Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 11:22 PM EST

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

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

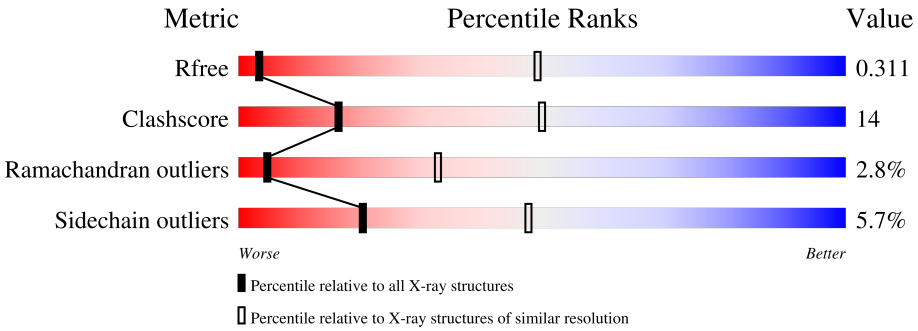
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	1083 (5.52-3.80)
Clashscore	141614	1156 (5.52-3.80)
Ramachandran outliers	138981	1092 (5.52-3.80)
Sidechain outliers	138945	1072 (5.50-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

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 (i)

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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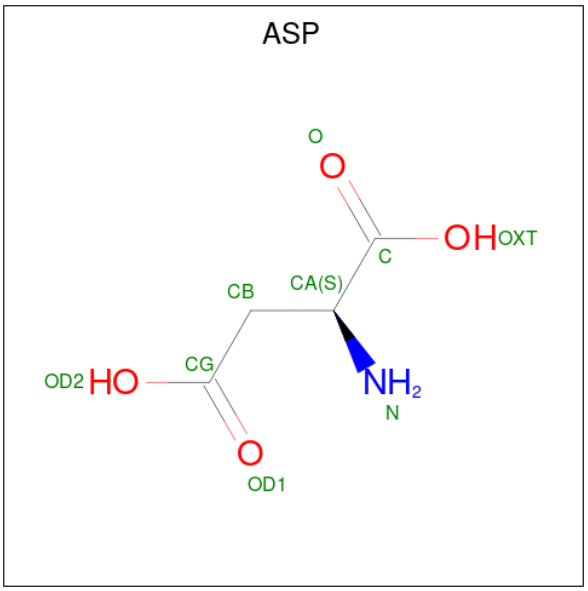
Chain	Residue	Modelled	Actual	Comment	Reference
D	422	ARG	-	expression tag	UNP O59010
E	37	HIS	ASP	engineered mutation	UNP O59010
E	40	HIS	LYS	engineered mutation	UNP O59010
E	125	HIS	LYS	engineered mutation	UNP O59010
E	132	HIS	LYS	engineered mutation	UNP O59010
E	198	CYS	VAL	engineered mutation	UNP 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: $C_4H_7NO_4$).



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 (three-letter code: NA) (formula: Na).

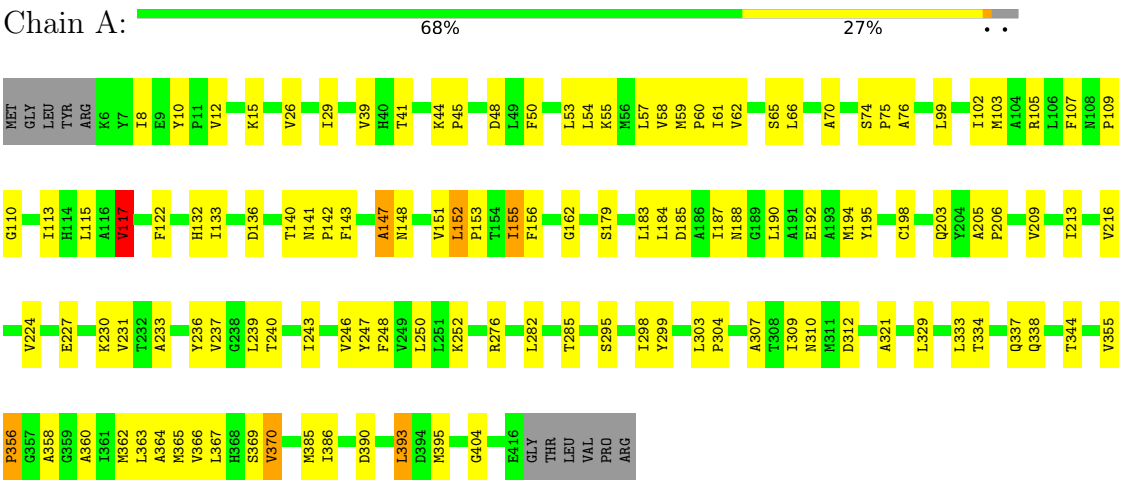
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	B	2	Total Na 2 2	0	0
3	C	2	Total Na 2 2	0	0
3	D	2	Total Na 2 2	0	0
3	E	2	Total Na 2 2	0	0
3	F	2	Total Na 2 2	0	0

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. 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.

