

Chain F: 38% 45% 12% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	116.96Å 116.96Å 313.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 3.50 15.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (15.00-3.50) 98.4 (15.00-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.249 , 0.294 0.249 , 0.289	Depositor DCC
R_{free} test set	2955 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	155.6	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 128.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.109 for -h,-k,l 0.389 for h,-h-k,-l 0.115 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18240	wwPDB-VP
Average B, all atoms (Å ²)	154.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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](#)

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

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	1.22	7/3087 (0.2%)	1.33	11/4213 (0.3%)
1	B	1.22	6/3087 (0.2%)	1.32	8/4213 (0.2%)
1	C	1.21	4/3087 (0.1%)	1.30	16/4213 (0.4%)
1	D	1.22	6/3087 (0.2%)	1.28	12/4213 (0.3%)
1	E	1.24	13/3087 (0.4%)	1.33	13/4213 (0.3%)
1	F	1.23	8/3087 (0.3%)	1.34	17/4213 (0.4%)
All	All	1.22	44/18522 (0.2%)	1.32	77/25278 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
All	All	0	3

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	32	HIS	ND1-CE1	9.30	1.41	1.32
1	C	152	LEU	C-O	-8.10	1.16	1.24
1	D	152	LEU	C-O	-7.84	1.17	1.24
1	F	350	ILE	CA-CB	6.71	1.62	1.54
1	A	361	ILE	CB-CG1	6.68	1.66	1.53
1	B	350	ILE	CA-CB	6.67	1.62	1.54
1	C	350	ILE	CA-CB	6.41	1.63	1.54
1	F	67	VAL	CA-C	6.39	1.60	1.52
1	A	32	HIS	ND1-CE1	6.32	1.38	1.32
1	E	378	ASN	CA-C	6.25	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	LEU	CA-C	6.20	1.60	1.52
1	E	32	HIS	CE1-NE2	6.19	1.38	1.32
1	D	151	VAL	C-O	-6.19	1.16	1.24
1	A	59	MET	N-CA	-5.97	1.42	1.46
1	A	378	ASN	CA-C	5.95	1.60	1.52
1	D	350	ILE	CA-CB	5.80	1.62	1.54
1	C	151	VAL	C-O	-5.76	1.17	1.24
1	E	32	HIS	CG-CD2	5.74	1.42	1.35
1	B	379	VAL	CA-CB	5.67	1.60	1.54
1	F	356	PRO	CA-C	5.58	1.59	1.52
1	A	128	PRO	CA-C	5.57	1.57	1.52
1	B	67	VAL	CA-C	5.53	1.59	1.52
1	E	264	HIS	N-CA	5.50	1.53	1.46
1	E	253	ILE	N-CA	5.48	1.53	1.46
1	D	128	PRO	CA-C	5.44	1.57	1.52
1	E	350	ILE	CA-CB	5.43	1.61	1.54
1	E	128	PRO	CA-C	5.40	1.57	1.52
1	E	409	THR	CA-C	5.39	1.59	1.52
1	A	350	ILE	CA-CB	5.38	1.61	1.54
1	A	409	THR	CA-C	5.35	1.59	1.52
1	E	253	ILE	CA-CB	5.33	1.60	1.54
1	B	52	ARG	N-CA	-5.33	1.40	1.46
1	D	356	PRO	CA-C	5.31	1.58	1.52
1	B	21	ILE	CA-CB	5.29	1.61	1.54
1	F	358	ALA	CA-CB	5.27	1.62	1.53
1	D	126	GLN	CA-C	5.26	1.59	1.52
1	E	177	ARG	NE-CZ	5.24	1.38	1.33
1	F	152	LEU	C-O	-5.19	1.19	1.24
1	E	361	ILE	CB-CG1	5.13	1.63	1.53
1	F	282	LEU	CA-C	5.10	1.59	1.52
1	F	212	LEU	N-CA	-5.09	1.41	1.47
1	C	126	GLN	CA-C	5.09	1.59	1.52
1	E	386	ILE	N-CA	5.06	1.52	1.46
1	F	86	VAL	CA-CB	5.03	1.61	1.54

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ASP	CA-C-N	9.46	131.67	119.84
1	A	376	ASP	C-N-CA	9.46	131.67	119.84
1	E	376	ASP	CA-C-N	9.22	131.36	119.84
1	E	376	ASP	C-N-CA	9.22	131.36	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	346	VAL	N-CA-C	-8.14	102.40	110.30
1	C	12	VAL	N-CA-C	7.52	117.64	110.42
1	B	376	ASP	CA-C-N	7.39	129.08	119.84
1	B	376	ASP	C-N-CA	7.39	129.08	119.84
1	D	12	VAL	N-CA-C	7.27	117.40	110.42
1	E	309	ILE	N-CA-C	6.84	119.65	111.09
1	E	143	PHE	N-CA-C	-6.73	103.87	111.07
1	A	175	LYS	N-CA-C	-6.68	105.26	113.41
1	B	390	ASP	N-CA-C	6.66	118.42	111.03
1	F	390	ASP	N-CA-C	6.61	118.17	110.97
1	F	376	ASP	CA-C-N	6.59	128.07	119.84
1	F	376	ASP	C-N-CA	6.59	128.07	119.84
1	D	309	ILE	N-CA-C	6.55	119.24	111.05
1	C	376	ASP	CA-C-N	6.45	127.90	119.84
1	C	376	ASP	C-N-CA	6.45	127.90	119.84
1	F	275	THR	CB-CA-C	-6.35	100.05	110.85
1	E	390	ASP	N-CA-C	6.35	117.89	110.97
1	A	390	ASP	N-CA-C	6.34	118.07	111.03
1	E	32	HIS	CE1-NE2-CD2	-6.27	102.73	109.00
1	E	12	VAL	N-CA-CB	6.20	117.37	110.62
1	D	58	VAL	CB-CA-C	-6.03	104.14	112.04
1	F	257	ASP	CA-C-N	6.02	125.73	119.05
1	F	257	ASP	C-N-CA	6.02	125.73	119.05
1	D	356	PRO	N-CA-C	5.92	119.73	110.80
1	C	358	ALA	N-CA-C	-5.81	106.15	113.18
1	D	143	PHE	N-CA-C	-5.80	104.86	111.07
1	C	58	VAL	CB-CA-C	-5.79	104.46	112.04
1	C	175	LYS	N-CA-C	-5.79	106.26	113.55
1	B	346	VAL	N-CA-C	-5.78	104.98	110.42
1	D	376	ASP	CA-C-N	5.75	127.03	119.84
1	D	376	ASP	C-N-CA	5.75	127.03	119.84
1	F	67	VAL	N-CA-C	5.72	115.85	110.30
1	D	407	THR	CB-CA-C	-5.68	101.37	110.79
1	F	58	VAL	CB-CA-C	-5.61	104.70	111.88
1	A	12	VAL	N-CA-CB	5.60	116.72	110.62
1	B	282	LEU	N-CA-C	5.59	122.17	109.81
1	C	356	PRO	N-CA-C	5.59	119.24	110.80
1	A	18	ILE	N-CA-C	5.59	115.78	110.53
1	F	282	LEU	N-CA-C	5.57	122.12	109.81
1	E	175	LYS	N-CA-C	-5.56	106.63	113.41
1	E	12	VAL	N-CA-C	5.54	115.67	110.30
1	D	92	THR	CB-CA-C	-5.50	101.55	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	213	ILE	N-CA-CB	5.42	121.50	110.82
1	A	92	THR	CB-CA-C	-5.41	101.65	110.85
1	C	143	PHE	N-CA-C	-5.41	104.62	111.11
1	F	131	VAL	CB-CA-C	-5.41	102.42	111.29
1	D	358	ALA	N-CA-C	-5.40	106.64	113.18
1	D	415	THR	CB-CA-C	-5.38	102.79	111.18
1	C	92	THR	CB-CA-C	-5.36	102.43	110.90
1	C	282	LEU	N-CA-C	5.34	121.62	109.81
1	C	275	THR	CB-CA-C	-5.32	100.96	110.70
1	E	282	LEU	N-CA-C	5.31	121.55	109.81
1	C	415	THR	CB-CA-C	-5.31	102.14	110.85
1	A	309	ILE	N-CA-C	5.29	117.66	111.05
1	A	12	VAL	N-CA-C	5.29	115.43	110.30
1	F	356	PRO	N-CA-C	5.29	118.78	110.80
1	E	379	VAL	N-CA-C	-5.27	105.19	110.30
1	A	143	PHE	N-CA-C	-5.27	105.43	111.07
1	D	131	VAL	CB-CA-C	-5.27	102.65	111.29
1	B	213	ILE	N-CA-CB	5.27	121.20	110.82
1	E	92	THR	CB-CA-C	-5.23	101.95	110.85
1	F	385	MET	CA-C-N	5.22	127.61	120.46
1	F	385	MET	C-N-CA	5.22	127.61	120.46
1	C	221	GLY	N-CA-C	-5.21	106.19	112.49
1	F	309	ILE	N-CA-C	5.21	117.60	111.09
1	A	350	ILE	N-CA-C	5.18	118.39	111.44
1	B	175	LYS	N-CA-C	-5.15	107.55	113.88
1	F	221	GLY	N-CA-C	-5.13	106.28	112.49
1	C	401	ASN	N-CA-C	-5.09	105.81	111.36
1	E	386	ILE	N-CA-C	5.07	115.79	110.62
1	B	131	VAL	CB-CA-C	-5.06	103.00	111.29
1	F	346	VAL	N-CA-C	-5.03	105.69	110.42
1	C	309	ILE	N-CA-C	5.03	119.13	111.89

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	124	PRO	Peptide
1	D	112	GLY	Peptide
1	D	124	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3028	0	3189	161	0
1	B	3028	0	3189	178	0
1	C	3028	0	3189	162	0
1	D	3028	0	3189	164	0
1	E	3028	0	3189	154	0
1	F	3028	0	3189	195	0
2	A	9	0	3	1	0
2	B	9	0	3	1	0
2	C	9	0	3	1	0
2	D	9	0	3	1	0
2	E	9	0	3	2	0
2	F	9	0	3	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	18240	0	19152	959	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 26.

