



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 04:45 pm GMT

PDB ID : 3V8G
Title : Crystal structure of an asymmetric trimer of a glutamate transporter homologue (GltPh)
Authors : Verdon, G.; Boudker, O.
Deposited on : 2011-12-22
Resolution : 4.66 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

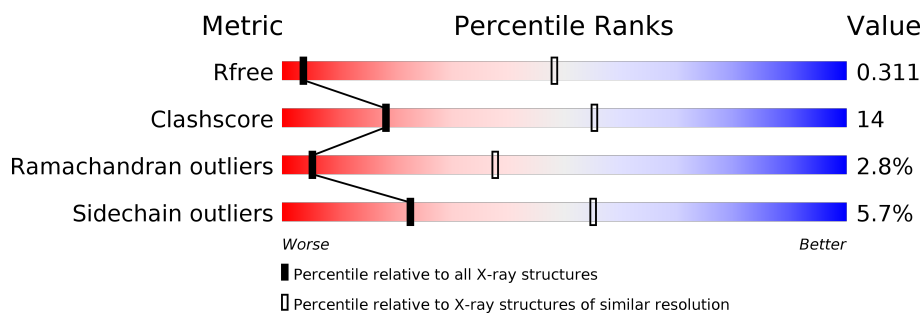
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.66 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}	111664	1090 (5.58-3.70)
Clashscore	122126	1019 (5.52-3.76)
Ramachandran outliers	120053	1104 (5.58-3.70)
Sidechain outliers	120020	1085 (5.58-3.70)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	422	68% 27% . .
1	B	422	67% 27% . .
1	C	422	52% 37% 6% 5%
1	D	422	68% 27% . .
1	E	422	68% 26% . 5%
1	F	422	52% 34% 7% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18038 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 sodium-coupled L-aspartate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3050	2007	492	533	18			
1	B	404	Total	C	N	O	S	0	0	0
			3001	1976	483	524	18			
1	C	400	Total	C	N	O	S	0	0	0
			2965	1955	475	518	17			
1	D	411	Total	C	N	O	S	0	0	0
			3050	2007	492	533	18			
1	E	403	Total	C	N	O	S	0	0	0
			2992	1971	481	522	18			
1	F	392	Total	C	N	O	S	0	0	0
			2914	1922	465	510	17			

There are 90 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	125	HIS	LYS	engineered mutation	UNP O59010
A	132	HIS	LYS	engineered mutation	UNP O59010
A	198	CYS	VAL	engineered mutation	UNP O59010
A	223	HIS	LYS	engineered mutation	UNP O59010
A	264	HIS	LYS	engineered mutation	UNP O59010
A	321	ALA	CYS	engineered mutation	UNP O59010
A	368	HIS	GLU	engineered mutation	UNP O59010
A	380	CYS	ALA	engineered mutation	UNP O59010
A	418	THR	-	EXPRESSION TAG	UNP O59010
A	419	LEU	-	EXPRESSION TAG	UNP O59010
A	420	VAL	-	EXPRESSION TAG	UNP O59010
A	421	PRO	-	EXPRESSION TAG	UNP O59010
A	422	ARG	-	EXPRESSION TAG	UNP O59010
B	37	HIS	ASP	engineered mutation	UNP O59010
B	40	HIS	LYS	engineered mutation	UNP O59010

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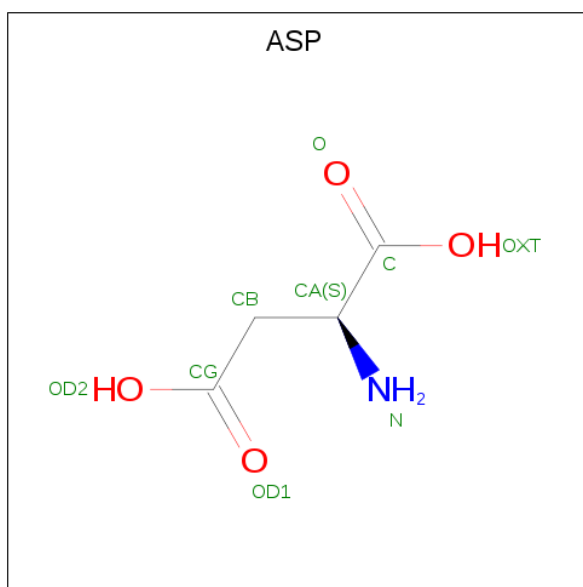
Chain	Residue	Modelled	Actual	Comment	Reference
B	125	HIS	LYS	engineered mutation	UNP O59010
B	132	HIS	LYS	engineered mutation	UNP O59010
B	198	CYS	VAL	engineered mutation	UNP O59010
B	223	HIS	LYS	engineered mutation	UNP O59010
B	264	HIS	LYS	engineered mutation	UNP O59010
B	321	ALA	CYS	engineered mutation	UNP O59010
B	368	HIS	GLU	engineered mutation	UNP O59010
B	380	CYS	ALA	engineered mutation	UNP O59010
B	418	THR	-	EXPRESSION TAG	UNP O59010
B	419	LEU	-	EXPRESSION TAG	UNP O59010
B	420	VAL	-	EXPRESSION TAG	UNP O59010
B	421	PRO	-	EXPRESSION TAG	UNP O59010
B	422	ARG	-	EXPRESSION TAG	UNP O59010
C	37	HIS	ASP	engineered mutation	UNP O59010
C	40	HIS	LYS	engineered mutation	UNP O59010
C	125	HIS	LYS	engineered mutation	UNP O59010
C	132	HIS	LYS	engineered mutation	UNP O59010
C	198	CYS	VAL	engineered mutation	UNP O59010
C	223	HIS	LYS	engineered mutation	UNP O59010
C	264	HIS	LYS	engineered mutation	UNP O59010
C	321	ALA	CYS	engineered mutation	UNP O59010
C	368	HIS	GLU	engineered mutation	UNP O59010
C	380	CYS	ALA	engineered mutation	UNP O59010
C	418	THR	-	EXPRESSION TAG	UNP O59010
C	419	LEU	-	EXPRESSION TAG	UNP O59010
C	420	VAL	-	EXPRESSION TAG	UNP O59010
C	421	PRO	-	EXPRESSION TAG	UNP O59010
C	422	ARG	-	EXPRESSION TAG	UNP O59010
D	37	HIS	ASP	engineered mutation	UNP O59010
D	40	HIS	LYS	engineered mutation	UNP O59010
D	125	HIS	LYS	engineered mutation	UNP O59010
D	132	HIS	LYS	engineered mutation	UNP O59010
D	198	CYS	VAL	engineered mutation	UNP O59010
D	223	HIS	LYS	engineered mutation	UNP O59010
D	264	HIS	LYS	engineered mutation	UNP O59010
D	321	ALA	CYS	engineered mutation	UNP O59010
D	368	HIS	GLU	engineered mutation	UNP O59010
D	380	CYS	ALA	engineered mutation	UNP O59010
D	418	THR	-	EXPRESSION TAG	UNP O59010
D	419	LEU	-	EXPRESSION TAG	UNP O59010
D	420	VAL	-	EXPRESSION TAG	UNP O59010
D	421	PRO	-	EXPRESSION TAG	UNP O59010

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Chain	Residue	Modelled	Actual	Comment	Reference
D	422	ARG	-	EXPRESSION TAG	UNP O59010
E	37	HIS	ASP	engineered mutation	UNP O59010
E	40	HIS	LYS	engineered mutation	UNP O59010
E	125	HIS	LYS	engineered mutation	UNP O59010
E	132	HIS	LYS	engineered mutation	UNP O59010
E	198	CYS	VAL	engineered mutation	UNP O59010
E	223	HIS	LYS	engineered mutation	UNP O59010
E	264	HIS	LYS	engineered mutation	UNP O59010
E	321	ALA	CYS	engineered mutation	UNP O59010
E	368	HIS	GLU	engineered mutation	UNP O59010
E	380	CYS	ALA	engineered mutation	UNP O59010
E	418	THR	-	EXPRESSION TAG	UNP O59010
E	419	LEU	-	EXPRESSION TAG	UNP O59010
E	420	VAL	-	EXPRESSION TAG	UNP O59010
E	421	PRO	-	EXPRESSION TAG	UNP O59010
E	422	ARG	-	EXPRESSION TAG	UNP O59010
F	37	HIS	ASP	engineered mutation	UNP O59010
F	40	HIS	LYS	engineered mutation	UNP O59010
F	125	HIS	LYS	engineered mutation	UNP O59010
F	132	HIS	LYS	engineered mutation	UNP O59010
F	198	CYS	VAL	engineered mutation	UNP O59010
F	223	HIS	LYS	engineered mutation	UNP O59010
F	264	HIS	LYS	engineered mutation	UNP O59010
F	321	ALA	CYS	engineered mutation	UNP O59010
F	368	HIS	GLU	engineered mutation	UNP O59010
F	380	CYS	ALA	engineered mutation	UNP O59010
F	418	THR	-	EXPRESSION TAG	UNP O59010
F	419	LEU	-	EXPRESSION TAG	UNP O59010
F	420	VAL	-	EXPRESSION TAG	UNP O59010
F	421	PRO	-	EXPRESSION TAG	UNP O59010
F	422	ARG	-	EXPRESSION TAG	UNP O59010

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: C₄H₇NO₄).