All (959) 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:B:265:ALA:HB1	1:B:266:LYS:HA	1.26	1.15
1:F:265:ALA:HB1	1:F:266:LYS:HA	1.25	1.13
1:E:265:ALA:HB1	1:E:266:LYS:HA	1.20	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ALA:HB1	1:A:266:LYS:HA	1.17	1.11
1:C:265:ALA:HB1	1:C:266:LYS:CA	1.84	1.07
1:D:265:ALA:HB1	1:D:266:LYS:CA	1.84	1.06
1:C:265:ALA:CB	1:C:266:LYS:HA	1.86	1.06
1:D:265:ALA:CB	1:D:266:LYS:HA	1.86	1.05
1:D:265:ALA:HB1	1:D:266:LYS:HA	1.06	1.05
1:A:265:ALA:HB1	1:A:266:LYS:CA	1.87	1.03
1:E:265:ALA:HB1	1:E:266:LYS:CA	1.87	1.03
1:F:265:ALA:HB1	1:F:266:LYS:CA	1.87	1.03
1:B:265:ALA:HB1	1:B:266:LYS:CA	1.87	1.02
1:C:265:ALA:HB1	1:C:266:LYS:HA	1.04	1.02
1:B:120:GLN:HB2	1:B:121:GLN:HA	1.43	1.00
1:F:120:GLN:HB2	1:F:121:GLN:HA	1.43	1.00
1:E:120:GLN:HB2	1:E:121:GLN:HA	1.45	0.99
1:F:265:ALA:CB	1:F:266:LYS:HA	1.93	0.97
1:B:265:ALA:CB	1:B:266:LYS:HA	1.94	0.96
1:D:120:GLN:HB2	1:D:121:GLN:HA	1.48	0.96
1:A:120:GLN:HB2	1:A:121:GLN:HA	1.48	0.96
1:D:264:HIS:CE1	1:D:265:ALA:HB2	2.01	0.96
1:E:265:ALA:CB	1:E:266:LYS:HA	1.97	0.95
1:A:265:ALA:CB	1:A:266:LYS:HA	1.96	0.95
1:E:264:HIS:CE1	1:E:265:ALA:HB2	2.03	0.94
1:C:120:GLN:HB2	1:C:121:GLN:HA	1.50	0.93
1:A:264:HIS:CE1	1:A:265:ALA:HB2	2.04	0.92
1:C:264:HIS:CE1	1:C:265:ALA:HB2	2.04	0.92
1:C:80:ARG:NH2	1:C:416:GLU:OE2	2.03	0.92
1:A:261:PHE:O	1:A:264:HIS:CD2	2.23	0.92
1:E:261:PHE:O	1:E:264:HIS:CD2	2.24	0.91
1:B:11:PRO:HG2	1:B:14:GLN:HG3	1.53	0.91
1:F:11:PRO:HG2	1:F:14:GLN:HG3	1.53	0.91
1:E:124:PRO:HB2	1:E:368:HIS:CE1	2.07	0.90
1:B:264:HIS:CE1	1:B:265:ALA:HB2	2.07	0.90
1:F:124:PRO:HB2	1:F:368:HIS:CE1	2.05	0.90
1:E:11:PRO:HG2	1:E:14:GLN:HG3	1.55	0.89
1:B:124:PRO:HB2	1:B:368:HIS:CE1	2.08	0.88
1:A:124:PRO:HB2	1:A:368:HIS:CE1	2.09	0.88
1:C:334:THR:O	1:C:338:GLN:HB2	1.74	0.88
1:C:124:PRO:HB2	1:C:368:HIS:CE1	2.09	0.87
1:D:334:THR:O	1:D:338:GLN:HB2	1.76	0.86
1:D:80:ARG:NH2	1:D:416:GLU:OE2	2.09	0.85
1:D:124:PRO:HB2	1:D:368:HIS:CE1	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:HIS:CE1	1:F:265:ALA:HB2	2.12	0.85
1:B:250:LEU:HA	1:B:253:ILE:HG22	1.58	0.85
1:F:235:VAL:HG22	1:F:320:VAL:HG11	1.59	0.83
1:D:36:ALA:HB1	1:D:219:GLU:HG2	1.62	0.82
1:D:97:VAL:HG11	1:D:342:VAL:HA	1.61	0.81
1:D:269:MET:SD	1:D:403:THR:OG1	2.37	0.81
1:A:36:ALA:HB1	1:A:219:GLU:HG2	1.62	0.81
1:E:36:ALA:HB1	1:E:219:GLU:HG2	1.63	0.81
1:D:261:PHE:O	1:D:264:HIS:CD2	2.34	0.80
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.64	0.80
1:C:28:LEU:HD13	1:C:217:MET:HG3	1.63	0.80
1:B:201:VAL:O	1:B:202:MET:HB2	1.82	0.79
1:F:250:LEU:HA	1:F:253:ILE:HG22	1.63	0.79
1:F:201:VAL:O	1:F:202:MET:HB2	1.82	0.79
1:A:11:PRO:HG2	1:A:14:GLN:HG3	1.65	0.79
1:D:28:LEU:HD13	1:D:217:MET:HG3	1.65	0.78
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.63	0.78
1:B:123:GLN:HG2	1:B:124:PRO:HA	1.64	0.78
1:E:81:VAL:HG21	1:E:298:ILE:HD12	1.65	0.78
1:C:261:PHE:O	1:C:264:HIS:CD2	2.37	0.77
1:B:59:MET:HE2	1:B:146:LEU:HA	1.66	0.77
1:D:81:VAL:HG21	1:D:298:ILE:HD12	1.65	0.77
1:D:266:LYS:CB	1:D:270:LEU:HG	2.15	0.77
1:F:59:MET:HE2	1:F:146:LEU:HA	1.66	0.77
1:D:201:VAL:O	1:D:202:MET:HB2	1.84	0.77
1:A:59:MET:HE2	1:A:146:LEU:HA	1.66	0.76
1:C:75:PRO:HG3	1:C:163:ILE:HG13	1.67	0.76
1:A:346:VAL:O	1:A:350:ILE:HG23	1.86	0.76
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.66	0.76
1:D:167:TYR:HB3	1:F:196:LYS:HE2	1.66	0.75
1:C:97:VAL:HG11	1:C:342:VAL:HA	1.67	0.75
1:F:269:MET:O	1:F:399:MET:HG3	1.86	0.75
1:E:28:LEU:HD13	1:E:217:MET:HG3	1.68	0.75
1:C:269:MET:SD	1:C:403:THR:OG1	2.43	0.75
1:B:196:LYS:HE2	1:C:167:TYR:HB3	1.70	0.74
1:D:11:PRO:HG2	1:D:14:GLN:HG3	1.68	0.74
1:F:36:ALA:HB1	1:F:219:GLU:HG2	1.67	0.74
1:C:350:ILE:N	1:C:351:GLY:HA3	2.02	0.74
1:D:121:GLN:N	1:D:122:PHE:HB3	2.03	0.73
1:A:250:LEU:HA	1:A:253:ILE:HG22	1.69	0.73
1:E:59:MET:HE2	1:E:146:LEU:HA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:HG2	1:C:124:PRO:HA	1.71	0.73
1:C:266:LYS:CB	1:C:270:LEU:HG	2.18	0.73
1:A:269:MET:O	1:A:399:MET:HG3	1.88	0.73
1:B:265:ALA:HB1	1:B:266:LYS:C	2.13	0.73
1:A:261:PHE:O	1:A:264:HIS:HD2	1.69	0.73
1:F:123:GLN:HG2	1:F:124:PRO:HA	1.71	0.73
1:F:28:LEU:HD13	1:F:217:MET:HG3	1.69	0.72
1:D:123:GLN:HG2	1:D:124:PRO:HA	1.72	0.72
1:F:66:LEU:HD21	1:F:159:ILE:HG13	1.72	0.72
1:F:264:HIS:CE1	1:F:288:VAL:HG11	2.25	0.72
1:B:350:ILE:N	1:B:351:GLY:HA3	2.04	0.72
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.72	0.72
1:C:36:ALA:HB1	1:C:219:GLU:HG2	1.70	0.71
1:F:265:ALA:HB1	1:F:266:LYS:C	2.14	0.71
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.71	0.71
1:C:382:ALA:HA	1:C:385:MET:HG3	1.73	0.71
1:F:350:ILE:N	1:F:351:GLY:HA3	2.05	0.71
1:D:350:ILE:N	1:D:351:GLY:HA3	2.05	0.71
1:A:123:GLN:HG2	1:A:124:PRO:HA	1.72	0.71
1:C:201:VAL:O	1:C:202:MET:HB2	1.91	0.71
1:F:334:THR:O	1:F:338:GLN:HB2	1.91	0.71
1:E:346:VAL:O	1:E:350:ILE:HG23	1.91	0.71
1:E:134:LEU:O	1:E:137:ILE:HG13	1.90	0.70
1:B:11:PRO:CG	1:B:14:GLN:HG3	2.21	0.70
1:C:269:MET:O	1:C:399:MET:HG3	1.91	0.70
1:D:58:VAL:HG22	1:D:283:PRO:HD3	1.72	0.70
1:F:11:PRO:CG	1:F:14:GLN:HG3	2.21	0.70
1:A:201:VAL:O	1:A:202:MET:HB2	1.91	0.70
1:F:81:VAL:HG21	1:F:298:ILE:HD12	1.72	0.70
1:B:81:VAL:HG21	1:B:298:ILE:HD12	1.74	0.70
1:D:250:LEU:HA	1:D:253:ILE:HG22	1.74	0.69
1:A:186:ALA:O	1:B:183:LEU:HD13	1.92	0.69
1:F:235:VAL:HG22	1:F:320:VAL:CG1	2.22	0.69
1:C:281:THR:HG22	1:C:285:THR:OG1	1.93	0.69
1:E:311:MET:HE1	1:E:354:GLY:HA2	1.74	0.69
1:A:167:TYR:HB3	1:C:196:LYS:HE2	1.74	0.69
1:B:36:ALA:HB1	1:B:219:GLU:HG2	1.75	0.68
1:E:121:GLN:N	1:E:122:PHE:HB3	2.09	0.68
1:A:146:LEU:HD13	1:B:143:PHE:CE1	2.28	0.68
1:B:269:MET:O	1:B:399:MET:HG3	1.93	0.68
1:D:155:ILE:HD11	1:D:304:PRO:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ALA:O	1:F:183:LEU:HD13	1.93	0.68
1:A:350:ILE:N	1:A:351:GLY:HA3	2.09	0.68
1:E:261:PHE:O	1:E:264:HIS:HD2	1.73	0.68
1:B:235:VAL:HG22	1:B:320:VAL:CG1	2.22	0.68
1:E:201:VAL:O	1:E:202:MET:HB2	1.93	0.68
1:C:121:GLN:N	1:C:122:PHE:HB3	2.09	0.67
1:E:250:LEU:HA	1:E:253:ILE:HG22	1.76	0.67
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.76	0.67
1:F:103:MET:HE3	1:F:238:GLY:HA2	1.75	0.67
1:D:196:LYS:HE2	1:E:167:TYR:HB3	1.75	0.67
1:C:9:GLU:OE2	1:C:9:GLU:HA	1.95	0.67
1:C:366:VAL:O	1:C:369:SER:OG	2.13	0.67
1:C:11:PRO:HG2	1:C:14:GLN:HG3	1.77	0.67
1:F:255:GLY:O	1:F:414:LYS:HE2	1.95	0.67
1:E:231:VAL:O	1:E:235:VAL:HG23	1.95	0.67
1:A:235:VAL:HG22	1:A:320:VAL:CG1	2.25	0.67
1:B:264:HIS:CE1	1:B:288:VAL:HG11	2.30	0.67
1:D:382:ALA:HA	1:D:385:MET:HG3	1.77	0.67
1:B:98:THR:O	1:B:102:ILE:HB	1.95	0.66
1:B:265:ALA:HB1	1:B:266:LYS:O	1.95	0.66
1:D:269:MET:O	1:D:399:MET:HG3	1.95	0.66
1:B:103:MET:HE3	1:B:238:GLY:HA2	1.76	0.66
1:E:123:GLN:HG2	1:E:124:PRO:HA	1.78	0.66
1:E:350:ILE:N	1:E:351:GLY:HA3	2.11	0.66
1:A:121:GLN:N	1:A:122:PHE:HB3	2.11	0.66
1:E:196:LYS:HE2	1:F:167:TYR:HB3	1.77	0.66
1:A:28:LEU:HD13	1:A:217:MET:HG3	1.78	0.65
1:F:311:MET:HE1	1:F:354:GLY:HA2	1.78	0.65
1:B:324:PHE:C	1:B:324:PHE:CD2	2.74	0.65
1:F:265:ALA:HB1	1:F:266:LYS:O	1.97	0.65
1:D:235:VAL:HG22	1:D:320:VAL:HG11	1.79	0.65
1:E:155:ILE:HD11	1:E:304:PRO:HB2	1.79	0.64
1:D:77:ARG:HH11	1:D:416:GLU:HG3	1.63	0.64
1:D:134:LEU:O	1:D:136:ASP:N	2.30	0.64
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.80	0.64
1:D:235:VAL:HG22	1:D:320:VAL:CG1	2.28	0.64
1:E:235:VAL:HG22	1:E:320:VAL:HG11	1.80	0.64
1:E:269:MET:O	1:E:399:MET:HG3	1.98	0.64
1:E:235:VAL:HG22	1:E:320:VAL:CG1	2.27	0.64
1:C:120:GLN:CB	1:C:121:GLN:HA	2.24	0.64
1:B:255:GLY:O	1:B:414:LYS:HE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:VAL:O	1:C:350:ILE:HG23	1.98	0.63
1:E:261:PHE:HD2	1:E:262:ILE:HD12	1.63	0.63
1:B:334:THR:O	1:B:338:GLN:HB2	1.98	0.63
1:B:134:LEU:O	1:B:137:ILE:HG13	1.97	0.63
1:C:235:VAL:HG22	1:C:320:VAL:CG1	2.29	0.63
1:C:243:ILE:HG22	1:C:244:LEU:HD23	1.81	0.63
1:D:120:GLN:CB	1:D:121:GLN:HA	2.24	0.63
1:E:265:ALA:HB1	1:E:266:LYS:C	2.24	0.63
1:C:355:VAL:HB	1:C:356:PRO:CD	2.29	0.63
1:A:276:ARG:O	2:A:501:ASP:N	2.32	0.63
1:D:281:THR:HG22	1:D:285:THR:OG1	1.98	0.63
1:A:134:LEU:O	1:A:137:ILE:HG13	1.97	0.63
1:D:120:GLN:C	1:D:122:PHE:HB3	2.23	0.63
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.81	0.62
1:B:311:MET:HE1	1:B:354:GLY:HA2	1.81	0.62
1:D:264:HIS:CE1	1:D:288:VAL:HG11	2.34	0.62
1:B:352:THR:HG22	1:B:353:ALA:O	1.99	0.62
1:C:264:HIS:CE1	1:C:288:VAL:HG11	2.34	0.62
1:E:269:MET:SD	1:E:403:THR:OG1	2.58	0.62
1:F:159:ILE:HD11	1:F:301:PHE:CD1	2.34	0.62
1:F:324:PHE:C	1:F:324:PHE:CD2	2.77	0.62
1:D:75:PRO:HG3	1:D:163:ILE:HG13	1.80	0.62
1:B:66:LEU:HD21	1:B:159:ILE:HG13	1.81	0.62
1:D:9:GLU:HA	1:D:9:GLU:OE2	2.00	0.62
1:D:58:VAL:HG22	1:D:283:PRO:CD	2.30	0.62
1:A:264:HIS:CE1	1:A:288:VAL:HG11	2.34	0.62
1:A:285:THR:HG22	1:A:303:LEU:HD13	1.82	0.62
1:D:138:VAL:O	1:D:138:VAL:HG12	1.98	0.62
1:E:146:LEU:HD13	1:F:143:PHE:CE1	2.35	0.62
1:F:63:PHE:O	1:F:67:VAL:HG23	2.00	0.62
1:B:205:ALA:N	1:B:206:PRO:HD2	2.15	0.61
1:D:125:LYS:HD3	1:D:125:LYS:N	2.15	0.61
1:A:231:VAL:O	1:A:235:VAL:HG23	2.00	0.61
1:E:50:PHE:CE1	1:E:205:ALA:HB2	2.35	0.61
1:C:254:TYR:CD2	1:C:411:ILE:HG23	2.35	0.61
1:D:254:TYR:CD2	1:D:411:ILE:HG23	2.34	0.61
1:D:261:PHE:O	1:D:264:HIS:HD2	1.81	0.61
1:D:355:VAL:HB	1:D:356:PRO:CD	2.30	0.61
1:B:123:GLN:HG2	1:B:124:PRO:CA	2.31	0.61
1:A:377:PRO:HB3	1:E:384:ALA:O	2.01	0.61
1:E:285:THR:HG22	1:E:303:LEU:HD13	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ARG:HB3	1:B:138:VAL:HG11	1.82	0.61
1:B:121:GLN:N	1:B:122:PHE:HB3	2.16	0.61
1:D:352:THR:HG22	1:D:353:ALA:O	2.00	0.61
1:C:58:VAL:HG22	1:C:283:PRO:HD3	1.83	0.60
1:E:264:HIS:CE1	1:E:288:VAL:HG11	2.35	0.60
1:F:352:THR:HG22	1:F:353:ALA:O	2.01	0.60
1:B:314:THR:OG1	2:B:501:ASP:OD2	2.17	0.60
1:C:110:GLY:N	1:C:227:GLU:OE1	2.34	0.60
1:E:36:ALA:HB1	1:E:219:GLU:CG	2.30	0.60
1:A:209:VAL:HG13	1:A:274:VAL:HG21	1.83	0.60
1:D:59:MET:HE2	1:D:146:LEU:HA	1.84	0.60
1:F:123:GLN:HG2	1:F:124:PRO:CA	2.31	0.60
1:C:261:PHE:O	1:C:264:HIS:HD2	1.84	0.60
1:D:196:LYS:HD2	1:E:168:LEU:HD23	1.85	0.59
1:B:159:ILE:HD11	1:B:301:PHE:CD1	2.37	0.59
1:E:11:PRO:CG	1:E:14:GLN:HG3	2.30	0.59
1:C:134:LEU:O	1:C:136:ASP:N	2.35	0.59
1:E:288:VAL:HG13	1:E:288:VAL:O	2.01	0.59
1:A:414:LYS:HG3	1:A:414:LYS:O	2.02	0.59
1:A:196:LYS:HE2	1:B:167:TYR:HB3	1.83	0.59
1:C:352:THR:HG22	1:C:353:ALA:O	2.02	0.59
1:C:137:ILE:HG22	1:C:152:LEU:HB3	1.84	0.59
1:C:190:LEU:O	1:C:191:ALA:C	2.44	0.59
1:F:97:VAL:HG11	1:F:342:VAL:HA	1.85	0.58
1:B:269:MET:SD	1:B:403:THR:OG1	2.61	0.58
1:E:414:LYS:O	1:E:414:LYS:HG3	2.02	0.58
1:B:77:ARG:O	1:B:78:LEU:C	2.45	0.58
1:A:269:MET:SD	1:A:403:THR:OG1	2.60	0.58
1:B:35:TYR:O	1:B:38:ALA:N	2.37	0.58
1:D:137:ILE:HG22	1:D:152:LEU:HB3	1.86	0.58
1:F:201:VAL:O	1:F:202:MET:CB	2.50	0.58
1:E:197:ILE:HG21	1:F:160:ILE:HG21	1.84	0.58
1:C:59:MET:HE2	1:C:146:LEU:HA	1.85	0.58
1:D:243:ILE:HG22	1:D:244:LEU:HD23	1.85	0.58
1:B:28:LEU:HD13	1:B:217:MET:HG3	1.85	0.58
1:C:58:VAL:HG22	1:C:283:PRO:CD	2.34	0.58
1:E:9:GLU:OE2	1:E:203:GLN:NE2	2.37	0.58
1:E:197:ILE:HG21	1:F:160:ILE:CG2	2.33	0.58
1:A:125:LYS:HD3	1:A:125:LYS:N	2.19	0.57
1:B:9:GLU:OE2	1:B:9:GLU:HA	2.03	0.57
1:C:81:VAL:HG23	1:C:412:VAL:HG12	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:VAL:O	1:D:202:MET:CB	2.53	0.57
1:A:103:MET:HE3	1:A:238:GLY:HA2	1.86	0.57
1:D:190:LEU:O	1:D:191:ALA:C	2.48	0.57
1:B:97:VAL:HG11	1:B:342:VAL:HA	1.86	0.57
1:D:125:LYS:HD3	1:D:125:LYS:H	1.69	0.57
1:F:263:LYS:C	1:F:265:ALA:H	2.12	0.57
1:A:36:ALA:HB1	1:A:219:GLU:CG	2.33	0.57
1:A:209:VAL:HA	1:A:274:VAL:HG11	1.86	0.57
1:A:311:MET:HE1	1:A:354:GLY:HA2	1.86	0.57
1:B:201:VAL:O	1:B:202:MET:CB	2.51	0.57
1:D:264:HIS:NE2	1:D:265:ALA:HB2	2.20	0.57
1:E:120:GLN:C	1:E:122:PHE:HB3	2.30	0.57
1:F:98:THR:O	1:F:102:ILE:HB	2.04	0.57
1:A:97:VAL:HG11	1:A:342:VAL:HA	1.86	0.57
1:C:139:PRO:HB3	1:C:153:PRO:HB3	1.86	0.57
1:A:265:ALA:HB1	1:A:266:LYS:C	2.30	0.57
1:C:120:GLN:C	1:C:122:PHE:HB3	2.29	0.57
1:D:260:SER:HA	1:D:263:LYS:CB	2.35	0.57
1:E:103:MET:HE3	1:E:238:GLY:HA2	1.87	0.57
1:C:77:ARG:HH11	1:C:416:GLU:HG3	1.69	0.56
1:B:261:PHE:O	1:B:264:HIS:CD2	2.59	0.56
1:B:120:GLN:CB	1:B:121:GLN:HA	2.25	0.56
1:C:50:PHE:HZ	1:C:271:THR:HG1	1.53	0.56
1:D:36:ALA:HB1	1:D:219:GLU:CG	2.35	0.56
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.87	0.56
1:B:186:ALA:O	1:C:183:LEU:HD13	2.05	0.56
1:C:247:TYR:OH	1:C:312:ASP:OD2	2.20	0.56
1:F:121:GLN:N	1:F:122:PHE:HB3	2.20	0.56
1:F:261:PHE:O	1:F:264:HIS:CD2	2.58	0.56
1:B:231:VAL:O	1:B:235:VAL:HG23	2.06	0.56
1:B:288:VAL:CG1	1:B:406:LEU:HD11	2.36	0.56
1:B:325:ILE:O	1:B:329:LEU:HG	2.05	0.56
1:C:250:LEU:HA	1:C:253:ILE:CG2	2.35	0.56
1:E:58:VAL:HG22	1:E:283:PRO:HD3	1.87	0.56
1:E:52:ARG:HB3	1:F:138:VAL:HG11	1.88	0.56
1:E:247:TYR:OH	1:E:312:ASP:OD2	2.18	0.56
1:F:77:ARG:O	1:F:78:LEU:C	2.48	0.56
1:F:120:GLN:CB	1:F:121:GLN:HA	2.26	0.56
1:F:205:ALA:N	1:F:206:PRO:HD2	2.21	0.56
1:A:120:GLN:C	1:A:122:PHE:HB3	2.31	0.56
1:E:97:VAL:HG11	1:E:342:VAL:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:VAL:HA	1:E:274:VAL:HG11	1.87	0.56
1:A:382:ALA:HA	1:A:385:MET:HG3	1.88	0.56
1:F:125:LYS:HD3	1:F:125:LYS:N	2.20	0.56
1:A:276:ARG:HD3	1:A:395:MET:CG	2.36	0.56
1:B:13:LEU:HD12	1:B:13:LEU:O	2.06	0.56
1:D:276:ARG:HG2	1:D:395:MET:HA	1.88	0.56
1:F:250:LEU:HA	1:F:253:ILE:CG2	2.35	0.56
1:B:73:ILE:HG22	1:B:78:LEU:HD22	1.87	0.55
1:B:85:ILE:HD13	1:B:408:GLY:O	2.07	0.55
1:C:249:VAL:O	1:C:253:ILE:HG22	2.06	0.55
1:D:73:ILE:HG23	1:D:74:SER:N	2.20	0.55
1:F:30:LEU:O	1:F:35:TYR:HB2	2.06	0.55
1:F:325:ILE:O	1:F:329:LEU:HG	2.06	0.55
1:A:168:LEU:HD23	1:C:196:LYS:HD2	1.88	0.55
1:B:89:TYR:CG	1:B:310:ASN:HB2	2.41	0.55
1:E:75:PRO:HG3	1:E:163:ILE:HG13	1.89	0.55
1:A:247:TYR:OH	1:A:312:ASP:OD2	2.19	0.55
1:E:104:ALA:HB2	1:E:320:VAL:HG23	1.89	0.55
1:A:250:LEU:HA	1:A:253:ILE:CG2	2.35	0.55
1:A:352:THR:HG22	1:A:353:ALA:O	2.06	0.55
1:F:9:GLU:OE2	1:F:9:GLU:HA	2.06	0.55
1:B:123:GLN:N	1:B:124:PRO:HA	2.21	0.55
1:B:250:LEU:HA	1:B:253:ILE:CG2	2.33	0.55
1:B:261:PHE:CD1	1:B:292:MET:HE1	2.42	0.55
1:D:346:VAL:O	1:D:350:ILE:HG23	2.07	0.55
1:A:16:ILE:HD11	1:A:205:ALA:CB	2.37	0.55
1:C:324:PHE:C	1:C:324:PHE:CD2	2.85	0.55
1:D:366:VAL:O	1:D:369:SER:OG	2.21	0.55
1:B:58:VAL:HG22	1:B:283:PRO:HD3	1.89	0.54
1:C:363:LEU:O	1:C:366:VAL:HG12	2.07	0.54
1:A:77:ARG:HH11	1:A:416:GLU:HG3	1.72	0.54
1:C:73:ILE:HG23	1:C:74:SER:N	2.21	0.54
1:D:137:ILE:O	1:D:139:PRO:HD3	2.07	0.54
1:D:57:LEU:HD22	1:D:194:MET:HE3	1.89	0.54
1:C:276:ARG:HD3	1:C:395:MET:CG	2.38	0.54
1:C:125:LYS:HD3	1:C:125:LYS:N	2.21	0.54
1:D:363:LEU:O	1:D:366:VAL:HG12	2.08	0.54
1:E:273:PHE:CE1	1:E:395:MET:HB3	2.43	0.54
1:F:125:LYS:HD3	1:F:125:LYS:H	1.73	0.54
1:A:113:ILE:HD13	1:E:113:ILE:HD13	1.88	0.54
1:E:276:ARG:HD3	1:E:395:MET:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HG21	1:B:160:ILE:HG21	1.89	0.54
1:B:263:LYS:C	1:B:265:ALA:H	2.16	0.54
1:E:367:LEU:HD22	1:E:372:LEU:HD11	1.88	0.54
1:F:215:TYR:CE1	1:F:219:GLU:OE1	2.60	0.54
1:F:257:ASP:OD2	1:F:259:ILE:HG13	2.08	0.54
1:A:201:VAL:O	1:A:202:MET:CB	2.56	0.54
1:A:288:VAL:O	1:A:288:VAL:HG13	2.07	0.54
1:B:122:PHE:C	1:B:124:PRO:HB3	2.33	0.54
1:B:125:LYS:HD3	1:B:125:LYS:N	2.23	0.53
1:E:352:THR:HG22	1:E:353:ALA:O	2.08	0.53
1:F:288:VAL:O	1:F:292:MET:HG2	2.08	0.53
1:C:276:ARG:HG2	1:C:395:MET:HA	1.90	0.53
1:D:23:GLY:HA2	1:D:210:PHE:CE2	2.43	0.53
1:D:324:PHE:C	1:D:324:PHE:CD2	2.86	0.53
1:E:209:VAL:HG13	1:E:274:VAL:HG21	1.90	0.53
1:E:324:PHE:C	1:E:324:PHE:CD2	2.86	0.53
1:B:39:VAL:O	1:B:43:VAL:HB	2.08	0.53
1:B:257:ASP:OD2	1:B:259:ILE:HG13	2.09	0.53
1:C:13:LEU:HD12	1:C:13:LEU:O	2.08	0.53
1:D:311:MET:HE1	1:D:354:GLY:HA2	1.91	0.53
1:C:311:MET:HE1	1:C:354:GLY:HA2	1.91	0.53
1:D:157:PHE:HD1	1:F:56:MET:HE3	1.74	0.53
1:F:134:LEU:O	1:F:136:ASP:N	2.42	0.53
1:A:261:PHE:HD2	1:A:262:ILE:HD12	1.72	0.53
1:A:324:PHE:C	1:A:324:PHE:CD2	2.86	0.53
1:A:355:VAL:HB	1:A:356:PRO:CD	2.38	0.53
1:C:317:TYR:HD1	1:C:318:GLN:N	2.07	0.53
1:D:247:TYR:OH	1:D:312:ASP:OD2	2.20	0.53
1:D:276:ARG:HD3	1:D:395:MET:CG	2.39	0.53
1:A:276:ARG:HD3	1:A:395:MET:HG2	1.91	0.53
1:F:363:LEU:O	1:F:366:VAL:HG12	2.08	0.53
1:A:81:VAL:HG23	1:A:412:VAL:HG12	1.89	0.53
1:B:215:TYR:CE1	1:B:219:GLU:OE1	2.61	0.53
1:C:264:HIS:NE2	1:C:265:ALA:HB2	2.24	0.53
1:E:334:THR:O	1:E:338:GLN:HB2	2.09	0.53
1:A:367:LEU:HD22	1:A:372:LEU:HD11	1.91	0.53
1:E:265:ALA:HB1	1:E:266:LYS:O	2.09	0.53
1:C:124:PRO:HB2	1:C:368:HIS:HE1	1.71	0.52
1:E:355:VAL:HB	1:E:356:PRO:CD	2.38	0.52
1:C:125:LYS:HD3	1:C:125:LYS:H	1.74	0.52
1:F:349:SER:C	1:F:351:GLY:HA3	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:HA	1:A:8:ILE:HD12	1.92	0.52
1:A:104:ALA:HB2	1:A:320:VAL:HG23	1.91	0.52
1:A:123:GLN:HG2	1:A:124:PRO:CA	2.39	0.52
1:B:120:GLN:C	1:B:122:PHE:HB3	2.34	0.52
1:E:367:LEU:HD22	1:E:372:LEU:CD1	2.39	0.52
1:E:382:ALA:HA	1:E:385:MET:HG3	1.92	0.52
1:A:209:VAL:HG22	1:A:274:VAL:HG11	1.91	0.52
1:A:334:THR:O	1:A:338:GLN:HB2	2.09	0.52
1:E:56:MET:CE	1:F:157:PHE:HD1	2.22	0.52
1:F:123:GLN:N	1:F:124:PRO:HA	2.22	0.52
1:D:250:LEU:HA	1:D:253:ILE:CG2	2.39	0.52
1:B:11:PRO:HG2	1:B:14:GLN:CG	2.35	0.52
1:B:63:PHE:O	1:B:67:VAL:HG23	2.10	0.52
1:C:201:VAL:O	1:C:202:MET:CB	2.58	0.52
1:D:13:LEU:O	1:D:13:LEU:HD12	2.09	0.52
1:F:81:VAL:HG23	1:F:412:VAL:HG12	1.91	0.52
1:F:85:ILE:O	1:F:88:TYR:HB3	2.10	0.52
1:F:191:ALA:O	1:F:195:TYR:HD1	1.93	0.52
1:D:64:ALA:HB1	1:D:191:ALA:HB2	1.91	0.52
1:E:85:ILE:CD1	1:E:408:GLY:O	2.58	0.52
1:B:124:PRO:HB2	1:B:368:HIS:HE1	1.73	0.51
1:B:264:HIS:ND1	1:B:264:HIS:C	2.68	0.51
1:A:56:MET:HE2	1:B:157:PHE:HD1	1.74	0.51
1:B:374:LEU:HA	1:B:379:VAL:HG11	1.92	0.51
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.45	0.51
1:A:72:SER:O	1:A:73:ILE:HD12	2.11	0.51
1:A:151:VAL:HG12	1:A:152:LEU:HD12	1.92	0.51
1:A:197:ILE:HG21	1:B:160:ILE:CG2	2.40	0.51
1:E:321:CYS:HB3	1:E:363:LEU:HD21	1.93	0.51
1:A:134:LEU:O	1:A:136:ASP:N	2.44	0.51
1:D:276:ARG:HD3	1:D:395:MET:HG2	1.93	0.51
1:F:261:PHE:CD1	1:F:292:MET:HE1	2.46	0.51
1:D:264:HIS:CE1	1:D:265:ALA:CB	2.87	0.51
1:D:55:LYS:HB2	1:E:140:THR:HG22	1.92	0.51
1:D:273:PHE:CE1	1:D:395:MET:HB3	2.46	0.51
1:E:276:ARG:HD3	1:E:395:MET:HG2	1.93	0.51
1:B:382:ALA:HA	1:B:385:MET:HG3	1.91	0.51
1:E:16:ILE:HD11	1:E:205:ALA:CB	2.41	0.51
1:F:276:ARG:O	1:F:356:PRO:HG3	2.10	0.51
1:F:301:PHE:CG	1:F:301:PHE:O	2.64	0.51
1:B:121:GLN:HB3	1:B:124:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ILE:CD1	1:B:361:ILE:N	2.74	0.51
1:D:103:MET:HE3	1:D:238:GLY:HA2	1.92	0.51
1:E:125:LYS:N	1:E:125:LYS:HD3	2.26	0.51
1:E:264:HIS:ND1	1:E:264:HIS:C	2.69	0.51
1:A:13:LEU:HD12	1:A:13:LEU:O	2.10	0.50
1:B:276:ARG:HD3	1:B:395:MET:HG2	1.93	0.50
1:C:103:MET:HE3	1:C:238:GLY:HA2	1.92	0.50
1:C:156:PHE:CD2	1:C:156:PHE:O	2.64	0.50
1:D:81:VAL:HG23	1:D:412:VAL:HG12	1.93	0.50
1:E:201:VAL:O	1:E:202:MET:CB	2.60	0.50
1:F:155:ILE:HD11	1:F:304:PRO:HB2	1.93	0.50
1:B:363:LEU:O	1:B:367:LEU:HG	2.12	0.50
1:D:165:ILE:O	1:D:168:LEU:N	2.44	0.50
1:D:288:VAL:HG13	1:D:288:VAL:O	2.10	0.50
1:E:317:TYR:CD1	1:E:317:TYR:C	2.89	0.50
1:F:174:GLU:CD	1:F:177:ARG:HE	2.20	0.50
1:A:136:ASP:HA	1:C:52:ARG:NH2	2.26	0.50
1:D:183:LEU:HD13	1:F:186:ALA:O	2.11	0.50
1:F:121:GLN:HB3	1:F:124:PRO:HD3	1.93	0.50
1:F:151:VAL:HG12	1:F:152:LEU:HD12	1.93	0.50
1:C:30:LEU:O	1:C:35:TYR:HB2	2.09	0.50
1:C:205:ALA:N	1:C:206:PRO:HD2	2.25	0.50
1:E:88:TYR:CZ	1:E:92:THR:HG21	2.47	0.50
1:F:173:ASN:OD1	1:F:176:VAL:HG13	2.11	0.50
1:B:298:ILE:HG21	1:B:413:ALA:HB2	1.92	0.50
1:D:265:ALA:HB1	1:D:266:LYS:C	2.35	0.50
1:F:77:ARG:HA	1:F:80:ARG:NH1	2.26	0.50
1:A:317:TYR:CD1	1:A:317:TYR:C	2.90	0.50
1:C:231:VAL:O	1:C:235:VAL:HG23	2.11	0.50
1:D:294:ILE:HG22	1:D:295:SER:N	2.26	0.50
1:D:321:CYS:SG	1:D:386:ILE:HG12	2.52	0.50
1:E:81:VAL:HG23	1:E:412:VAL:HG12	1.93	0.50
1:F:35:TYR:O	1:F:38:ALA:N	2.45	0.50
1:A:11:PRO:CG	1:A:14:GLN:HG3	2.39	0.50
1:A:139:PRO:HB3	1:A:153:PRO:HB3	1.94	0.50
1:A:408:GLY:O	1:A:412:VAL:HG23	2.12	0.50
1:C:209:VAL:HA	1:C:274:VAL:HG11	1.94	0.50
1:C:251:LEU:HD13	1:C:258:PRO:HA	1.94	0.50
1:C:265:ALA:HB1	1:C:266:LYS:C	2.35	0.50
1:C:137:ILE:O	1:C:139:PRO:HD3	2.12	0.50
1:F:120:GLN:C	1:F:122:PHE:HB3	2.37	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:HIS:NE2	1:A:265:ALA:HB2	2.26	0.50
1:B:53:LEU:O	1:B:56:MET:HB3	2.11	0.50
1:B:125:LYS:HD3	1:B:125:LYS:H	1.76	0.50
1:E:56:MET:HE2	1:F:157:PHE:HD1	1.77	0.50
1:F:10:TYR:CD2	1:F:11:PRO:HD2	2.47	0.50
1:F:139:PRO:HB3	1:F:153:PRO:HB3	1.94	0.50
1:A:125:LYS:HD3	1:A:125:LYS:H	1.76	0.49
1:A:363:LEU:O	1:A:366:VAL:HG12	2.12	0.49
1:B:73:ILE:HG23	1:B:74:SER:N	2.27	0.49
1:C:64:ALA:HB1	1:C:191:ALA:HB2	1.94	0.49
1:D:134:LEU:C	1:D:136:ASP:N	2.70	0.49
1:A:73:ILE:HG22	1:A:78:LEU:HD22	1.93	0.49
1:B:264:HIS:NE2	1:B:265:ALA:HB2	2.27	0.49
1:C:57:LEU:HD22	1:C:194:MET:HE3	1.95	0.49
1:C:305:LEU:HG	1:C:305:LEU:O	2.12	0.49
1:F:89:TYR:CG	1:F:310:ASN:HB2	2.47	0.49
1:A:137:ILE:O	1:A:139:PRO:HD3	2.12	0.49
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.77	0.49
1:D:249:VAL:O	1:D:253:ILE:HG22	2.12	0.49
1:F:346:VAL:O	1:F:350:ILE:HG23	2.11	0.49
1:F:414:LYS:HG3	1:F:414:LYS:O	2.13	0.49
1:B:85:ILE:O	1:B:88:TYR:HB3	2.12	0.49
1:C:260:SER:HA	1:C:263:LYS:CB	2.43	0.49
1:D:11:PRO:HG2	1:D:14:GLN:CG	2.39	0.49
1:E:276:ARG:O	2:E:501:ASP:N	2.44	0.49
1:A:183:LEU:HD13	1:C:186:ALA:O	2.13	0.49
1:A:195:TYR:O	1:A:198:VAL:HG12	2.13	0.49
1:C:24:ALA:O	1:C:28:LEU:HB2	2.11	0.49
1:F:66:LEU:HD13	1:F:300:SER:O	2.11	0.49
1:B:139:PRO:HB3	1:B:153:PRO:HB3	1.95	0.49
1:C:317:TYR:CD1	1:C:317:TYR:C	2.91	0.49
1:F:111:ALA:N	1:F:327:ASN:HB3	2.27	0.49
1:F:122:PHE:C	1:F:124:PRO:HB3	2.37	0.49
1:F:298:ILE:HG21	1:F:413:ALA:HB2	1.94	0.49
1:D:110:GLY:N	1:D:227:GLU:OE1	2.46	0.49
1:D:298:ILE:HG21	1:D:413:ALA:HB2	1.95	0.49
1:A:16:ILE:HD11	1:A:205:ALA:HB1	1.94	0.49
1:A:75:PRO:HG3	1:A:163:ILE:HG13	1.95	0.49
1:C:77:ARG:O	1:C:78:LEU:C	2.56	0.49
1:D:97:VAL:HG22	1:D:315:ALA:O	2.13	0.49
1:D:264:HIS:ND1	1:D:264:HIS:C	2.70	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:THR:O	1:E:102:ILE:HB	2.12	0.49
1:F:288:VAL:CG1	1:F:406:LEU:HD11	2.43	0.49
1:F:311:MET:HE1	1:F:353:ALA:O	2.13	0.49
1:A:9:GLU:OE2	1:A:203:GLN:NE2	2.46	0.49
1:A:56:MET:CE	1:B:157:PHE:HD1	2.25	0.49
1:B:68:VAL:O	1:B:71:ALA:N	2.46	0.49
1:B:113:ILE:HD13	1:D:113:ILE:HD13	1.95	0.49
1:D:24:ALA:O	1:D:28:LEU:HB2	2.12	0.49
1:D:121:GLN:HB3	1:D:124:PRO:HD3	1.94	0.49
1:B:30:LEU:O	1:B:35:TYR:HB2	2.13	0.49
1:B:349:SER:C	1:B:351:GLY:HA3	2.37	0.49
1:D:139:PRO:HB3	1:D:153:PRO:HB3	1.95	0.49
1:E:125:LYS:HD3	1:E:125:LYS:H	1.78	0.49
1:F:48:ASP:O	1:F:49:LEU:C	2.56	0.49
1:A:384:ALA:O	1:E:377:PRO:HB3	2.13	0.48
1:B:288:VAL:HG12	1:B:406:LEU:HD11	1.93	0.48
1:F:276:ARG:HD3	1:F:395:MET:HG2	1.95	0.48
1:A:10:TYR:CD2	1:A:11:PRO:HD2	2.49	0.48
1:A:321:CYS:HB3	1:A:363:LEU:HD21	1.95	0.48
1:B:48:ASP:O	1:B:51:VAL:N	2.46	0.48
1:B:266:LYS:CB	1:B:270:LEU:HG	2.43	0.48
1:E:77:ARG:HH11	1:E:416:GLU:HG3	1.77	0.48
1:F:322:THR:HG23	1:F:367:LEU:HD23	1.94	0.48
1:A:146:LEU:HB3	1:B:143:PHE:CD1	2.49	0.48
1:B:246:VAL:O	1:B:250:LEU:HB2	2.14	0.48
1:C:273:PHE:CE1	1:C:395:MET:HB3	2.48	0.48
1:C:321:CYS:SG	1:C:386:ILE:HG12	2.53	0.48
1:D:23:GLY:CA	1:D:210:PHE:CE2	2.96	0.48
1:D:271:THR:O	1:D:275:THR:OG1	2.27	0.48
1:E:13:LEU:HD12	1:E:13:LEU:O	2.13	0.48
1:E:134:LEU:O	1:E:136:ASP:N	2.47	0.48
1:E:197:ILE:O	1:E:200:GLY:N	2.47	0.48
1:E:250:LEU:HA	1:E:253:ILE:CG2	2.40	0.48
1:F:285:THR:HG22	1:F:303:LEU:HD13	1.96	0.48
1:A:249:VAL:O	1:A:253:ILE:HG22	2.14	0.48
1:D:282:LEU:HD13	1:D:307:ALA:HB2	1.95	0.48
1:E:123:GLN:HG2	1:E:124:PRO:CA	2.42	0.48
1:E:254:TYR:CD2	1:E:411:ILE:HG23	2.49	0.48
1:B:223:HIS:HD2	1:D:378:ASN:ND2	2.09	0.48
1:E:139:PRO:HB3	1:E:153:PRO:HB3	1.95	0.48
1:B:288:VAL:O	1:B:292:MET:HG2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:VAL:O	1:E:253:ILE:HG22	2.14	0.48
1:B:60:PRO:HG3	1:C:143:PHE:CZ	2.48	0.48
1:E:6:LYS:HA	1:E:8:ILE:HD12	1.94	0.48
1:F:377:PRO:O	1:F:381:ALA:N	2.45	0.48
1:C:276:ARG:HD3	1:C:395:MET:HG2	1.96	0.48
1:F:282:LEU:HD13	1:F:307:ALA:HB2	1.94	0.48
1:A:35:TYR:O	1:A:38:ALA:N	2.47	0.48
1:A:264:HIS:ND1	1:A:264:HIS:C	2.72	0.48
1:A:266:LYS:CB	1:A:270:LEU:HG	2.44	0.48
1:C:138:VAL:HG12	1:C:138:VAL:O	2.12	0.48
1:D:120:GLN:HB2	1:D:121:GLN:CA	2.33	0.48
1:D:376:ASP:O	1:D:379:VAL:HB	2.14	0.48
1:E:195:TYR:O	1:E:198:VAL:HG12	2.14	0.48
1:F:374:LEU:HA	1:F:379:VAL:HG11	1.96	0.48
1:D:186:ALA:O	1:E:183:LEU:HD13	2.14	0.48
1:F:67:VAL:HG11	1:F:187:ILE:HD13	1.96	0.48
1:A:254:TYR:CD2	1:A:411:ILE:HG23	2.50	0.47
1:B:84:LYS:HD2	1:B:412:VAL:HG13	1.95	0.47
1:C:266:LYS:O	1:C:268:ALA:N	2.47	0.47
1:C:317:TYR:HD1	1:C:317:TYR:C	2.22	0.47
1:D:24:ALA:N	1:D:213:ILE:HD13	2.29	0.47
1:D:157:PHE:HD1	1:F:56:MET:CE	2.27	0.47
1:F:264:HIS:NE2	1:F:265:ALA:HB2	2.29	0.47
1:C:165:ILE:O	1:C:168:LEU:N	2.47	0.47
1:A:235:VAL:HG22	1:A:320:VAL:HG13	1.94	0.47
1:F:99:LEU:O	1:F:103:MET:HG2	2.13	0.47
1:F:246:VAL:O	1:F:250:LEU:HB2	2.14	0.47
1:A:157:PHE:O	1:A:160:ILE:N	2.47	0.47
1:C:123:GLN:HG2	1:C:124:PRO:CA	2.41	0.47
1:E:121:GLN:HB3	1:E:124:PRO:HD3	1.96	0.47
1:E:134:LEU:O	1:E:137:ILE:CG1	2.60	0.47
1:E:157:PHE:O	1:E:160:ILE:N	2.48	0.47
1:F:58:VAL:HG22	1:F:283:PRO:HD3	1.95	0.47
1:F:343:LEU:HD12	1:F:347:LEU:HD23	1.96	0.47
1:B:48:ASP:O	1:B:49:LEU:C	2.57	0.47
1:C:121:GLN:HB3	1:C:124:PRO:HD3	1.96	0.47
1:C:378:ASN:OD1	1:F:385:MET:HA	2.15	0.47
1:D:124:PRO:HB2	1:D:368:HIS:HE1	1.75	0.47
1:F:263:LYS:O	1:F:265:ALA:N	2.48	0.47
1:B:303:LEU:HD21	1:B:406:LEU:HD23	1.96	0.47
1:D:88:TYR:CZ	1:D:92:THR:HG21	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:ILE:HG22	1:F:78:LEU:HD22	1.95	0.47
1:B:317:TYR:HA	1:B:320:VAL:CG1	2.45	0.47
1:B:414:LYS:O	1:B:414:LYS:HG3	2.15	0.47
1:C:134:LEU:C	1:C:136:ASP:N	2.72	0.47
1:C:264:HIS:ND1	1:C:264:HIS:C	2.72	0.47
1:D:134:LEU:O	1:D:135:LEU:C	2.55	0.47
1:D:136:ASP:HA	1:F:52:ARG:NH2	2.30	0.47
1:D:231:VAL:O	1:D:235:VAL:HG23	2.14	0.47
1:E:317:TYR:C	1:E:317:TYR:HD1	2.23	0.47
1:F:84:LYS:HD2	1:F:412:VAL:HG13	1.96	0.47
1:F:134:LEU:O	1:F:135:LEU:C	2.56	0.47
1:F:231:VAL:O	1:F:235:VAL:HG23	2.15	0.47
1:B:264:HIS:CE1	1:B:265:ALA:CB	2.92	0.47
1:B:346:VAL:O	1:B:350:ILE:HG23	2.15	0.47
1:C:376:ASP:O	1:C:379:VAL:HB	2.14	0.47
1:D:16:ILE:HD11	1:D:205:ALA:CB	2.45	0.47
1:F:8:ILE:O	1:F:9:GLU:OE1	2.32	0.47
1:B:99:LEU:O	1:B:103:MET:HG2	2.14	0.47
1:D:209:VAL:HA	1:D:274:VAL:HG11	1.97	0.47
1:D:251:LEU:HD13	1:D:258:PRO:HA	1.96	0.47
1:E:10:TYR:CD2	1:E:11:PRO:HD2	2.50	0.47
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.96	0.47
1:B:24:ALA:N	1:B:213:ILE:HD13	2.30	0.47
1:B:66:LEU:HD13	1:B:300:SER:O	2.14	0.47
1:C:258:PRO:O	1:C:261:PHE:HB3	2.15	0.47
1:C:276:ARG:HD3	1:C:395:MET:HG3	1.97	0.47
1:D:143:PHE:CE1	1:F:146:LEU:HD13	2.50	0.47
1:F:73:ILE:HG23	1:F:74:SER:N	2.29	0.47
1:F:361:ILE:N	1:F:361:ILE:CD1	2.78	0.47
1:B:81:VAL:HG23	1:B:412:VAL:HG12	1.97	0.46
1:B:348:ALA:O	1:B:352:THR:N	2.47	0.46
1:C:288:VAL:O	1:C:288:VAL:HG13	2.15	0.46
1:D:376:ASP:O	1:D:379:VAL:N	2.49	0.46
1:A:315:ALA:HB2	1:A:349:SER:OG	2.14	0.46
1:B:78:LEU:HD13	1:B:78:LEU:HA	1.70	0.46
1:B:173:ASN:OD1	1:B:176:VAL:HG13	2.15	0.46
1:C:63:PHE:O	1:C:67:VAL:HG23	2.15	0.46
1:C:294:ILE:HG22	1:C:295:SER:N	2.30	0.46
1:D:355:VAL:O	2:D:501:ASP:N	2.49	0.46
1:A:317:TYR:C	1:A:317:TYR:HD1	2.24	0.46
1:C:378:ASN:ND2	1:F:223:HIS:HD2	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:ALA:O	1:F:183:LEU:CD1	2.63	0.46
1:A:144:GLY:O	1:A:145:ALA:C	2.59	0.46
1:D:66:LEU:HA	1:D:300:SER:OG	2.16	0.46
1:D:266:LYS:O	1:D:268:ALA:N	2.48	0.46
1:C:123:GLN:HG2	1:C:125:LYS:H	1.80	0.46
1:E:16:ILE:HD11	1:E:205:ALA:HB1	1.97	0.46
1:F:104:ALA:HB2	1:F:320:VAL:HG23	1.97	0.46
1:F:134:LEU:C	1:F:136:ASP:N	2.74	0.46
1:F:155:ILE:HG22	1:F:156:PHE:N	2.30	0.46
1:F:264:HIS:ND1	1:F:264:HIS:C	2.73	0.46
1:A:56:MET:HE2	1:B:157:PHE:CD1	2.51	0.46
1:C:134:LEU:O	1:C:135:LEU:C	2.57	0.46
1:E:30:LEU:O	1:E:35:TYR:HB2	2.14	0.46
1:D:134:LEU:C	1:D:136:ASP:H	2.22	0.46
1:D:281:THR:O	1:D:282:LEU:C	2.59	0.46
1:E:73:ILE:HG22	1:E:78:LEU:HD22	1.97	0.46
1:F:311:MET:HE2	2:F:501:ASP:OXT	2.16	0.46
1:A:110:GLY:N	1:A:227:GLU:OE1	2.46	0.46
1:A:190:LEU:O	1:A:191:ALA:C	2.56	0.46
1:B:35:TYR:O	1:B:38:ALA:HB3	2.16	0.46
1:B:301:PHE:O	1:B:301:PHE:CG	2.69	0.46
1:C:120:GLN:HB2	1:C:121:GLN:CA	2.33	0.46
1:D:299:TYR:C	1:D:299:TYR:CD2	2.94	0.46