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

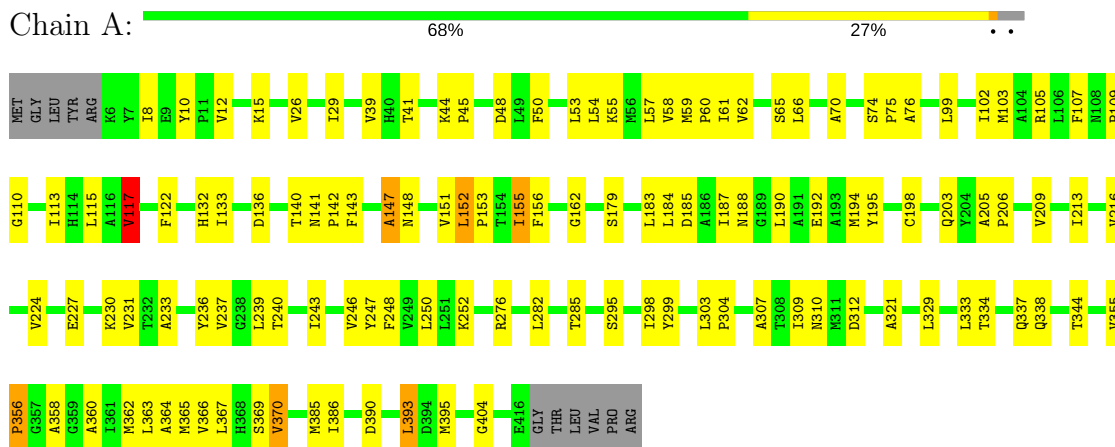
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

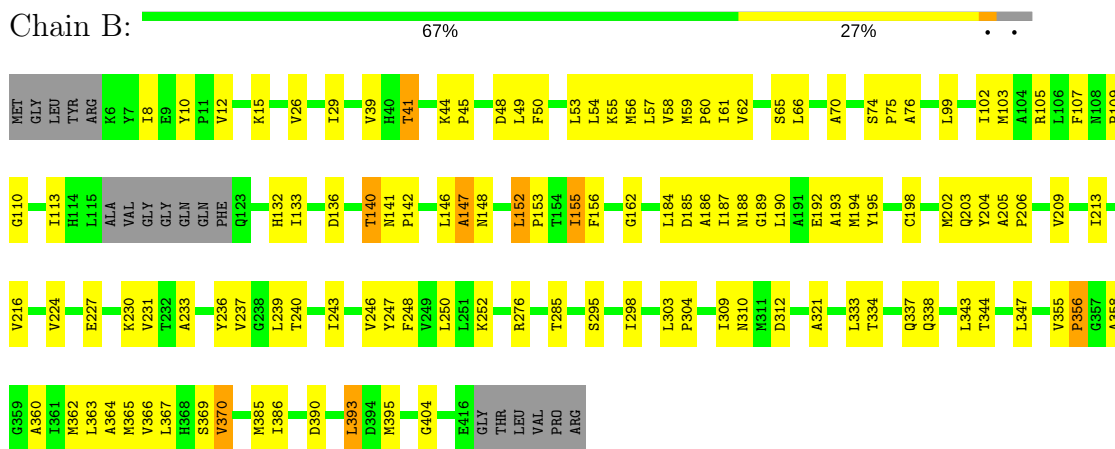
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

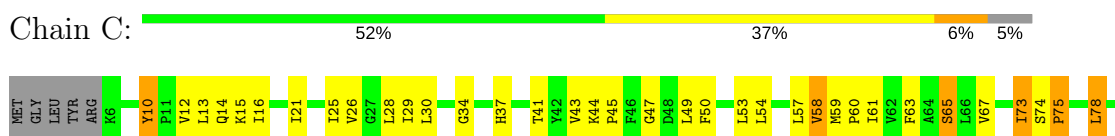
- Molecule 1: sodium-coupled L-aspartate transporter

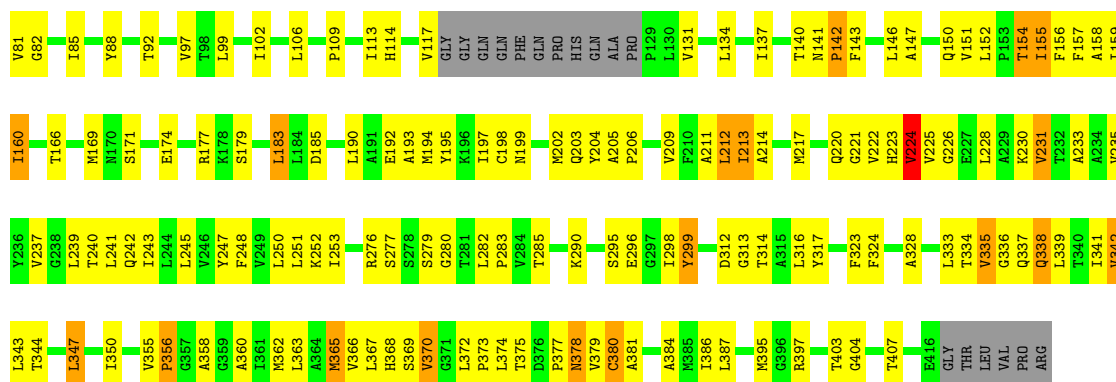


- Molecule 1: sodium-coupled L-aspartate transporter

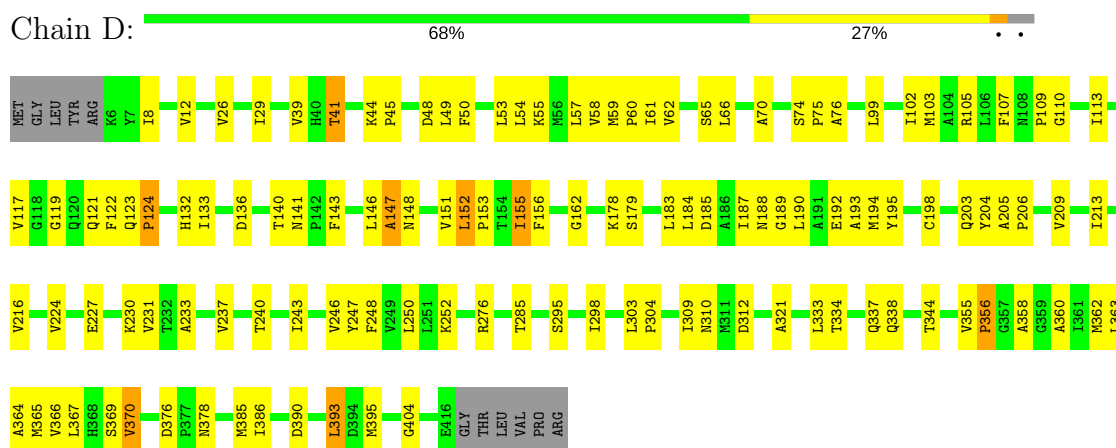


- Molecule 1: sodium-coupled L-aspartate transporter

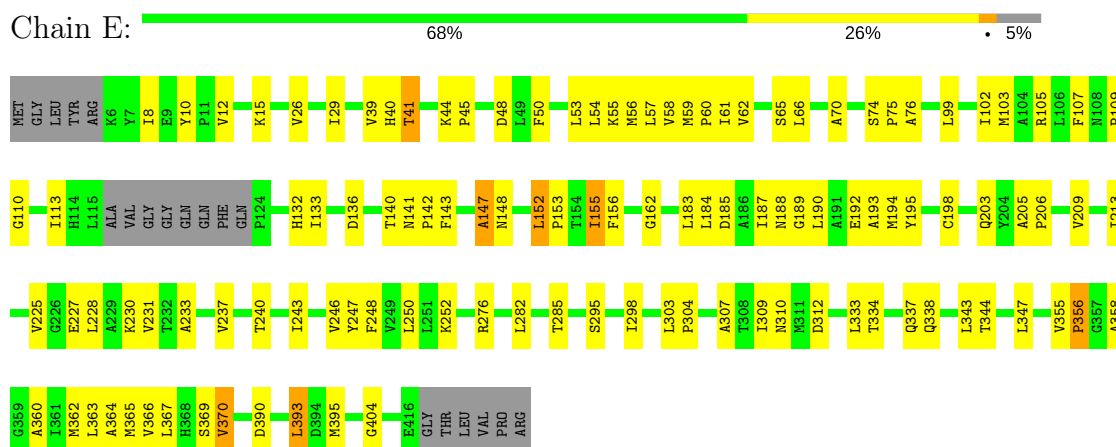




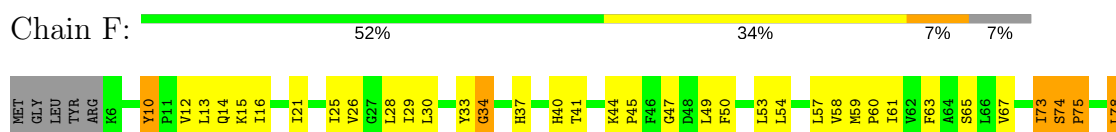
• Molecule 1: sodium-coupled L-aspartate transporter