1:A:386:ILE:HA	1:A:389:ILE:HG22	1.96	0.46
1:B:165:ILE:O	1:B:166:THR:C	2.59	0.46
1:C:24:ALA:N	1:C:213:ILE:HD13	2.31	0.46
1:C:85:ILE:HG13	1:C:89:TYR:CE1	2.51	0.46
1:D:115:LEU:HB2	1:D:328:ALA:O	2.16	0.46
1:E:235:VAL:HG22	1:E:320:VAL:HG13	1.98	0.46
1:B:66:LEU:HA	1:B:300:SER:OG	2.16	0.45
1:E:264:HIS:NE2	1:E:265:ALA:HB2	2.30	0.45
1:F:317:TYR:HA	1:F:320:VAL:CG1	2.46	0.45
1:B:74:SER:O	1:B:77:ARG:N	2.49	0.45
1:B:363:LEU:O	1:B:366:VAL:HG12	2.15	0.45
1:D:64:ALA:CB	1:D:191:ALA:HB2	2.45	0.45
1:E:48:ASP:O	1:E:51:VAL:N	2.49	0.45
1:D:123:GLN:HG2	1:D:124:PRO:CA	2.42	0.45
1:F:282:LEU:HB3	1:F:283:PRO:HD3	1.99	0.45
1:A:50:PHE:CE1	1:A:205:ALA:HB2	2.51	0.45
1:F:288:VAL:HG12	1:F:406:LEU:HD11	1.97	0.45
1:B:85:ILE:CD1	1:B:408:GLY:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:TYR:O	1:B:321:CYS:N	2.47	0.45
1:E:209:VAL:HG22	1:E:274:VAL:HG11	1.97	0.45
1:F:72:SER:O	1:F:73:ILE:HD12	2.16	0.45
1:F:85:ILE:HD13	1:F:408:GLY:O	2.16	0.45
1:F:190:LEU:O	1:F:193:ALA:N	2.49	0.45
1:B:7:TYR:HB2	1:B:8:ILE:C	2.41	0.45
1:B:174:GLU:CD	1:B:177:ARG:HE	2.24	0.45
1:D:144:GLY:O	1:D:147:ALA:N	2.49	0.45
1:E:266:LYS:CB	1:E:270:LEU:HG	2.47	0.45
1:F:53:LEU:O	1:F:56:MET:HB3	2.16	0.45
1:F:303:LEU:HD21	1:F:406:LEU:HD23	1.99	0.45
1:F:333:LEU:HD22	1:F:341:ILE:HD11	1.98	0.45
1:A:266:LYS:O	1:A:268:ALA:N	2.50	0.45
1:D:337:GLN:O	1:D:338:GLN:C	2.60	0.45
1:F:66:LEU:CD2	1:F:159:ILE:HG13	2.45	0.45
1:F:78:LEU:HD13	1:F:78:LEU:HA	1.75	0.45
1:A:30:LEU:O	1:A:35:TYR:HB2	2.16	0.45
1:A:276:ARG:HD3	1:A:395:MET:HG3	1.99	0.45
1:B:400:VAL:HG12	1:B:400:VAL:O	2.17	0.45
1:C:298:ILE:HG21	1:C:413:ALA:HB2	1.99	0.45
1:F:89:TYR:CD2	1:F:310:ASN:HB2	2.52	0.45
1:D:145:ALA:O	1:D:150:GLN:HB2	2.17	0.45
1:F:178:LYS:O	1:F:182:THR:OG1	2.35	0.45
1:F:190:LEU:O	1:F:191:ALA:C	2.60	0.45
1:D:256:ILE:HD13	1:D:410:ALA:HB1	1.98	0.45
1:F:41:THR:HG22	1:F:42:TYR:CD1	2.52	0.45
1:F:209:VAL:HG13	1:F:274:VAL:HG21	1.98	0.45
1:D:212:LEU:CB	1:D:274:VAL:HG13	2.46	0.44
1:D:305:LEU:O	1:D:305:LEU:HG	2.17	0.44
1:A:262:ILE:O	1:A:265:ALA:HB3	2.17	0.44
1:F:273:PHE:CE1	1:F:395:MET:HB3	2.52	0.44
1:B:77:ARG:HA	1:B:80:ARG:NH1	2.32	0.44
1:B:111:ALA:N	1:B:327:ASN:HB3	2.33	0.44
1:B:276:ARG:HD3	1:B:395:MET:CG	2.47	0.44
1:B:282:LEU:HD13	1:B:307:ALA:HB2	1.98	0.44
1:D:374:LEU:HA	1:D:379:VAL:HG11	1.99	0.44
1:E:146:LEU:HB3	1:F:143:PHE:CD1	2.53	0.44
1:E:216:VAL:HG12	1:E:392:ILE:HD12	2.00	0.44
1:F:13:LEU:HD12	1:F:13:LEU:O	2.17	0.44
1:F:264:HIS:CE1	1:F:265:ALA:CB	2.94	0.44
1:F:311:MET:CE	1:F:354:GLY:HA2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:382:ALA:HA	1:F:385:MET:HG3	1.97	0.44
1:B:81:VAL:HG21	1:B:298:ILE:HG23	1.99	0.44
1:B:191:ALA:O	1:B:195:TYR:HD1	1.99	0.44
1:C:337:GLN:O	1:C:338:GLN:C	2.61	0.44
1:D:30:LEU:O	1:D:35:TYR:HB2	2.17	0.44
1:F:74:SER:O	1:F:75:PRO:C	2.61	0.44
1:F:333:LEU:HD12	1:F:333:LEU:H	1.83	0.44
1:A:144:GLY:O	1:A:147:ALA:N	2.50	0.44
1:A:265:ALA:HB1	1:A:266:LYS:O	2.17	0.44
1:A:273:PHE:CE1	1:A:395:MET:HB3	2.53	0.44
1:D:414:LYS:O	1:D:414:LYS:HG3	2.17	0.44
1:F:337:GLN:O	1:F:341:ILE:N	2.48	0.44
1:A:231:VAL:HG23	1:A:320:VAL:HG22	1.99	0.44
1:B:67:VAL:HG11	1:B:187:ILE:HD13	2.00	0.44
1:C:198:VAL:HG13	1:C:287:ARG:HD3	2.00	0.44
1:D:282:LEU:HB3	1:D:283:PRO:HD3	2.00	0.44
1:D:282:LEU:O	1:D:283:PRO:C	2.58	0.44
1:D:285:THR:HG22	1:D:303:LEU:HD13	1.99	0.44
1:F:7:TYR:HB2	1:F:8:ILE:C	2.42	0.44
1:F:81:VAL:HG21	1:F:298:ILE:HG23	2.00	0.44
1:A:140:THR:HG22	1:C:55:LYS:HB2	1.99	0.44
1:B:377:PRO:O	1:B:381:ALA:N	2.48	0.44
1:C:299:TYR:CD2	1:C:299:TYR:C	2.95	0.44
1:D:52:ARG:NH2	1:E:136:ASP:HA	2.32	0.44
1:D:325:ILE:HD11	1:D:383:TYR:HA	1.99	0.44
1:E:315:ALA:HB2	1:E:349:SER:OG	2.18	0.44
1:F:124:PRO:HB2	1:F:368:HIS:NE2	2.32	0.44
1:F:165:ILE:O	1:F:166:THR:C	2.61	0.44
1:F:77:ARG:HA	1:F:80:ARG:HH12	1.83	0.44
1:D:77:ARG:O	1:D:78:LEU:C	2.60	0.44
1:D:165:ILE:O	1:D:166:THR:C	2.59	0.44
1:E:394:ASP:OD1	2:E:501:ASP:N	2.51	0.44
1:B:10:TYR:CD2	1:B:11:PRO:HD2	2.53	0.43
1:E:144:GLY:O	1:E:145:ALA:C	2.61	0.43
1:F:215:TYR:CE1	1:F:219:GLU:CD	2.96	0.43
1:A:281:THR:O	1:A:283:PRO:N	2.51	0.43
1:E:50:PHE:CZ	1:E:54:LEU:HD11	2.52	0.43
1:F:23:GLY:HA2	1:F:210:PHE:CE2	2.53	0.43
1:A:107:PHE:HE1	1:A:237:VAL:HG11	1.84	0.43
1:C:72:SER:O	1:C:73:ILE:HD12	2.18	0.43
1:D:63:PHE:O	1:D:67:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:ALA:O	1:E:195:TYR:HD1	2.01	0.43
1:E:205:ALA:N	1:E:206:PRO:HD2	2.33	0.43
1:F:48:ASP:O	1:F:51:VAL:N	2.52	0.43
1:A:228:LEU:HB3	1:A:389:ILE:HD13	1.99	0.43
1:C:325:ILE:O	1:C:329:LEU:HG	2.18	0.43
1:C:374:LEU:HA	1:C:379:VAL:HG11	2.00	0.43
1:D:146:LEU:HD13	1:E:143:PHE:CE1	2.53	0.43
1:E:123:GLN:N	1:E:124:PRO:HA	2.33	0.43
1:F:263:LYS:C	1:F:265:ALA:N	2.73	0.43
1:A:282:LEU:HD13	1:A:307:ALA:HB2	2.01	0.43
1:B:263:LYS:O	1:B:265:ALA:N	2.52	0.43
1:C:262:ILE:O	1:C:265:ALA:HB3	2.19	0.43
1:C:311:MET:HE2	2:C:501:ASP:OXT	2.19	0.43
1:D:157:PHE:O	1:D:160:ILE:N	2.50	0.43
1:C:73:ILE:CG2	1:C:74:SER:N	2.81	0.43
1:F:202:MET:HA	1:F:205:ALA:HB2	2.01	0.43
1:E:9:GLU:OE2	1:E:9:GLU:HA	2.18	0.43
1:F:43:VAL:C	1:F:45:PRO:HD2	2.43	0.43
1:A:85:ILE:HG13	1:A:89:TYR:CE1	2.54	0.43
1:A:367:LEU:HD22	1:A:372:LEU:CD1	2.48	0.43
1:B:50:PHE:CZ	1:B:54:LEU:HD11	2.54	0.43
1:C:134:LEU:O	1:C:137:ILE:HG13	2.19	0.43
1:D:321:CYS:HB3	1:D:363:LEU:HD21	2.01	0.43
1:F:28:LEU:HD12	1:F:28:LEU:HA	1.87	0.43
1:A:297:GLY:O	1:A:298:ILE:HD13	2.19	0.43
1:B:43:VAL:C	1:B:45:PRO:HD2	2.44	0.43
1:C:253:ILE:HG23	1:C:254:TYR:HD1	1.84	0.43
1:F:391:ALA:HA	1:F:394:ASP:CB	2.49	0.43
1:B:7:TYR:HD2	1:B:9:GLU:OE2	2.02	0.42
1:D:294:ILE:HG22	1:D:295:SER:H	1.83	0.42
1:E:337:GLN:O	1:E:341:ILE:N	2.52	0.42
1:F:68:VAL:O	1:F:71:ALA:N	2.52	0.42
1:A:228:LEU:HB3	1:A:389:ILE:CD1	2.50	0.42
1:A:374:LEU:HA	1:A:379:VAL:HG11	2.01	0.42
1:C:134:LEU:C	1:C:136:ASP:H	2.26	0.42
1:D:101:ILE:O	1:D:105:ARG:HG2	2.18	0.42
1:E:72:SER:O	1:E:73:ILE:HD12	2.19	0.42
1:A:174:GLU:CD	1:A:177:ARG:HE	2.26	0.42
1:A:251:LEU:HD13	1:A:258:PRO:HA	2.01	0.42
1:C:128:PRO:C	1:C:130:LEU:H	2.26	0.42
1:C:157:PHE:O	1:C:160:ILE:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:276:ARG:HD3	1:E:395:MET:HG3	2.00	0.42
1:F:74:SER:O	1:F:77:ARG:N	2.52	0.42
1:F:134:LEU:O	1:F:137:ILE:HG13	2.18	0.42
1:F:228:LEU:HB3	1:F:389:ILE:CD1	2.50	0.42
1:A:32:HIS:HB2	1:A:222:VAL:HG12	2.01	0.42
1:A:400:VAL:O	1:A:400:VAL:HG12	2.20	0.42
1:B:117:VAL:CG1	1:B:378:ASN:HB2	2.49	0.42
1:B:385:MET:HA	1:D:378:ASN:OD1	2.19	0.42
1:C:66:LEU:HA	1:C:300:SER:OG	2.20	0.42
1:C:282:LEU:HD13	1:C:307:ALA:HB2	2.01	0.42
1:D:134:LEU:O	1:D:137:ILE:HG13	2.20	0.42
1:E:281:THR:O	1:E:283:PRO:N	2.52	0.42
1:F:382:ALA:O	1:F:385:MET:HG3	2.19	0.42
1:B:58:VAL:HG22	1:B:283:PRO:CD	2.49	0.42
1:B:123:GLN:N	1:B:124:PRO:CA	2.82	0.42
1:B:276:ARG:O	1:B:356:PRO:HG3	2.18	0.42
1:E:24:ALA:N	1:E:213:ILE:HD13	2.35	0.42
1:E:58:VAL:HG22	1:E:283:PRO:CD	2.49	0.42
1:E:210:PHE:CD1	1:E:210:PHE:C	2.97	0.42
1:A:98:THR:O	1:A:102:ILE:HB	2.18	0.42
1:B:228:LEU:HB3	1:B:389:ILE:CD1	2.50	0.42
1:D:258:PRO:O	1:D:261:PHE:HB3	2.18	0.42
1:D:408:GLY:O	1:D:412:VAL:HG23	2.20	0.42
1:F:348:ALA:O	1:F:352:THR:N	2.52	0.42
1:B:215:TYR:CE1	1:B:219:GLU:CD	2.98	0.42
1:C:64:ALA:CB	1:C:191:ALA:HB2	2.49	0.42
1:D:253:ILE:HG23	1:D:254:TYR:HD1	1.84	0.42
1:E:7:TYR:N	1:E:8:ILE:HA	2.34	0.42
1:F:24:ALA:O	1:F:28:LEU:HB2	2.20	0.42
1:F:216:VAL:HG12	1:F:392:ILE:HD12	2.02	0.42
1:F:399:MET:HE2	1:F:399:MET:HB3	1.96	0.42
1:A:28:LEU:HD12	1:A:28:LEU:HA	1.86	0.42
1:A:79:GLY:O	1:A:83:VAL:HG23	2.20	0.42
1:A:113:ILE:HD12	1:A:114:HIS:H	1.85	0.42
1:B:209:VAL:HG22	1:B:274:VAL:HG11	2.02	0.42
1:C:285:THR:HG22	1:C:303:LEU:HD13	2.00	0.42
1:F:39:VAL:O	1:F:43:VAL:HB	2.20	0.42
1:B:337:GLN:O	1:B:341:ILE:N	2.50	0.42
1:C:81:VAL:HG23	1:C:412:VAL:CG1	2.48	0.42
1:D:128:PRO:C	1:D:130:LEU:H	2.27	0.42
1:F:276:ARG:HD3	1:F:395:MET:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:TYR:CD2	1:B:310:ASN:HB2	2.55	0.42
1:B:136:ASP:C	1:B:138:VAL:N	2.78	0.42
1:D:376:ASP:C	1:D:376:ASP:OD1	2.63	0.42
1:E:64:ALA:CB	1:E:191:ALA:HB2	2.50	0.42
1:E:250:LEU:CA	1:E:253:ILE:HG22	2.49	0.42
1:E:297:GLY:O	1:E:298:ILE:HD13	2.20	0.42
1:F:7:TYR:CD2	1:F:9:GLU:OE2	2.73	0.42
1:F:391:ALA:HA	1:F:394:ASP:HB3	2.01	0.42
1:A:138:VAL:HG11	1:C:52:ARG:HB3	2.02	0.41
1:A:261:PHE:CD1	1:A:292:MET:HE1	2.55	0.41
1:C:75:PRO:HG3	1:C:163:ILE:CG1	2.45	0.41
1:C:295:SER:OG	1:C:298:ILE:HG12	2.20	0.41
1:D:156:PHE:O	1:D:156:PHE:CD2	2.73	0.41
1:E:28:LEU:HD12	1:E:28:LEU:HA	1.89	0.41
1:E:134:LEU:C	1:E:136:ASP:N	2.78	0.41
1:E:137:ILE:O	1:E:139:PRO:HD3	2.20	0.41
1:F:7:TYR:HD2	1:F:9:GLU:OE2	2.02	0.41
1:F:363:LEU:O	1:F:367:LEU:HG	2.20	0.41
1:A:146:LEU:O	1:B:141:ASN:ND2	2.49	0.41
1:B:216:VAL:HG12	1:B:392:ILE:HD12	2.02	0.41
1:E:190:LEU:O	1:E:191:ALA:C	2.60	0.41
1:F:24:ALA:N	1:F:213:ILE:HD13	2.35	0.41
1:F:115:LEU:HD22	1:F:378:ASN:ND2	2.34	0.41
1:B:333:LEU:H	1:B:333:LEU:HD12	1.86	0.41
1:C:165:ILE:O	1:C:166:THR:C	2.62	0.41
1:C:202:MET:HA	1:C:205:ALA:HB2	2.01	0.41
1:E:89:TYR:CD2	1:E:310:ASN:HB2	2.55	0.41
1:E:113:ILE:HD12	1:E:114:HIS:H	1.85	0.41
1:B:52:ARG:NH2	1:C:136:ASP:HA	2.36	0.41
1:C:228:LEU:HB3	1:C:389:ILE:HD13	2.02	0.41
1:C:317:TYR:CD1	1:C:318:GLN:N	2.88	0.41
1:D:209:VAL:HG13	1:D:274:VAL:HG21	2.02	0.41
1:E:66:LEU:HD21	1:E:159:ILE:HG13	2.03	0.41
1:E:228:LEU:HB3	1:E:389:ILE:CD1	2.51	0.41
1:A:134:LEU:C	1:A:136:ASP:N	2.78	0.41
1:A:174:GLU:OE1	1:A:177:ARG:NE	2.53	0.41
1:B:74:SER:O	1:B:75:PRO:C	2.64	0.41
1:B:146:LEU:O	1:B:148:ASN:N	2.53	0.41
1:B:190:LEU:O	1:B:191:ALA:C	2.62	0.41
1:B:299:TYR:CD2	1:B:299:TYR:C	2.97	0.41
1:C:77:ARG:HA	1:C:80:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:ALA:N	1:D:206:PRO:HD2	2.34	0.41
1:A:66:LEU:HA	1:A:300:SER:OG	2.21	0.41
1:A:337:GLN:O	1:A:341:ILE:N	2.53	0.41
1:A:398:THR:HA	1:A:401:ASN:ND2	2.36	0.41
1:C:209:VAL:HG13	1:C:274:VAL:HG21	2.02	0.41
1:C:212:LEU:CB	1:C:274:VAL:HG13	2.50	0.41
1:C:261:PHE:HD2	1:C:262:ILE:HD12	1.85	0.41
1:E:124:PRO:CB	1:E:368:HIS:CE1	2.92	0.41
1:E:398:THR:HA	1:E:401:ASN:ND2	2.36	0.41
1:F:9:GLU:OE2	1:F:203:GLN:NE2	2.54	0.41
1:F:110:GLY:N	1:F:227:GLU:OE1	2.48	0.41
1:F:123:GLN:N	1:F:124:PRO:CA	2.84	0.41
1:A:43:VAL:HG11	1:A:214:ALA:CB	2.50	0.41
1:A:78:LEU:HD13	1:A:78:LEU:HA	1.82	0.41
1:C:193:ALA:O	1:C:196:LYS:HB2	2.21	0.41
1:C:261:PHE:CD1	1:C:292:MET:HE1	2.55	0.41
1:E:56:MET:HE2	1:F:157:PHE:CD1	2.55	0.41
1:E:111:ALA:N	1:E:327:ASN:HB3	2.35	0.41
1:E:159:ILE:HD11	1:E:301:PHE:CD1	2.56	0.41
1:F:190:LEU:O	1:F:193:ALA:HB3	2.21	0.41
1:A:51:VAL:HG22	1:A:275:THR:HG23	2.02	0.41
1:A:346:VAL:O	1:A:350:ILE:CG2	2.65	0.41
1:B:391:ALA:HA	1:B:394:ASP:HB3	2.02	0.41
1:D:123:GLN:HG2	1:D:125:LYS:H	1.86	0.41
1:D:344:THR:HA	1:D:347:LEU:HB2	2.03	0.41
1:E:15:LYS:NZ	1:E:206:PRO:HG3	2.35	0.41
1:E:183:LEU:HG	1:E:187:ILE:HD12	2.02	0.41
1:F:61:ILE:O	1:F:286:MET:HE1	2.20	0.41
1:A:66:LEU:HD21	1:A:159:ILE:HG13	2.03	0.41
1:A:85:ILE:CD1	1:A:408:GLY:O	2.69	0.41
1:A:123:GLN:N	1:A:124:PRO:HA	2.36	0.41
1:A:210:PHE:CD1	1:A:210:PHE:C	2.99	0.41
1:B:7:TYR:CD2	1:B:9:GLU:OE2	2.74	0.41
1:B:77:ARG:HH11	1:B:416:GLU:HG3	1.85	0.41
1:B:263:LYS:C	1:B:265:ALA:N	2.78	0.41
1:C:11:PRO:HG2	1:C:14:GLN:CG	2.47	0.41
1:C:23:GLY:HA2	1:C:210:PHE:CE2	2.55	0.41
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.56	0.41
1:C:256:ILE:HD13	1:C:410:ALA:HB1	2.03	0.41
1:C:325:ILE:HD11	1:C:383:TYR:HA	2.02	0.41
1:D:77:ARG:HA	1:D:80:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:TYR:C	1:D:317:TYR:CD1	2.99	0.41
1:E:122:PHE:C	1:E:124:PRO:HB3	2.46	0.41
1:E:228:LEU:HB3	1:E:389:ILE:HD13	2.03	0.41
1:E:261:PHE:CD1	1:E:292:MET:HE1	2.56	0.41
1:F:129:PRO:O	1:F:130:LEU:C	2.64	0.41
1:F:317:TYR:O	1:F:321:CYS:N	2.50	0.41
1:A:9:GLU:OE2	1:A:9:GLU:HA	2.21	0.41
1:B:19:GLY:O	1:B:23:GLY:N	2.51	0.41
1:B:49:LEU:O	1:B:52:ARG:HB2	2.21	0.41
1:D:117:VAL:CG1	1:D:378:ASN:HB2	2.51	0.41
1:D:276:ARG:HD3	1:D:395:MET:HG3	2.02	0.41
1:E:322:THR:HG21	1:E:341:ILE:CD1	2.51	0.41
1:F:248:PHE:O	1:F:252:LYS:HB2	2.21	0.41
1:F:314:THR:HG22	1:F:318:GLN:NE2	2.36	0.41
1:A:286:MET:HA	1:A:303:LEU:HD12	2.03	0.40
1:B:7:TYR:HB2	1:B:8:ILE:O	2.21	0.40
1:C:16:ILE:HD11	1:C:205:ALA:CB	2.51	0.40
1:C:97:VAL:HB	1:C:342:VAL:HG22	2.03	0.40
1:C:350:ILE:N	1:C:351:GLY:CA	2.81	0.40
1:D:212:LEU:HB2	1:D:274:VAL:HG13	2.02	0.40
1:E:197:ILE:CG2	1:F:160:ILE:CG2	2.99	0.40
1:E:400:VAL:O	1:E:400:VAL:HG12	2.21	0.40
1:F:73:ILE:CG2	1:F:74:SER:N	2.84	0.40
1:F:128:PRO:C	1:F:130:LEU:H	2.28	0.40
1:F:210:PHE:CD1	1:F:210:PHE:C	2.98	0.40
1:F:257:ASP:HA	1:F:258:PRO:HD3	1.93	0.40
1:A:11:PRO:HG2	1:A:14:GLN:CG	2.45	0.40
1:A:64:ALA:CB	1:A:191:ALA:HB2	2.52	0.40
1:A:215:TYR:O	1:A:218:ALA:N	2.54	0.40
1:B:134:LEU:C	1:B:136:ASP:N	2.79	0.40
1:B:137:ILE:O	1:B:139:PRO:HD3	2.21	0.40
1:B:209:VAL:HG13	1:B:274:VAL:HG21	2.03	0.40
1:B:265:ALA:CB	1:B:266:LYS:O	2.68	0.40
1:B:346:VAL:O	1:B:347:LEU:C	2.64	0.40
1:C:35:TYR:O	1:C:38:ALA:N	2.54	0.40
1:C:349:SER:C	1:C:351:GLY:HA3	2.46	0.40
1:D:85:ILE:HG13	1:D:89:TYR:CE1	2.56	0.40
1:D:143:PHE:CZ	1:F:60:PRO:HG3	2.55	0.40
1:B:35:TYR:O	1:B:36:ALA:C	2.64	0.40
1:B:191:ALA:O	1:B:192:GLU:C	2.62	0.40
1:C:123:GLN:N	1:C:124:PRO:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:PHE:O	1:F:264:HIS:HD2	2.02	0.40
1:C:16:ILE:HD11	1:C:205:ALA:HB3	2.04	0.40
1:C:98:THR:O	1:C:102:ILE:HB	2.22	0.40
1:A:134:LEU:O	1:A:137:ILE:CG1	2.66	0.40
1:A:257:ASP:HA	1:A:258:PRO:HD3	1.98	0.40
1:A:296:GLU:HA	1:A:299:TYR:CE1	2.56	0.40
1:B:241:LEU:O	1:B:245:LEU:HB2	2.22	0.40
1:B:285:THR:HG22	1:B:303:LEU:HD13	2.04	0.40
1:B:402:VAL:HG22	4:B:601:HOH:O	2.22	0.40
1:D:195:TYR:O	1:D:198:VAL:HG12	2.22	0.40
1:D:242:GLN:O	1:D:243:ILE:C	2.65	0.40
1:E:299:TYR:CD2	1:E:299:TYR:C	2.99	0.40
1:F:237:VAL:O	1:F:241:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/425 (96%)	330 (81%)	63 (15%)	16 (4%)	2	20
1	B	409/425 (96%)	326 (80%)	59 (14%)	24 (6%)	1	12
1	C	409/425 (96%)	328 (80%)	63 (15%)	18 (4%)	2	17
1	D	409/425 (96%)	331 (81%)	56 (14%)	22 (5%)	1	14
1	E	409/425 (96%)	328 (80%)	68 (17%)	13 (3%)	3	24
1	F	409/425 (96%)	321 (78%)	66 (16%)	22 (5%)	1	14
All	All	2454/2550 (96%)	1964 (80%)	375 (15%)	115 (5%)	2	17

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ALA
1	A	124	PRO
1	A	127	ALA
1	A	267	ASP
1	B	68	VAL
1	B	124	PRO
1	B	127	ALA
1	B	282	LEU
1	C	116	ALA
1	C	124	PRO
1	C	127	ALA
1	C	130	LEU
1	C	135	LEU
1	C	267	ASP
1	C	282	LEU
1	D	124	PRO
1	D	127	ALA
1	D	130	LEU
1	D	135	LEU
1	D	267	ASP
1	E	116	ALA
1	E	124	PRO
1	E	127	ALA
1	E	149	GLY
1	E	267	ASP
1	E	282	LEU
1	F	68	VAL
1	F	124	PRO
1	F	127	ALA
1	F	267	ASP
1	F	282	LEU
1	A	130	LEU
1	A	135	LEU
1	A	149	GLY
1	A	150	GLN
1	A	282	LEU
1	B	56	MET
1	B	115	LEU
1	B	116	ALA
1	B	130	LEU
1	B	149	GLY
1	B	200	GLY
1	B	202	MET

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Mol	Chain	Res	Type
1	B	264	HIS
1	B	267	ASP
1	C	149	GLY
1	C	172	GLU
1	C	202	MET
1	D	116	ALA
1	D	149	GLY
1	D	202	MET
1	D	282	LEU
1	E	130	LEU
1	E	135	LEU
1	E	150	GLN
1	F	34	GLY
1	F	115	LEU
1	F	116	ALA
1	F	130	LEU
1	F	149	GLY
1	F	155	ILE
1	F	202	MET
1	F	264	HIS
1	B	155	ILE
1	C	155	ILE
1	C	220	GLN
1	D	155	ILE
1	E	34	GLY
1	E	56	MET
1	E	202	MET
1	F	135	LEU
1	F	150	GLN
1	F	200	GLY
1	F	334	THR
1	A	34	GLY
1	A	115	LEU
1	A	202	MET
1	B	150	GLN
1	B	334	THR
1	C	68	VAL
1	C	150	GLN
1	D	172	GLU
1	D	220	GLN
1	F	56	MET
1	F	220	GLN