• Molecule 1: sodium-coupled L-aspartate transporter



• Molecule 1: sodium-coupled L-aspartate transporter



V355	P356	G357	A358	G359	A360	I361	M362	L363	A364	M365	V366	L367	H368	S369	V370	G371	L372	M378	V379	C380	A381		A384	M385	I386	L387	D390	D394	M395	G396	R397	T403	G404	T407	E416	GLY	THR	LEU	VAL	PRO	ARG								
G238	L239	T240	L241	Q242	I243	L244	L245	V246	Y247	F248	V249	L250	L251	K252	L253	R276	S277	S278	S279	G280	T281	L282	P283	K290	S295	E296	G297	L298	T299	D312	G313	T314	A315	L316	Y317	F323	F324	T334	V335	G336	Q337	Q338	L339	T340	V342	L343	T344	L347	I350
F157	A158	I159	I160	T166	M169	N170	S171	E174	R177	L183	L184	D185	L190	A191	E192	A193	M194	Y195	K196	I197	C198	N199	M202	Q203	Y204	A205	P206	V209	L212	I213	A214	Y215	V216	M217	Q220	G221	V222	H223	V224	V225	G226	K230	V231	T232	A233	A234	V237		
V81	G82	I85	Y88	T92	V97	T98	L99	I102	L106	F107	N108	P109	GLY	ALA	GLY	ILE	HIS	LEU	ALA	VAL	GLY	GLY	GLN	GLN	PHE	GLN	PRO	HIS	GLN	ALA	PRO	P129	L130	V131	L134	I137	T140	N141	P142	L146	A147	Q150	V151	T154	I155	F156			

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.69Å 119.63Å 223.41Å 90.00° 113.77° 90.00°	Depositor
Resolution (Å)	15.00 – 4.66 68.15 – 4.66	Depositor EDS
% Data completeness (in resolution range)	73.1 (15.00-4.66) 66.2 (68.15-4.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 4.65Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.255 , 0.294 0.291 , 0.311	Depositor DCC
R_{free} test set	1029 reflections (5.29%)	wwPDB-VP
Wilson B-factor (Å ²)	255.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 436.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	18038	wwPDB-VP
Average B, all atoms (Å ²)	283.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.37	0/3110	0.54	0/4241
1	B	0.37	0/3059	0.53	0/4171
1	C	0.41	0/3020	0.61	0/4116
1	D	0.37	0/3110	0.53	0/4241
1	E	0.37	0/3050	0.53	0/4158
1	F	0.40	0/2968	0.60	0/4045
All	All	0.38	0/18317	0.56	0/24972

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	C	0	2
1	F	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	223	HIS	Peptide
1	C	224	VAL	Peptide
1	F	223	HIS	Peptide
1	F	224	VAL	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	3050	0	3223	81	0
1	B	3001	0	3177	79	0
1	C	2965	0	3147	129	0
1	D	3050	0	3223	82	0
1	E	2992	0	3170	74	0
1	F	2914	0	3093	121	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
2	C	9	0	3	0	0
2	D	9	0	3	0	0
2	E	9	0	3	0	0
2	F	9	0	3	0	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
All	All	18038	0	19051	532	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 14.

All (532) 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:D:243:ILE:HA	1:D:247:TYR:HD2	1.30	0.96
1:E:243:ILE:HA	1:E:247:TYR:HD2	1.30	0.95
1:B:243:ILE:HA	1:B:247:TYR:HD2	1.29	0.95
1:A:243:ILE:HA	1:A:247:TYR:HD2	1.31	0.92
1:C:134:LEU:O	1:C:137:ILE:HG12	1.71	0.90
1:F:192:GLU:HA	1:F:195:TYR:HD2	1.38	0.88
1:C:59:MET:HB2	1:C:60:PRO:HD3	1.58	0.84
1:F:134:LEU:O	1:F:137:ILE:HG12	1.76	0.84
1:F:59:MET:HB2	1:F:60:PRO:HD3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:HA	1:C:195:TYR:HD2	1.45	0.80
1:F:59:MET:HB2	1:F:60:PRO:CD	2.12	0.79
1:F:192:GLU:HA	1:F:195:TYR:CD2	2.18	0.79
1:C:198:CYS:O	1:C:202:MET:HG2	1.84	0.78
1:C:113:ILE:HA	1:F:40:HIS:CE1	2.18	0.78
1:D:243:ILE:HA	1:D:247:TYR:CD2	2.19	0.76
1:D:152:LEU:H	1:D:152:LEU:HD12	1.50	0.76
1:C:59:MET:HB2	1:C:60:PRO:CD	2.15	0.76
1:B:152:LEU:HD12	1:B:152:LEU:H	1.51	0.75
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.18	0.75
1:D:121:GLN:HG3	1:D:378:ASN:ND2	2.02	0.75
1:A:152:LEU:HD12	1:A:152:LEU:H	1.51	0.75
1:C:113:ILE:HA	1:F:40:HIS:HE1	1.50	0.75
1:E:243:ILE:HA	1:E:247:TYR:CD2	2.18	0.75
1:C:282:LEU:H	1:C:283:PRO:CD	2.01	0.74
1:F:334:THR:H	1:F:337:GLN:HE21	1.35	0.74
1:F:198:CYS:O	1:F:202:MET:HG2	1.87	0.73
1:E:152:LEU:HD12	1:E:152:LEU:H	1.54	0.73
1:A:243:ILE:HA	1:A:247:TYR:CD2	2.21	0.72
1:F:282:LEU:H	1:F:283:PRO:CD	2.02	0.72
1:C:334:THR:H	1:C:337:GLN:HE21	1.37	0.71
1:C:192:GLU:HA	1:C:195:TYR:CD2	2.26	0.71
1:C:290:LYS:HE3	1:C:299:TYR:OH	1.91	0.71
1:A:122:PHE:HD2	1:A:329:LEU:CD2	2.04	0.71
1:F:379:VAL:O	1:F:381:ALA:N	2.21	0.70
1:C:109:PRO:HB2	1:C:324:PHE:HD1	1.57	0.70
1:F:109:PRO:HB2	1:F:324:PHE:HD1	1.57	0.69
1:F:363:LEU:O	1:F:366:VAL:HG12	1.92	0.69
1:D:344:THR:HB	1:D:366:VAL:HG23	1.75	0.69
1:C:282:LEU:N	1:C:283:PRO:CD	2.56	0.69
1:B:147:ALA:O	1:C:141:ASN:ND2	2.25	0.69
1:A:233:ALA:O	1:A:237:VAL:HG22	1.93	0.68
1:D:233:ALA:O	1:D:237:VAL:HG22	1.93	0.68
1:D:369:SER:O	1:D:370:VAL:HB	1.93	0.68
1:F:282:LEU:N	1:F:283:PRO:CD	2.57	0.68
1:F:290:LYS:HE3	1:F:299:TYR:OH	1.93	0.68
1:B:233:ALA:O	1:B:237:VAL:HG22	1.93	0.67
1:A:369:SER:O	1:A:370:VAL:HB	1.94	0.67
1:A:59:MET:HG3	1:B:141:ASN:ND2	2.09	0.67
1:E:233:ALA:O	1:E:237:VAL:HG22	1.93	0.67
1:E:344:THR:HB	1:E:366:VAL:HG23	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:THR:HB	1:A:366:VAL:HG23	1.75	0.67
1:D:190:LEU:N	1:E:183:LEU:CD1	2.59	0.66
1:E:369:SER:O	1:E:370:VAL:HB	1.96	0.66
1:C:114:HIS:HA	1:C:328:ALA:O	1.95	0.66
1:D:122:PHE:HB2	1:D:376:ASP:OD1	1.95	0.65
1:D:334:THR:O	1:D:337:GLN:HG2	1.96	0.65
1:D:59:MET:HG3	1:E:141:ASN:ND2	2.10	0.65
1:B:344:THR:HB	1:B:366:VAL:HG23	1.78	0.65
1:F:360:ALA:O	1:F:363:LEU:HB3	1.97	0.65
1:B:369:SER:O	1:B:370:VAL:HB	1.96	0.64
1:C:360:ALA:O	1:C:363:LEU:HB3	1.97	0.64
1:C:209:VAL:O	1:C:213:ILE:HG13	1.98	0.64
1:C:363:LEU:O	1:C:366:VAL:HG12	1.98	0.64
1:C:224:VAL:H	1:C:228:LEU:HD12	1.62	0.64
1:C:335:VAL:HA	1:C:338:GLN:HB2	1.79	0.63
1:F:335:VAL:HA	1:F:338:GLN:HB2	1.80	0.63
1:D:62:VAL:O	1:D:66:LEU:HG	1.99	0.63
1:D:55:LYS:O	1:D:58:VAL:HG12	1.99	0.63
1:E:152:LEU:HB2	1:E:153:PRO:HD3	1.81	0.63
1:F:61:ILE:HD11	1:F:279:SER:HB2	1.80	0.63
1:C:169:MET:O	1:C:177:ARG:HG2	1.99	0.63
1:F:109:PRO:HB3	1:F:230:LYS:HB3	1.80	0.62
1:C:324:PHE:CD2	1:C:386:ILE:HD11	2.34	0.62
1:C:109:PRO:HB3	1:C:230:LYS:HB3	1.81	0.62
1:B:334:THR:O	1:B:337:GLN:HG2	1.99	0.62
1:B:152:LEU:HB2	1:B:153:PRO:HD3	1.81	0.62
1:F:276:ARG:HD3	1:F:395:MET:HG2	1.82	0.62
1:F:169:MET:O	1:F:177:ARG:HG2	2.00	0.62
1:F:44:LYS:N	1:F:45:PRO:HD2	2.14	0.62
1:C:61:ILE:HG22	1:C:194:MET:HB3	1.79	0.62
1:E:192:GLU:HA	1:E:195:TYR:CD2	2.35	0.62
1:F:166:THR:O	1:F:169:MET:HB2	2.00	0.61
1:A:61:ILE:HG13	1:A:62:VAL:N	2.16	0.61
1:A:334:THR:O	1:A:337:GLN:HG2	2.01	0.61
1:A:62:VAL:O	1:A:66:LEU:HG	2.00	0.61
1:C:166:THR:O	1:C:169:MET:HB2	2.00	0.61
1:E:61:ILE:HG13	1:E:62:VAL:N	2.15	0.61
1:D:61:ILE:HG13	1:D:62:VAL:N	2.15	0.61
1:F:209:VAL:O	1:F:213:ILE:HG13	2.00	0.61
1:C:339:LEU:O	1:C:342:VAL:HG12	2.00	0.61
1:E:55:LYS:O	1:E:58:VAL:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:THR:O	1:E:337:GLN:HG2	2.01	0.61
1:C:369:SER:O	1:C:370:VAL:HB	2.00	0.60
1:D:141:ASN:ND2	1:F:147:ALA:O	2.33	0.60
1:A:152:LEU:HB2	1:A:153:PRO:HD3	1.84	0.60
1:D:99:LEU:HA	1:D:102:ILE:HD12	1.83	0.60
1:C:344:THR:HB	1:C:366:VAL:HG23	1.82	0.60
1:D:192:GLU:HA	1:D:195:TYR:CD2	2.36	0.60
1:A:192:GLU:HA	1:A:195:TYR:CD2	2.37	0.60
1:C:226:GLY:O	1:C:230:LYS:N	2.34	0.60
1:C:276:ARG:HD3	1:C:395:MET:HG2	1.84	0.60
1:F:324:PHE:CD2	1:F:386:ILE:HD11	2.36	0.60
1:A:122:PHE:HD2	1:A:329:LEU:HD23	1.67	0.60
1:C:61:ILE:HD11	1:C:279:SER:HB2	1.82	0.60
1:F:344:THR:HB	1:F:366:VAL:HG23	1.83	0.60
1:B:55:LYS:O	1:B:58:VAL:HG12	2.02	0.59
1:C:338:GLN:HA	1:C:341:ILE:HD12	1.84	0.59
1:E:62:VAL:O	1:E:66:LEU:HG	2.02	0.59
1:B:192:GLU:HA	1:B:195:TYR:CD2	2.36	0.59
1:B:62:VAL:O	1:B:66:LEU:HG	2.01	0.59
1:D:152:LEU:HB2	1:D:153:PRO:HD3	1.84	0.59
1:C:44:LYS:N	1:C:45:PRO:HD2	2.17	0.59
1:A:55:LYS:O	1:A:58:VAL:HG12	2.02	0.58
1:F:358:ALA:O	1:F:362:MET:HG2	2.03	0.58
1:F:369:SER:O	1:F:370:VAL:HB	2.04	0.58
1:B:99:LEU:HA	1:B:102:ILE:HD12	1.85	0.58
1:A:103:MET:HE2	1:A:237:VAL:HG23	1.85	0.58
1:B:61:ILE:HG13	1:B:62:VAL:N	2.19	0.58
1:B:44:LYS:N	1:B:45:PRO:HD2	2.19	0.58
1:E:99:LEU:HA	1:E:102:ILE:HD12	1.85	0.58
1:F:10:TYR:HB2	1:F:15:LYS:HD3	1.85	0.58
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.86	0.58
1:D:179:SER:HA	1:F:185:ASP:OD1	2.04	0.57
1:F:226:GLY:O	1:F:230:LYS:N	2.37	0.57
1:C:159:ILE:HG22	1:C:160:ILE:N	2.19	0.57
1:E:195:TYR:HA	1:E:198:CYS:SG	2.44	0.57
1:E:227:GLU:O	1:E:231:VAL:HG23	2.04	0.57
1:F:61:ILE:HG22	1:F:194:MET:HB3	1.85	0.57
1:A:183:LEU:CD1	1:C:190:LEU:N	2.68	0.57
1:A:99:LEU:HA	1:A:102:ILE:HD12	1.86	0.57
1:C:150:GLN:O	1:C:154:THR:OG1	2.22	0.57
1:D:53:LEU:O	1:D:57:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:N	1:D:45:PRO:HD2	2.19	0.57
1:A:44:LYS:N	1:A:45:PRO:HD2	2.20	0.57
1:E:103:MET:CE	1:E:237:VAL:HG23	2.35	0.57
1:F:250:LEU:HA	1:F:253:ILE:HG22	1.87	0.56
1:A:141:ASN:ND2	1:C:147:ALA:O	2.38	0.56
1:E:44:LYS:N	1:E:45:PRO:HD2	2.20	0.56
1:B:190:LEU:O	1:B:194:MET:HG2	2.06	0.56
1:C:379:VAL:O	1:C:381:ALA:N	2.25	0.56
1:C:379:VAL:C	1:C:381:ALA:H	2.08	0.56
1:D:190:LEU:O	1:D:194:MET:HG2	2.05	0.56
1:F:339:LEU:O	1:F:342:VAL:HG12	2.05	0.56
1:F:384:ALA:HA	1:F:387:LEU:HB3	1.88	0.56
1:A:122:PHE:HD2	1:A:329:LEU:HD21	1.69	0.56
1:A:103:MET:CE	1:A:237:VAL:HG23	2.36	0.56
1:A:227:GLU:O	1:A:231:VAL:HG23	2.06	0.56
1:C:47:GLY:O	1:C:50:PHE:HB3	2.06	0.56
1:B:184:LEU:HA	1:B:187:ILE:HD12	1.88	0.56
1:B:227:GLU:O	1:B:231:VAL:HG23	2.06	0.55
1:C:282:LEU:H	1:C:283:PRO:HD2	1.70	0.55
1:B:195:TYR:HA	1:B:198:CYS:SG	2.46	0.55
1:C:282:LEU:N	1:C:283:PRO:HD2	2.22	0.55
1:F:67:VAL:HG22	1:F:158:ALA:HB1	1.87	0.55
1:A:190:LEU:O	1:A:194:MET:HG2	2.06	0.55
1:B:53:LEU:O	1:B:57:LEU:HG	2.06	0.55
1:F:338:GLN:HA	1:F:341:ILE:HD12	1.88	0.55
1:C:67:VAL:HG22	1:C:158:ALA:HB1	1.87	0.55
1:F:282:LEU:N	1:F:283:PRO:HD2	2.22	0.55
1:F:97:VAL:HG21	1:F:342:VAL:HA	1.89	0.55
1:D:103:MET:CE	1:D:237:VAL:HG23	2.37	0.55
1:F:282:LEU:H	1:F:283:PRO:HD2	1.71	0.55
1:D:103:MET:HE2	1:D:237:VAL:HG23	1.90	0.54
1:F:379:VAL:C	1:F:381:ALA:H	2.07	0.54
1:A:184:LEU:HA	1:A:187:ILE:HD12	1.90	0.54
1:C:248:PHE:HA	1:C:251:LEU:HD12	1.90	0.54
1:E:53:LEU:O	1:E:57:LEU:HG	2.08	0.53
1:A:360:ALA:O	1:A:363:LEU:HB3	2.08	0.53
1:B:132:HIS:O	1:B:136:ASP:N	2.39	0.53
1:A:155:ILE:HG22	1:A:156:PHE:N	2.23	0.53
1:A:53:LEU:O	1:A:57:LEU:HG	2.07	0.53
1:C:377:PRO:HG3	1:F:361:ILE:HG12	1.91	0.53
1:E:360:ALA:O	1:E:363:LEU:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:PHE:HA	1:F:251:LEU:HD12	1.91	0.53
1:C:10:TYR:HB2	1:C:15:LYS:HD3	1.91	0.53
1:E:190:LEU:O	1:E:194:MET:HG2	2.08	0.53
1:C:75:PRO:HG3	1:C:78:LEU:HD23	1.91	0.53
1:F:150:GLN:O	1:F:154:THR:OG1	2.27	0.53
1:B:103:MET:CE	1:B:237:VAL:HG23	2.39	0.53