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Mol	Chain	Res	Type
1	A	56	MET
1	B	34	GLY
1	B	135	LEU
1	B	146	LEU
1	B	220	GLN
1	D	36	ALA
1	D	115	LEU
1	D	150	GLN
1	F	352	THR
1	C	60	PRO
1	D	371	GLY
1	A	377	PRO
1	C	370	VAL
1	F	222	VAL
1	B	60	PRO
1	B	371	GLY
1	C	371	GLY
1	C	373	PRO
1	D	60	PRO
1	D	68	VAL
1	D	370	VAL
1	F	60	PRO
1	B	377	PRO
1	D	129	PRO
1	D	373	PRO
1	A	155	ILE
1	A	371	GLY
1	D	377	PRO
1	B	373	PRO
1	E	370	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	316/330 (96%)	241 (76%)	75 (24%)	1 4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	316/330 (96%)	239 (76%)	77 (24%)	1	4
1	C	316/330 (96%)	245 (78%)	71 (22%)	1	5
1	D	316/330 (96%)	242 (77%)	74 (23%)	1	4
1	E	316/330 (96%)	242 (77%)	74 (23%)	1	4
1	F	316/330 (96%)	236 (75%)	80 (25%)	0	3
All	All	1896/1980 (96%)	1445 (76%)	451 (24%)	1	4