1:E:61:ILE:HG13	1:E:62:VAL:H	1.73	0.53
1:F:29:ILE:HG13	1:F:30:LEU:N	2.24	0.52
1:D:146:LEU:HD11	1:E:143:PHE:CE1	2.45	0.52
1:D:227:GLU:O	1:D:231:VAL:HG23	2.10	0.52
1:F:54:LEU:HD23	1:F:277:SER:HB2	1.92	0.52
1:A:26:VAL:HA	1:A:29:ILE:HG12	1.91	0.52
1:D:26:VAL:HA	1:D:29:ILE:HG12	1.92	0.52
1:F:47:GLY:O	1:F:50:PHE:HB3	2.10	0.52
1:C:151:VAL:O	1:C:154:THR:OG1	2.28	0.52
1:D:209:VAL:O	1:D:213:ILE:HG13	2.10	0.52
1:D:61:ILE:HG13	1:D:62:VAL:H	1.73	0.52
1:F:159:ILE:HG22	1:F:160:ILE:N	2.25	0.51
1:F:75:PRO:HG3	1:F:78:LEU:HD23	1.92	0.51
1:C:199:ASN:HA	1:C:202:MET:HG2	1.91	0.51
1:F:290:LYS:HE3	1:F:299:TYR:HH	1.74	0.51
1:B:133:ILE:HA	1:B:136:ASP:HB2	1.90	0.51
1:E:155:ILE:HG22	1:E:156:PHE:N	2.26	0.51
1:D:360:ALA:O	1:D:363:LEU:HB3	2.10	0.51
1:D:50:PHE:O	1:D:54:LEU:HD12	2.11	0.51
1:C:205:ALA:N	1:C:206:PRO:HD2	2.26	0.51
1:C:224:VAL:N	1:C:228:LEU:HD12	2.26	0.51
1:D:184:LEU:HA	1:D:187:ILE:HD12	1.92	0.51
1:B:58:VAL:HG13	1:B:59:MET:N	2.26	0.51
1:D:133:ILE:HA	1:D:136:ASP:HB2	1.93	0.51
1:B:246:VAL:O	1:B:250:LEU:HG	2.11	0.51
1:D:190:LEU:CA	1:E:183:LEU:HD11	2.40	0.51
1:F:205:ALA:N	1:F:206:PRO:HD2	2.26	0.51
1:A:246:VAL:O	1:A:250:LEU:HG	2.11	0.51
1:D:155:ILE:HG22	1:D:156:PHE:N	2.25	0.51
1:C:61:ILE:CG2	1:C:194:MET:HB3	2.41	0.51
1:B:390:ASP:HA	1:B:393:LEU:HD12	1.93	0.50
1:C:82:GLY:HA2	1:C:85:ILE:HG22	1.92	0.50
1:D:147:ALA:O	1:E:141:ASN:ND2	2.44	0.50
1:C:29:ILE:HG13	1:C:30:LEU:N	2.26	0.50
1:D:132:HIS:O	1:D:136:ASP:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:GLY:HA2	1:F:85:ILE:HG22	1.93	0.50
1:F:313:GLY:C	1:F:397:ARG:HG3	2.31	0.50
1:A:133:ILE:HA	1:A:136:ASP:HB2	1.94	0.50
1:B:360:ALA:O	1:B:363:LEU:HB3	2.12	0.50
1:A:132:HIS:O	1:A:136:ASP:N	2.42	0.50
1:C:380:CYS:CB	1:F:380:CYS:CB	2.89	0.50
1:D:190:LEU:N	1:E:183:LEU:HD11	2.26	0.50
1:D:246:VAL:O	1:D:250:LEU:HG	2.12	0.50
1:E:26:VAL:HA	1:E:29:ILE:HG12	1.92	0.50
1:E:56:MET:HA	1:F:140:THR:O	2.11	0.50
1:F:75:PRO:HA	1:F:78:LEU:N	2.27	0.50
1:E:390:ASP:HA	1:E:393:LEU:HD12	1.93	0.50
1:C:384:ALA:HA	1:C:387:LEU:HB3	1.93	0.50
1:E:184:LEU:HA	1:E:187:ILE:HD12	1.93	0.50
1:F:199:ASN:HA	1:F:202:MET:HG2	1.93	0.50
1:A:61:ILE:HG13	1:A:62:VAL:H	1.76	0.50
1:D:205:ALA:N	1:D:206:PRO:HD2	2.26	0.50
1:D:333:LEU:HA	1:D:337:GLN:NE2	2.27	0.50
1:D:58:VAL:HG13	1:D:59:MET:N	2.27	0.50
1:E:133:ILE:HA	1:E:136:ASP:HB2	1.94	0.50
1:B:26:VAL:HA	1:B:29:ILE:HG12	1.93	0.49
1:E:58:VAL:HG13	1:E:59:MET:N	2.27	0.49
1:A:205:ALA:N	1:A:206:PRO:HD2	2.27	0.49
1:D:105:ARG:HH21	1:D:338:GLN:HE22	1.61	0.49
1:D:247:TYR:CE1	1:D:404:GLY:HA2	2.47	0.49
1:E:246:VAL:O	1:E:250:LEU:HG	2.12	0.49
1:A:58:VAL:HG13	1:A:59:MET:N	2.28	0.49
1:D:183:LEU:CD1	1:F:190:LEU:N	2.75	0.49
1:D:195:TYR:HA	1:D:198:CYS:SG	2.51	0.49
1:A:247:TYR:CE1	1:A:404:GLY:HA2	2.48	0.49
1:C:13:LEU:HD22	1:C:14:GLN:NE2	2.28	0.49
1:C:97:VAL:HG21	1:C:342:VAL:HA	1.95	0.49
1:C:358:ALA:O	1:C:362:MET:HG2	2.13	0.49
1:D:189:GLY:O	1:D:193:ALA:N	2.24	0.49
1:E:50:PHE:O	1:E:54:LEU:HD12	2.13	0.49
1:A:362:MET:O	1:A:365:MET:HB3	2.13	0.49
1:E:247:TYR:CE1	1:E:404:GLY:HA2	2.48	0.49
1:F:344:THR:HA	1:F:347:LEU:HD22	1.95	0.49
1:A:61:ILE:O	1:A:65:SER:HB3	2.13	0.49
1:B:103:MET:HE2	1:B:237:VAL:HG23	1.93	0.49
1:B:56:MET:HE2	1:C:157:PHE:HD1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:MET:HE2	1:E:237:VAL:HG23	1.94	0.49
1:A:50:PHE:O	1:A:54:LEU:HD12	2.12	0.49
1:B:205:ALA:N	1:B:206:PRO:HD2	2.28	0.49
1:C:75:PRO:HA	1:C:78:LEU:N	2.28	0.48
1:E:132:HIS:O	1:E:136:ASP:N	2.42	0.48
1:E:205:ALA:N	1:E:206:PRO:HD2	2.28	0.48
1:F:347:LEU:HA	1:F:350:ILE:HD12	1.95	0.48
1:B:50:PHE:O	1:B:54:LEU:HD12	2.13	0.48
1:B:59:MET:HB2	1:B:60:PRO:HD3	1.96	0.48
1:E:147:ALA:O	1:F:141:ASN:ND2	2.47	0.48
1:B:209:VAL:O	1:B:213:ILE:HG13	2.13	0.48
1:C:347:LEU:HA	1:C:350:ILE:HD12	1.95	0.48
1:E:189:GLY:O	1:E:193:ALA:N	2.27	0.48
1:F:26:VAL:HA	1:F:29:ILE:HG12	1.96	0.48
1:F:365:MET:HA	1:F:368:HIS:HB2	1.96	0.48
1:A:122:PHE:CD2	1:A:329:LEU:HD21	2.48	0.48
1:B:309:ILE:HG22	1:B:310:ASN:N	2.29	0.48
1:A:183:LEU:HD11	1:C:190:LEU:N	2.29	0.48
1:A:390:ASP:HA	1:A:393:LEU:HD12	1.96	0.48
1:B:61:ILE:HG13	1:B:62:VAL:H	1.79	0.48
1:C:344:THR:HA	1:C:347:LEU:HD22	1.95	0.48
1:E:309:ILE:HG22	1:E:310:ASN:N	2.29	0.48
1:A:115:LEU:HD12	1:A:117:VAL:HG13	1.96	0.47
1:A:105:ARG:HH21	1:A:338:GLN:HE22	1.62	0.47
1:B:110:GLY:O	1:B:113:ILE:HG22	2.14	0.47
1:F:102:ILE:O	1:F:106:LEU:HG	2.14	0.47
1:C:102:ILE:O	1:C:106:LEU:HG	2.14	0.47
1:B:187:ILE:O	1:B:190:LEU:HB3	2.14	0.47
1:D:390:ASP:HA	1:D:393:LEU:HD12	1.95	0.47
1:E:209:VAL:O	1:E:213:ILE:HG13	2.15	0.47
1:B:147:ALA:HA	1:C:143:PHE:HB3	1.96	0.47
1:D:309:ILE:HG22	1:D:310:ASN:N	2.30	0.47
1:B:155:ILE:HG22	1:B:156:PHE:N	2.29	0.47
1:B:333:LEU:HA	1:B:337:GLN:NE2	2.29	0.47
1:A:333:LEU:HA	1:A:337:GLN:NE2	2.29	0.47
1:B:247:TYR:CE1	1:B:404:GLY:HA2	2.49	0.47
1:C:240:THR:HA	1:C:243:ILE:HD12	1.96	0.47
1:C:299:TYR:CD2	1:C:299:TYR:C	2.87	0.47
1:F:13:LEU:HD22	1:F:14:GLN:NE2	2.30	0.47
1:C:295:SER:HB3	1:C:298:ILE:HD13	1.96	0.47
1:B:295:SER:HB3	1:B:298:ILE:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ILE:O	1:D:65:SER:HB3	2.15	0.47
1:F:50:PHE:HB2	1:F:204:TYR:HE2	1.79	0.47
1:C:363:LEU:O	1:C:367:LEU:HG	2.14	0.47
1:E:295:SER:HB3	1:E:298:ILE:HD13	1.96	0.47
1:F:378:ASN:OD1	1:F:378:ASN:N	2.43	0.47
1:A:309:ILE:HG22	1:A:310:ASN:N	2.30	0.47
1:B:107:PHE:O	1:B:109:PRO:HD3	2.15	0.47
1:B:362:MET:O	1:B:365:MET:HB3	2.14	0.47
1:C:54:LEU:HD23	1:C:277:SER:HB2	1.96	0.47
1:E:333:LEU:HA	1:E:337:GLN:NE2	2.30	0.47
1:E:39:VAL:C	1:E:41:THR:H	2.18	0.47
1:F:61:ILE:CG2	1:F:194:MET:HB3	2.45	0.47
1:F:194:MET:HA	1:F:197:ILE:HD12	1.97	0.46
1:F:198:CYS:SG	1:F:280:GLY:O	2.74	0.46
1:F:295:SER:HB3	1:F:298:ILE:HD13	1.97	0.46
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.50	0.46
1:A:209:VAL:O	1:A:213:ILE:HG13	2.15	0.46
1:C:26:VAL:HA	1:C:29:ILE:HG12	1.96	0.46
1:C:99:LEU:HD22	1:C:316:LEU:HD11	1.97	0.46
1:F:75:PRO:HA	1:F:78:LEU:H	1.81	0.46
1:A:107:PHE:O	1:A:109:PRO:HD3	2.16	0.46
1:D:143:PHE:CE2	1:F:146:LEU:HD21	2.50	0.46
1:B:189:GLY:O	1:B:193:ALA:N	2.26	0.46
1:F:192:GLU:CA	1:F:195:TYR:HD2	2.20	0.46
1:A:364:ALA:HA	1:A:367:LEU:HD12	1.97	0.46
1:E:187:ILE:O	1:E:190:LEU:HB3	2.15	0.46
1:F:193:ALA:O	1:F:197:ILE:HG13	2.16	0.46
1:C:198:CYS:SG	1:C:280:GLY:O	2.74	0.46
1:F:21:ILE:O	1:F:25:ILE:HD12	2.15	0.46
1:C:247:TYR:OH	1:C:404:GLY:HA3	2.16	0.46
1:C:378:ASN:N	1:C:378:ASN:OD1	2.42	0.46
1:C:50:PHE:HB2	1:C:204:TYR:HE2	1.80	0.46
1:B:105:ARG:HH21	1:B:338:GLN:HE22	1.63	0.46
1:C:194:MET:HA	1:C:197:ILE:HD12	1.97	0.46
1:E:362:MET:O	1:E:365:MET:HB3	2.15	0.46
1:C:282:LEU:HA	1:C:285:THR:OG1	2.17	0.45
1:D:295:SER:HB3	1:D:298:ILE:HD13	1.97	0.45
1:D:8:ILE:HG23	1:D:8:ILE:O	2.17	0.45
1:E:61:ILE:O	1:E:65:SER:HB3	2.17	0.45
1:F:151:VAL:O	1:F:154:THR:OG1	2.28	0.45
1:A:185:ASP:O	1:A:188:ASN:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HG23	1:A:8:ILE:O	2.16	0.45
1:B:8:ILE:O	1:B:8:ILE:HG23	2.16	0.45
1:C:282:LEU:H	1:C:283:PRO:HD3	1.79	0.45
1:D:369:SER:O	1:D:370:VAL:CB	2.64	0.45
1:D:39:VAL:C	1:D:41:THR:H	2.20	0.45
1:F:282:LEU:H	1:F:283:PRO:HD3	1.81	0.45
1:F:99:LEU:HD22	1:F:316:LEU:HD11	1.99	0.45
1:B:61:ILE:O	1:B:65:SER:HB3	2.17	0.45
1:D:276:ARG:HD3	1:D:395:MET:HG2	1.99	0.45
1:E:276:ARG:HD3	1:E:395:MET:HG2	1.98	0.45
1:F:299:TYR:CD2	1:F:299:TYR:C	2.89	0.45
1:A:59:MET:HB2	1:A:60:PRO:HD3	1.98	0.45
1:C:365:MET:HA	1:C:368:HIS:HB2	1.98	0.45
1:F:379:VAL:C	1:F:381:ALA:N	2.69	0.45
1:B:186:ALA:O	1:C:183:LEU:HG	2.16	0.45
1:D:107:PHE:O	1:D:109:PRO:HD3	2.16	0.45
1:F:233:ALA:O	1:F:237:VAL:HG22	2.17	0.45
1:B:39:VAL:C	1:B:41:THR:H	2.21	0.45
1:C:313:GLY:C	1:C:397:ARG:HG3	2.37	0.45
1:F:240:THR:HA	1:F:243:ILE:HD12	1.99	0.45
1:F:355:VAL:CG1	1:F:356:PRO:HD2	2.47	0.45
1:F:363:LEU:O	1:F:367:LEU:HG	2.17	0.45
1:A:295:SER:HB3	1:A:298:ILE:HD13	1.98	0.45
1:A:276:ARG:HD3	1:A:395:MET:HG2	1.99	0.45
1:A:39:VAL:C	1:A:41:THR:H	2.20	0.44
1:F:355:VAL:HG12	1:F:356:PRO:HD2	1.99	0.44
1:F:88:TYR:CZ	1:F:92:THR:HG21	2.52	0.44
1:C:239:LEU:O	1:C:242:GLN:HB3	2.16	0.44
1:C:355:VAL:CG1	1:C:356:PRO:HD2	2.48	0.44
1:C:73:ILE:HG23	1:C:73:ILE:O	2.17	0.44
1:F:12:VAL:O	1:F:13:LEU:C	2.55	0.44
1:D:362:MET:O	1:D:365:MET:HB3	2.17	0.44
1:D:216:VAL:HG11	1:D:385:MET:HG2	2.00	0.44
1:F:49:LEU:O	1:F:53:LEU:HG	2.17	0.44
1:C:21:ILE:O	1:C:25:ILE:HD12	2.17	0.44
1:C:290:LYS:HE3	1:C:299:TYR:HH	1.81	0.44
1:D:364:ALA:HA	1:D:367:LEU:HD12	1.98	0.44
1:A:303:LEU:N	1:A:304:PRO:HD2	2.32	0.44
1:D:321:ALA:HB1	1:D:386:ILE:HD13	2.00	0.44
1:F:334:THR:HG22	1:F:337:GLN:NE2	2.32	0.44
1:F:53:LEU:O	1:F:57:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:C	1:C:214:ALA:H	2.21	0.44
1:C:61:ILE:O	1:C:65:SER:HB3	2.18	0.44
1:E:75:PRO:HA	1:E:76:ALA:HA	1.63	0.44
1:E:8:ILE:O	1:E:8:ILE:HG23	2.17	0.44
1:A:369:SER:O	1:A:370:VAL:CB	2.65	0.44
1:C:355:VAL:HG12	1:C:356:PRO:HD2	2.00	0.44
1:B:303:LEU:N	1:B:304:PRO:HD2	2.33	0.44
1:D:303:LEU:N	1:D:304:PRO:HD2	2.32	0.44
1:E:243:ILE:HG22	1:E:248:PHE:CE1	2.53	0.44
1:E:355:VAL:HG13	1:E:356:PRO:HD2	2.00	0.44
1:E:107:PHE:O	1:E:109:PRO:HD3	2.17	0.43
1:F:28:LEU:HD22	1:F:217:MET:HB3	2.00	0.43
1:F:390:ASP:O	1:F:394:ASP:N	2.45	0.43
1:C:28:LEU:HD22	1:C:217:MET:HB3	1.99	0.43
1:C:334:THR:N	1:C:337:GLN:HE21	2.11	0.43
1:E:364:ALA:HA	1:E:367:LEU:HD12	1.99	0.43
1:C:12:VAL:O	1:C:13:LEU:C	2.56	0.43
1:A:216:VAL:HG12	1:A:224:VAL:HG11	2.00	0.43
1:A:363:LEU:HA	1:A:366:VAL:HG12	2.00	0.43
1:D:143:PHE:CE1	1:F:146:LEU:HD11	2.53	0.43
1:F:16:ILE:HG23	1:F:206:PRO:HA	2.00	0.43
1:D:243:ILE:HG22	1:D:248:PHE:CE1	2.53	0.43
1:F:171:SER:O	1:F:177:ARG:HG3	2.19	0.43
1:A:187:ILE:O	1:A:190:LEU:HB3	2.19	0.43
1:A:75:PRO:HA	1:A:76:ALA:HA	1.61	0.43
1:C:49:LEU:O	1:C:53:LEU:HG	2.18	0.43
1:F:313:GLY:O	1:F:397:ARG:HG3	2.18	0.43
1:B:75:PRO:HA	1:B:76:ALA:HA	1.62	0.43
1:A:70:ALA:HB3	1:A:162:GLY:HA3	2.01	0.43
1:A:147:ALA:O	1:B:141:ASN:ND2	2.52	0.43
1:B:141:ASN:HA	1:B:142:PRO:HD2	1.84	0.43
1:B:355:VAL:HG13	1:B:356:PRO:HD2	2.01	0.43
1:D:75:PRO:HA	1:D:76:ALA:HA	1.63	0.43
1:E:10:TYR:HB2	1:E:15:LYS:HD2	2.01	0.43
1:F:141:ASN:HA	1:F:142:PRO:HD2	1.76	0.43
1:F:334:THR:C	1:F:336:GLY:H	2.22	0.43
1:A:240:THR:HA	1:A:243:ILE:HD12	2.00	0.43
1:B:10:TYR:HB2	1:B:15:LYS:HD2	2.01	0.43
1:C:109:PRO:O	1:C:324:PHE:HA	2.19	0.43
1:C:231:VAL:O	1:C:235:VAL:HG23	2.19	0.43
1:C:334:THR:C	1:C:336:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ILE:O	1:D:190:LEU:HB3	2.19	0.43
1:C:296:GLU:HA	1:C:299:TYR:CE1	2.54	0.43
1:D:59:MET:HB2	1:D:60:PRO:HD3	2.01	0.43
1:B:243:ILE:HG22	1:B:248:PHE:CE1	2.54	0.42
1:B:364:ALA:HA	1:B:367:LEU:HD12	2.01	0.42
1:F:107:PHE:HB2	1:F:234:ALA:HB2	2.01	0.42
1:F:60:PRO:HB2	1:F:194:MET:HE2	2.01	0.42
1:A:243:ILE:HG22	1:A:248:PHE:CE1	2.54	0.42
1:A:321:ALA:HB1	1:A:386:ILE:HD13	2.00	0.42
1:B:276:ARG:HD3	1:B:395:MET:HG2	2.01	0.42
1:C:379:VAL:C	1:C:381:ALA:N	2.72	0.42
1:D:190:LEU:H	1:E:183:LEU:CD1	2.30	0.42
1:E:70:ALA:HB3	1:E:162:GLY:HA3	2.00	0.42
1:B:140:THR:HG23	1:B:141:ASN:H	1.84	0.42
1:A:183:LEU:CD1	1:C:190:LEU:H	2.32	0.42
1:D:70:ALA:HB3	1:D:162:GLY:HA3	2.01	0.42
1:D:363:LEU:HA	1:D:366:VAL:HG12	2.00	0.42
1:E:363:LEU:HA	1:E:366:VAL:HG12	2.01	0.42
1:F:61:ILE:HG22	1:F:194:MET:CB	2.50	0.42
1:A:110:GLY:O	1:A:113:ILE:HG22	2.20	0.42
1:A:393:LEU:H	1:A:393:LEU:HG	1.72	0.42
1:C:171:SER:O	1:C:177:ARG:HG3	2.20	0.42
1:E:185:ASP:O	1:E:188:ASN:O	2.38	0.42
1:E:369:SER:O	1:E:370:VAL:CB	2.66	0.42
1:F:247:TYR:OH	1:F:404:GLY:HA3	2.19	0.42
1:C:334:THR:HG22	1:C:337:GLN:NE2	2.34	0.42
1:E:105:ARG:HH21	1:E:338:GLN:HE22	1.67	0.42
1:B:146:LEU:HD21	1:C:143:PHE:CZ	2.54	0.42
1:B:369:SER:O	1:B:370:VAL:CB	2.66	0.42
1:C:57:LEU:O	1:C:58:VAL:C	2.58	0.42
1:E:303:LEU:N	1:E:304:PRO:HD2	2.34	0.42
1:E:282:LEU:HD13	1:E:307:ALA:HB2	2.02	0.42
1:E:59:MET:HB2	1:E:60:PRO:HD3	2.00	0.42
1:F:212:LEU:C	1:F:214:ALA:H	2.23	0.42
1:A:10:TYR:HB2	1:A:15:LYS:HD2	2.01	0.42
1:A:179:SER:HA	1:C:185:ASP:OD1	2.20	0.42
1:A:236:TYR:HA	1:A:239:LEU:HD12	2.02	0.42
1:B:240:THR:HA	1:B:243:ILE:HD12	2.01	0.42
1:D:190:LEU:H	1:E:183:LEU:HD12	1.85	0.42
1:B:49:LEU:HD23	1:B:204:TYR:OH	2.20	0.42
1:B:321:ALA:HB1	1:B:386:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:HA	1:B:366:VAL:HG12	2.02	0.42
1:C:141:ASN:HA	1:C:142:PRO:HD2	1.75	0.42
1:C:152:LEU:O	1:C:155:ILE:HB	2.20	0.42
1:C:373:PRO:C	1:C:375:THR:H	2.23	0.42
1:D:216:VAL:HG12	1:D:224:VAL:HG11	2.02	0.42
1:D:243:ILE:O	1:D:248:PHE:HD1	2.03	0.42
1:F:296:GLU:HA	1:F:299:TYR:CE1	2.55	0.42
1:F:314:THR:HG23	1:F:397:ARG:HD3	2.02	0.42
1:B:216:VAL:HG12	1:B:224:VAL:HG11	2.02	0.42
1:F:54:LEU:N	1:F:54:LEU:HD12	2.35	0.42
1:C:16:ILE:HG23	1:C:206:PRO:HA	2.01	0.41
1:C:243:ILE:HG13	1:C:243:ILE:H	1.61	0.41
1:C:61:ILE:HG22	1:C:194:MET:CB	2.46	0.41
1:E:225:VAL:HA	1:E:228:LEU:HD12	2.02	0.41
1:F:334:THR:N	1:F:337:GLN:HE21	2.11	0.41
1:C:198:CYS:O	1:C:202:MET:CG	2.63	0.41
1:F:155:ILE:O	1:F:156:PHE:C	2.58	0.41
1:F:403:THR:O	1:F:407:THR:OG1	2.36	0.41
1:B:216:VAL:HG11	1:B:385:MET:HG2	2.02	0.41
1:C:50:PHE:O	1:C:54:LEU:HD13	2.20	0.41
1:D:110:GLY:O	1:D:113:ILE:HG22	2.19	0.41
1:F:33:TYR:HB2	1:F:34:GLY:H	1.69	0.41
1:C:233:ALA:O	1:C:237:VAL:HG22	2.21	0.41
1:F:73:ILE:O	1:F:73:ILE:HG23	2.21	0.41
1:B:185:ASP:OD1	1:C:179:SER:HA	2.20	0.41
1:E:240:THR:HA	1:E:243:ILE:HD12	2.03	0.41
1:A:299:TYR:HB2	1:A:303:LEU:HD23	2.02	0.41
1:B:198:CYS:O	1:B:202:MET:HG2	2.21	0.41
1:D:185:ASP:O	1:D:188:ASN:O	2.39	0.41
1:E:141:ASN:HA	1:E:142:PRO:HD2	1.82	0.41
1:B:243:ILE:O	1:B:248:PHE:HD1	2.04	0.41
1:E:243:ILE:O	1:E:248:PHE:HD1	2.03	0.41
1:F:85:ILE:O	1:F:88:TYR:HB3	2.21	0.41
1:B:185:ASP:O	1:B:188:ASN:O	2.38	0.41
1:C:43:VAL:O	1:C:211:ALA:HB1	2.21	0.41
1:F:213:ILE:HA	1:F:216:VAL:HB	2.03	0.41
1:B:70:ALA:HB3	1:B:162:GLY:HA3	2.03	0.41
1:B:236:TYR:HA	1:B:239:LEU:HD12	2.03	0.41
1:C:193:ALA:O	1:C:197:ILE:HG13	2.21	0.41
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.56	0.41
1:C:75:PRO:HA	1:C:78:LEU:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:LEU:HD23	1:D:204:TYR:OH	2.21	0.41
1:E:343:LEU:O	1:E:347:LEU:HD13	2.21	0.41
1:F:341:ILE:C	1:F:343:LEU:N	2.73	0.41
1:F:63:PHE:O	1:F:67:VAL:HG23	2.21	0.41
1:A:282:LEU:HD13	1:A:307:ALA:HB2	2.03	0.41
1:B:309:ILE:HG22	1:B:310:ASN:H	1.86	0.41
1:C:276:ARG:HG2	1:C:395:MET:HA	2.03	0.41
1:C:333:LEU:HA	1:C:337:GLN:HE21	1.85	0.41
1:E:110:GLY:O	1:E:113:ILE:HG22	2.20	0.41
1:A:151:VAL:HG12	1:A:155:ILE:HD13	2.03	0.40
1:C:190:LEU:O	1:C:194:MET:HG2	2.21	0.40
1:D:240:THR:HA	1:D:243:ILE:HD12	2.02	0.40
1:A:155:ILE:O	1:A:156:PHE:C	2.59	0.40
1:A:195:TYR:HA	1:A:198:CYS:SG	2.60	0.40
1:B:393:LEU:HG	1:B:393:LEU:H	1.73	0.40
1:D:123:GLN:HA	1:D:124:PRO:HD2	1.79	0.40
1:F:239:LEU:O	1:F:242:GLN:HB3	2.22	0.40
1:F:74:SER:O	1:F:75:PRO:C	2.59	0.40
1:A:243:ILE:O	1:A:248:PHE:HD1	2.04	0.40
1:A:355:VAL:HG13	1:A:356:PRO:HD2	2.03	0.40
1:A:216:VAL:HG11	1:A:385:MET:HG2	2.02	0.40
1:C:403:THR:O	1:C:407:THR:OG1	2.35	0.40
1:D:183:LEU:HD11	1:F:190:LEU:HB2	2.03	0.40
1:A:143:PHE:CE2	1:C:146:LEU:HD21	2.56	0.40
1:C:155:ILE:HD12	1:C:155:ILE:H	1.87	0.40
1:D:151:VAL:HG12	1:D:155:ILE:HD13	2.04	0.40
1:D:355:VAL:HG13	1:D:356:PRO:HD2	2.03	0.40
1:F:129:PRO:HB2	1:F:130:LEU:H	1.54	0.40
1:B:343:LEU:O	1:B:347:LEU:HD13	2.22	0.40
1:C:155:ILE:O	1:C:156:PHE:C	2.59	0.40
1:D:309:ILE:HG22	1:D:310:ASN:H	1.87	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	409/422 (97%)	357 (87%)	44 (11%)	8 (2%)	8	45
1	B	400/422 (95%)	350 (88%)	44 (11%)	6 (2%)	11	50
1	C	396/422 (94%)	302 (76%)	75 (19%)	19 (5%)	2	26
1	D	409/422 (97%)	356 (87%)	44 (11%)	9 (2%)	7	42
1	E	399/422 (94%)	350 (88%)	42 (10%)	7 (2%)	9	47
1	F	388/422 (92%)	296 (76%)	73 (19%)	19 (5%)	2	26
All	All	2401/2532 (95%)	2011 (84%)	322 (13%)	68 (3%)	5	38