All (451) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	9	GLU
1	A	13	LEU
1	A	15	LYS
1	A	16	ILE
1	A	17	LEU
1	A	25	ILE
1	A	28	LEU
1	A	29	ILE
1	A	61	ILE
1	A	62	VAL
1	A	73	ILE
1	A	77	ARG
1	A	78	LEU
1	A	80	ARG
1	A	90	LEU
1	A	99	LEU
1	A	102	ILE
1	A	105	ARG
1	A	106	LEU
1	A	113	ILE
1	A	120	GLN
1	A	122	PHE
1	A	123	GLN
1	A	125	LYS
1	A	131	VAL
1	A	137	ILE
1	A	140	THR
1	A	148	ASN
1	A	151	VAL

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Mol	Chain	Res	Type
1	A	159	ILE
1	A	163	ILE
1	A	175	LYS
1	A	178	LYS
1	A	182	THR
1	A	197	ILE
1	A	198	VAL
1	A	207	ILE
1	A	213	ILE
1	A	215	TYR
1	A	232	THR
1	A	237	VAL
1	A	241	LEU
1	A	242	GLN
1	A	243	ILE
1	A	245	LEU
1	A	249	VAL
1	A	250	LEU
1	A	253	ILE
1	A	260	SER
1	A	269	MET
1	A	274	VAL
1	A	287	ARG
1	A	288	VAL
1	A	290	LYS
1	A	295	SER
1	A	296	GLU
1	A	317	TYR
1	A	320	VAL
1	A	333	LEU
1	A	338	GLN
1	A	344	THR
1	A	350	ILE
1	A	355	VAL
1	A	361	ILE
1	A	365	MET
1	A	372	LEU
1	A	375	THR
1	A	385	MET
1	A	386	ILE
1	A	387	LEU
1	A	389	ILE

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Mol	Chain	Res	Type
1	A	392	ILE
1	A	402	VAL
1	A	415	THR
1	B	6	LYS
1	B	9	GLU
1	B	13	LEU
1	B	15	LYS
1	B	16	ILE
1	B	17	LEU
1	B	25	ILE
1	B	28	LEU
1	B	29	ILE
1	B	61	ILE
1	B	62	VAL
1	B	72	SER
1	B	73	ILE
1	B	74	SER
1	B	77	ARG
1	B	78	LEU
1	B	80	ARG
1	B	90	LEU
1	B	99	LEU
1	B	102	ILE
1	B	105	ARG
1	B	113	ILE
1	B	120	GLN
1	B	122	PHE
1	B	123	GLN
1	B	125	LYS
1	B	131	VAL
1	B	137	ILE
1	B	140	THR
1	B	148	ASN
1	B	151	VAL
1	B	159	ILE
1	B	175	LYS
1	B	176	VAL
1	B	178	LYS
1	B	182	THR
1	B	207	ILE
1	B	213	ILE
1	B	215	TYR

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Mol	Chain	Res	Type
1	B	231	VAL
1	B	232	THR
1	B	237	VAL
1	B	241	LEU
1	B	242	GLN
1	B	245	LEU
1	B	249	VAL
1	B	253	ILE
1	B	260	SER
1	B	264	HIS
1	B	269	MET
1	B	274	VAL
1	B	283	PRO
1	B	288	VAL
1	B	290	LYS
1	B	295	SER
1	B	296	GLU
1	B	300	SER
1	B	308	THR
1	B	317	TYR
1	B	320	VAL
1	B	333	LEU
1	B	334	THR
1	B	338	GLN
1	B	340	THR
1	B	350	ILE
1	B	355	VAL
1	B	361	ILE
1	B	365	MET
1	B	372	LEU
1	B	375	THR
1	B	385	MET
1	B	386	ILE
1	B	387	LEU
1	B	389	ILE
1	B	392	ILE
1	B	402	VAL
1	B	415	THR
1	C	6	LYS
1	C	9	GLU
1	C	15	LYS
1	C	17	LEU