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	ALA
1	A	370	VAL
1	B	358	ALA
1	B	370	VAL
1	C	75	PRO
1	C	131	VAL
1	C	225	VAL
1	C	380	CYS
1	D	358	ALA
1	D	370	VAL
1	E	358	ALA
1	E	370	VAL
1	F	75	PRO
1	F	131	VAL
1	F	224	VAL
1	F	225	VAL
1	F	380	CYS
1	A	74	SER
1	A	117	VAL
1	B	74	SER
1	C	34	GLY
1	C	78	LEU
1	C	356	PRO
1	D	74	SER
1	D	117	VAL
1	D	119	GLY
1	E	74	SER

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Mol	Chain	Res	Type
1	F	34	GLY
1	F	78	LEU
1	B	356	PRO
1	C	220	GLN
1	C	221	GLY
1	D	356	PRO
1	F	58	VAL
1	F	220	GLN
1	F	221	GLY
1	F	356	PRO
1	A	147	ALA
1	A	356	PRO
1	B	147	ALA
1	C	58	VAL
1	C	213	ILE
1	C	335	VAL
1	E	147	ALA
1	E	356	PRO
1	F	335	VAL
1	C	63	PHE
1	D	124	PRO
1	D	147	ALA
1	D	155	ILE
1	F	147	ALA
1	F	213	ILE
1	F	222	VAL
1	A	155	ILE
1	C	374	LEU
1	E	40	HIS
1	E	155	ILE
1	B	155	ILE
1	C	10	TYR
1	C	155	ILE
1	F	155	ILE
1	C	222	VAL
1	F	10	TYR
1	F	142	PRO
1	C	142	PRO
1	C	370	VAL
1	F	370	VAL
1	A	142	PRO

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	321/330 (97%)	309 (96%)	12 (4%)	37	65
1	B	317/330 (96%)	305 (96%)	12 (4%)	36	65
1	C	312/330 (94%)	281 (90%)	31 (10%)	8	33
1	D	321/330 (97%)	308 (96%)	13 (4%)	34	63
1	E	316/330 (96%)	304 (96%)	12 (4%)	36	65
1	F	308/330 (93%)	279 (91%)	29 (9%)	9	35
All	All	1895/1980 (96%)	1786 (94%)	109 (6%)	23	54

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	48	ASP
1	A	117	VAL
1	A	140	THR
1	A	148	ASN
1	A	152	LEU
1	A	203	GLN
1	A	230	LYS
1	A	252	LYS
1	A	285	THR
1	A	312	ASP
1	A	393	LEU
1	B	12	VAL
1	B	41	THR
1	B	48	ASP
1	B	140	THR
1	B	148	ASN
1	B	152	LEU
1	B	203	GLN
1	B	230	LYS
1	B	252	LYS
1	B	285	THR

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Mol	Chain	Res	Type
1	B	312	ASP
1	B	393	LEU
1	C	37	HIS
1	C	41	THR
1	C	65	SER
1	C	73	ILE
1	C	74	SER
1	C	81	VAL
1	C	117	VAL
1	C	140	THR
1	C	154	THR
1	C	160	ILE
1	C	174	GLU
1	C	183	LEU
1	C	203	GLN
1	C	212	LEU
1	C	224	VAL
1	C	231	VAL
1	C	241	LEU
1	C	245	LEU
1	C	252	LYS
1	C	299	TYR
1	C	312	ASP
1	C	314	THR
1	C	317	TYR
1	C	323	PHE
1	C	338	GLN
1	C	342	VAL
1	C	343	LEU
1	C	347	LEU
1	C	365	MET
1	C	372	LEU
1	C	378	ASN
1	D	12	VAL
1	D	41	THR
1	D	48	ASP
1	D	140	THR
1	D	148	ASN
1	D	152	LEU
1	D	178	LYS
1	D	203	GLN
1	D	230	LYS

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Mol	Chain	Res	Type
1	D	252	LYS
1	D	285	THR
1	D	312	ASP
1	D	393	LEU
1	E	12	VAL
1	E	41	THR
1	E	48	ASP
1	E	140	THR
1	E	148	ASN
1	E	152	LEU
1	E	203	GLN
1	E	230	LYS
1	E	252	LYS
1	E	285	THR
1	E	312	ASP
1	E	393	LEU
1	F	37	HIS
1	F	41	THR
1	F	65	SER
1	F	73	ILE
1	F	74	SER
1	F	81	VAL
1	F	129	PRO
1	F	140	THR
1	F	154	THR
1	F	160	ILE
1	F	174	GLU
1	F	183	LEU
1	F	203	GLN
1	F	212	LEU
1	F	231	VAL
1	F	245	LEU
1	F	252	LYS
1	F	299	TYR
1	F	312	ASP
1	F	314	THR
1	F	317	TYR
1	F	323	PHE
1	F	338	GLN
1	F	342	VAL
1	F	343	LEU
1	F	347	LEU

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Mol	Chain	Res	Type
1	F	365	MET
1	F	372	LEU
1	F	378	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	203	GLN
1	A	338	GLN
1	B	108	ASN
1	B	203	GLN
1	B	338	GLN
1	C	108	ASN
1	C	337	GLN
1	D	108	ASN
1	D	203	GLN
1	D	337	GLN
1	D	338	GLN
1	E	108	ASN
1	E	203	GLN
1	E	338	GLN
1	F	40	HIS
1	F	108	ASN
1	F	223	HIS
1	F	337	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	A	501	-	1,8,8	0.20	0	1,10,10	0.54	0
2	ASP	B	501	-	1,8,8	0.26	0	1,10,10	0.62	0
2	ASP	C	501	-	1,8,8	0.17	0	1,10,10	0.58	0
2	ASP	D	501	-	1,8,8	0.23	0	1,10,10	0.55	0
2	ASP	E	501	-	1,8,8	0.24	0	1,10,10	0.56	0
2	ASP	F	501	-	1,8,8	0.17	0	1,10,10	0.72	0

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	A	501	-	-	0/2/8/8	0/0/0/0
2	ASP	B	501	-	-	0/2/8/8	0/0/0/0
2	ASP	C	501	-	-	0/2/8/8	0/0/0/0
2	ASP	D	501	-	-	0/2/8/8	0/0/0/0
2	ASP	E	501	-	-	0/2/8/8	0/0/0/0
2	ASP	F	501	-	-	0/2/8/8	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.