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Mol	Chain	Res	Type
1	C	28	LEU
1	C	29	ILE
1	C	61	ILE
1	C	62	VAL
1	C	72	SER
1	C	73	ILE
1	C	74	SER
1	C	78	LEU
1	C	80	ARG
1	C	90	LEU
1	C	91	LEU
1	C	99	LEU
1	C	102	ILE
1	C	105	ARG
1	C	113	ILE
1	C	120	GLN
1	C	122	PHE
1	C	125	LYS
1	C	126	GLN
1	C	130	LEU
1	C	131	VAL
1	C	137	ILE
1	C	148	ASN
1	C	151	VAL
1	C	159	ILE
1	C	163	ILE
1	C	175	LYS
1	C	182	THR
1	C	207	ILE
1	C	213	ILE
1	C	230	LYS
1	C	231	VAL
1	C	232	THR
1	C	237	VAL
1	C	242	GLN
1	C	243	ILE
1	C	245	LEU
1	C	249	VAL
1	C	253	ILE
1	C	260	SER
1	C	269	MET
1	C	271	THR

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Mol	Chain	Res	Type
1	C	274	VAL
1	C	283	PRO
1	C	287	ARG
1	C	288	VAL
1	C	290	LYS
1	C	295	SER
1	C	296	GLU
1	C	317	TYR
1	C	320	VAL
1	C	333	LEU
1	C	338	GLN
1	C	344	THR
1	C	350	ILE
1	C	355	VAL
1	C	361	ILE
1	C	365	MET
1	C	372	LEU
1	C	374	LEU
1	C	375	THR
1	C	385	MET
1	C	386	ILE
1	C	387	LEU
1	C	389	ILE
1	C	392	ILE
1	C	415	THR
1	D	6	LYS
1	D	9	GLU
1	D	13	LEU
1	D	15	LYS
1	D	16	ILE
1	D	17	LEU
1	D	28	LEU
1	D	29	ILE
1	D	61	ILE
1	D	62	VAL
1	D	72	SER
1	D	73	ILE
1	D	74	SER
1	D	78	LEU
1	D	80	ARG
1	D	90	LEU
1	D	91	LEU

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Mol	Chain	Res	Type
1	D	99	LEU
1	D	102	ILE
1	D	105	ARG
1	D	113	ILE
1	D	120	GLN
1	D	122	PHE
1	D	123	GLN
1	D	125	LYS
1	D	130	LEU
1	D	131	VAL
1	D	137	ILE
1	D	148	ASN
1	D	151	VAL
1	D	152	LEU
1	D	159	ILE
1	D	163	ILE
1	D	166	THR
1	D	175	LYS
1	D	182	THR
1	D	207	ILE
1	D	213	ILE
1	D	231	VAL
1	D	232	THR
1	D	237	VAL
1	D	242	GLN
1	D	243	ILE
1	D	245	LEU
1	D	249	VAL
1	D	253	ILE
1	D	260	SER
1	D	269	MET
1	D	274	VAL
1	D	283	PRO
1	D	287	ARG
1	D	288	VAL
1	D	290	LYS
1	D	295	SER
1	D	296	GLU
1	D	299	TYR
1	D	300	SER
1	D	308	THR
1	D	317	TYR

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Mol	Chain	Res	Type
1	D	320	VAL
1	D	333	LEU
1	D	334	THR
1	D	338	GLN
1	D	350	ILE
1	D	355	VAL
1	D	361	ILE
1	D	365	MET
1	D	372	LEU
1	D	375	THR
1	D	386	ILE
1	D	387	LEU
1	D	389	ILE
1	D	392	ILE
1	D	415	THR
1	E	6	LYS
1	E	9	GLU
1	E	15	LYS
1	E	16	ILE
1	E	17	LEU
1	E	25	ILE
1	E	28	LEU
1	E	29	ILE
1	E	39	VAL
1	E	57	LEU
1	E	61	ILE
1	E	73	ILE
1	E	77	ARG
1	E	78	LEU
1	E	80	ARG
1	E	90	LEU
1	E	99	LEU
1	E	102	ILE
1	E	105	ARG
1	E	106	LEU
1	E	113	ILE
1	E	120	GLN
1	E	122	PHE
1	E	123	GLN
1	E	125	LYS
1	E	131	VAL
1	E	137	ILE

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Mol	Chain	Res	Type
1	E	140	THR
1	E	148	ASN
1	E	151	VAL
1	E	159	ILE
1	E	163	ILE
1	E	175	LYS
1	E	176	VAL
1	E	178	LYS
1	E	182	THR
1	E	197	ILE
1	E	207	ILE
1	E	213	ILE
1	E	232	THR
1	E	237	VAL
1	E	241	LEU
1	E	242	GLN
1	E	243	ILE
1	E	245	LEU
1	E	249	VAL
1	E	250	LEU
1	E	253	ILE
1	E	260	SER
1	E	264	HIS
1	E	274	VAL
1	E	287	ARG
1	E	288	VAL
1	E	290	LYS
1	E	295	SER
1	E	296	GLU
1	E	317	TYR
1	E	333	LEU
1	E	334	THR
1	E	338	GLN
1	E	344	THR
1	E	350	ILE
1	E	355	VAL
1	E	361	ILE
1	E	365	MET
1	E	372	LEU
1	E	375	THR
1	E	385	MET
1	E	386	ILE

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Mol	Chain	Res	Type
1	E	387	LEU
1	E	389	ILE
1	E	392	ILE
1	E	402	VAL
1	E	415	THR
1	F	6	LYS
1	F	9	GLU
1	F	13	LEU
1	F	15	LYS
1	F	16	ILE
1	F	17	LEU
1	F	28	LEU
1	F	29	ILE
1	F	61	ILE
1	F	62	VAL
1	F	73	ILE
1	F	74	SER
1	F	77	ARG
1	F	78	LEU
1	F	80	ARG
1	F	90	LEU
1	F	99	LEU
1	F	102	ILE
1	F	105	ARG
1	F	113	ILE
1	F	120	GLN
1	F	122	PHE
1	F	123	GLN
1	F	125	LYS
1	F	126	GLN
1	F	130	LEU
1	F	131	VAL
1	F	135	LEU
1	F	137	ILE
1	F	140	THR
1	F	148	ASN
1	F	151	VAL
1	F	155	ILE
1	F	163	ILE
1	F	166	THR
1	F	175	LYS
1	F	176	VAL

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Mol	Chain	Res	Type
1	F	182	THR
1	F	207	ILE
1	F	213	ILE
1	F	215	TYR
1	F	231	VAL
1	F	232	THR
1	F	237	VAL
1	F	241	LEU
1	F	242	GLN
1	F	245	LEU
1	F	249	VAL
1	F	253	ILE
1	F	260	SER
1	F	264	HIS
1	F	269	MET
1	F	274	VAL
1	F	283	PRO
1	F	288	VAL
1	F	290	LYS
1	F	295	SER
1	F	296	GLU
1	F	300	SER
1	F	305	LEU
1	F	308	THR
1	F	317	TYR
1	F	320	VAL
1	F	333	LEU
1	F	334	THR
1	F	335	VAL
1	F	338	GLN
1	F	350	ILE
1	F	355	VAL
1	F	361	ILE
1	F	365	MET
1	F	372	LEU
1	F	375	THR
1	F	385	MET
1	F	386	ILE
1	F	387	LEU
1	F	389	ILE
1	F	392	ILE
1	F	402	VAL

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Mol	Chain	Res	Type
1	F	415	THR

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	121	GLN
1	A	123	GLN
1	A	148	ASN
1	A	223	HIS
1	A	242	GLN
1	A	264	HIS
1	A	310	ASN
1	B	108	ASN
1	B	120	GLN
1	B	121	GLN
1	B	203	GLN
1	B	223	HIS
1	B	242	GLN
1	B	378	ASN
1	C	150	GLN
1	C	327	ASN
1	C	368	HIS
1	D	121	GLN
1	D	148	ASN
1	D	150	GLN
1	D	203	GLN
1	D	223	HIS
1	D	242	GLN
1	D	327	ASN
1	D	368	HIS
1	E	121	GLN
1	E	123	GLN
1	E	223	HIS
1	E	242	GLN
1	E	264	HIS
1	E	310	ASN
1	F	108	ASN
1	F	120	GLN
1	F	121	GLN
1	F	148	ASN
1	F	203	GLN
1	F	223	HIS

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Mol	Chain	Res	Type
1	F	242	GLN
1	F	327	ASN
1	F	378	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	ASP	B	501	-	7,8,8	1.22	0	6,10,10	1.49	1 (16%)
2	ASP	E	501	-	7,8,8	1.29	1 (14%)	6,10,10	1.64	1 (16%)
2	ASP	D	501	-	7,8,8	1.24	0	6,10,10	1.54	1 (16%)
2	ASP	A	501	-	7,8,8	1.22	0	6,10,10	1.65	2 (33%)
2	ASP	F	501	-	7,8,8	1.33	0	6,10,10	1.41	1 (16%)
2	ASP	C	501	-	7,8,8	1.17	0	6,10,10	1.77	1 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ASP	B	501	-	-	4/8/8/8	-
2	ASP	E	501	-	-	4/8/8/8	-
2	ASP	D	501	-	-	4/8/8/8	-
2	ASP	A	501	-	-	4/8/8/8	-
2	ASP	F	501	-	-	4/8/8/8	-
2	ASP	C	501	-	-	4/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	ASP	OXT-C	-2.13	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	ASP	OXT-C-O	-3.90	115.22	124.08
2	D	501	ASP	OXT-C-O	-3.38	116.42	124.08
2	E	501	ASP	OXT-C-O	-3.16	116.91	124.08
2	F	501	ASP	OXT-C-O	-3.06	117.14	124.08
2	B	501	ASP	OXT-C-O	-3.00	117.28	124.08
2	A	501	ASP	OXT-C-O	-2.93	117.43	124.08
2	A	501	ASP	OD2-CG-CB	2.12	120.59	114.00

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	501	ASP	CA-CB-CG-OD1
2	D	501	ASP	CA-CB-CG-OD1
2	D	501	ASP	CA-CB-CG-OD2
2	D	501	ASP	C-CA-CB-CG
2	A	501	ASP	N-CA-CB-CG
2	B	501	ASP	N-CA-CB-CG
2	C	501	ASP	N-CA-CB-CG
2	D	501	ASP	N-CA-CB-CG
2	F	501	ASP	N-CA-CB-CG
2	A	501	ASP	CA-CB-CG-OD1
2	A	501	ASP	CA-CB-CG-OD2

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Mol	Chain	Res	Type	Atoms
2	B	501	ASP	CA-CB-CG-OD1
2	C	501	ASP	CA-CB-CG-OD2
2	F	501	ASP	CA-CB-CG-OD1
2	F	501	ASP	CA-CB-CG-OD2
2	B	501	ASP	CA-CB-CG-OD2
2	E	501	ASP	CA-CB-CG-OD2
2	A	501	ASP	C-CA-CB-CG
2	B	501	ASP	C-CA-CB-CG
2	C	501	ASP	C-CA-CB-CG
2	E	501	ASP	C-CA-CB-CG
2	F	501	ASP	C-CA-CB-CG
2	E	501	ASP	CA-CB-CG-OD1
2	E	501	ASP	N-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	ASP	1	0
2	E	501	ASP	2	0
2	D	501	ASP	1	0
2	A	501	ASP	1	0
2	F	501	ASP	1	0
2	C	501	ASP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	411/425 (96%)	-1.25	0 100 100	117, 165, 200, 226	0
1	B	411/425 (96%)	-1.24	0 100 100	108, 147, 181, 213	0
1	C	411/425 (96%)	-1.23	0 100 100	108, 147, 182, 215	0
1	D	411/425 (96%)	-1.25	0 100 100	111, 147, 182, 217	0
1	E	411/425 (96%)	-1.24	0 100 100	119, 165, 200, 224	0
1	F	411/425 (96%)	-1.24	0 100 100	105, 146, 182, 211	0
All	All	2466/2550 (96%)	-1.24	0 100 100	105, 153, 190, 226	0

There are no RSRZ outliers to report.

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ASP	C	501	9/9	0.97	0.13	122,127,130,136	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ASP	D	501	9/9	0.98	0.12	122,128,130,137	0
3	NA	A	502	1/1	0.98	0.07	124,124,124,124	0
3	NA	B	502	1/1	0.98	0.07	105,105,105,105	0
3	NA	C	503	1/1	0.98	0.15	137,137,137,137	0
3	NA	F	502	1/1	0.98	0.06	108,108,108,108	0
2	ASP	A	501	9/9	0.99	0.10	135,140,146,150	0
3	NA	A	503	1/1	0.99	0.08	155,155,155,155	0
2	ASP	B	501	9/9	0.99	0.05	124,127,131,132	0
3	NA	C	502	1/1	0.99	0.07	106,106,106,106	0
2	ASP	E	501	9/9	0.99	0.10	132,140,145,148	0
3	NA	D	503	1/1	0.99	0.12	132,132,132,132	0
3	NA	E	502	1/1	0.99	0.08	123,123,123,123	0
3	NA	E	503	1/1	0.99	0.12	155,155,155,155	0
2	ASP	F	501	9/9	0.99	0.07	125,127,130,132	0
3	NA	B	503	1/1	1.00	0.06	140,140,140,140	0
3	NA	D	502	1/1	1.00	0.03	106,106,106,106	0
3	NA	F	503	1/1	1.00	0.04	140,140,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.