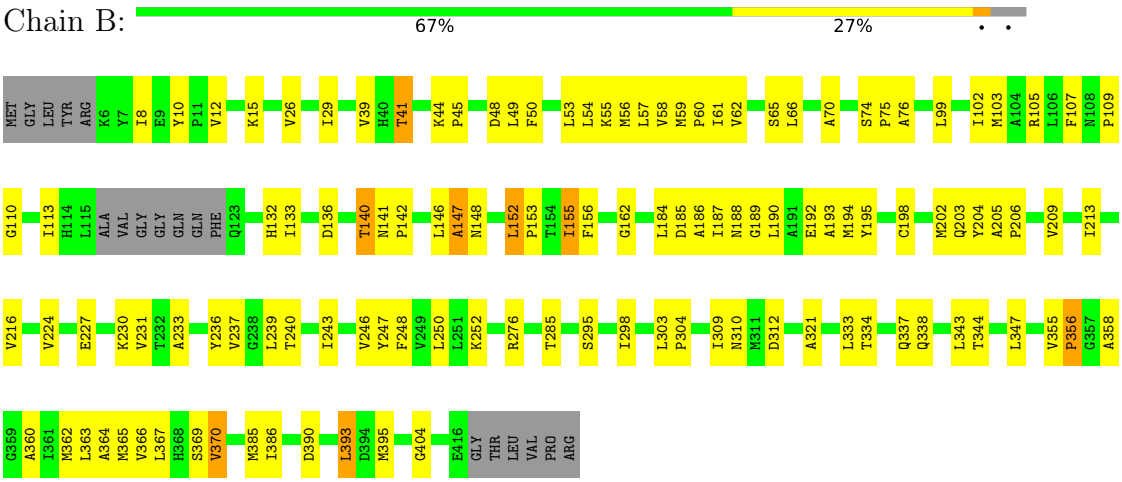
• Molecule 1: sodium-coupled L-aspartate transporter

Chain A:



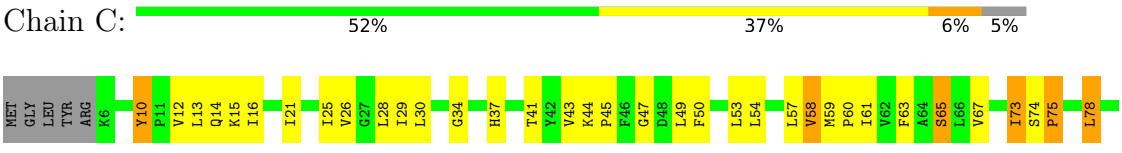
• Molecule 1: sodium-coupled L-aspartate transporter

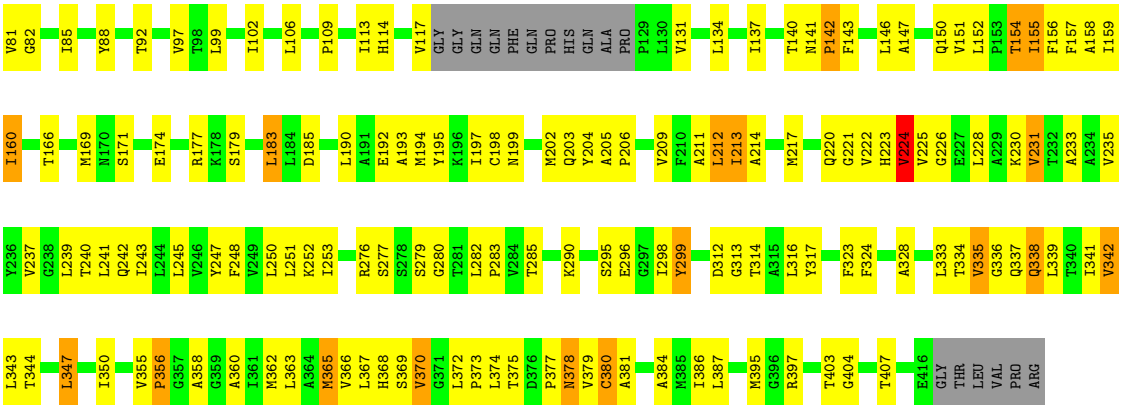
Chain B:



• Molecule 1: sodium-coupled L-aspartate transporter

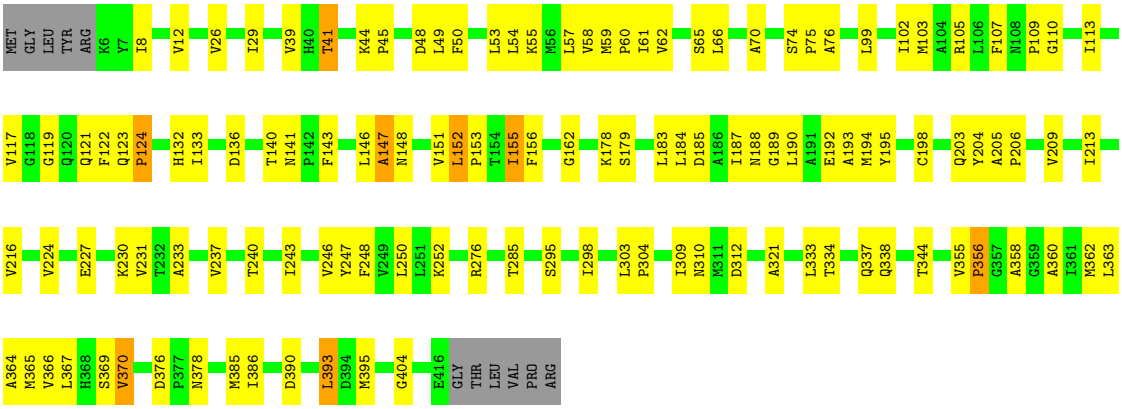
Chain C:





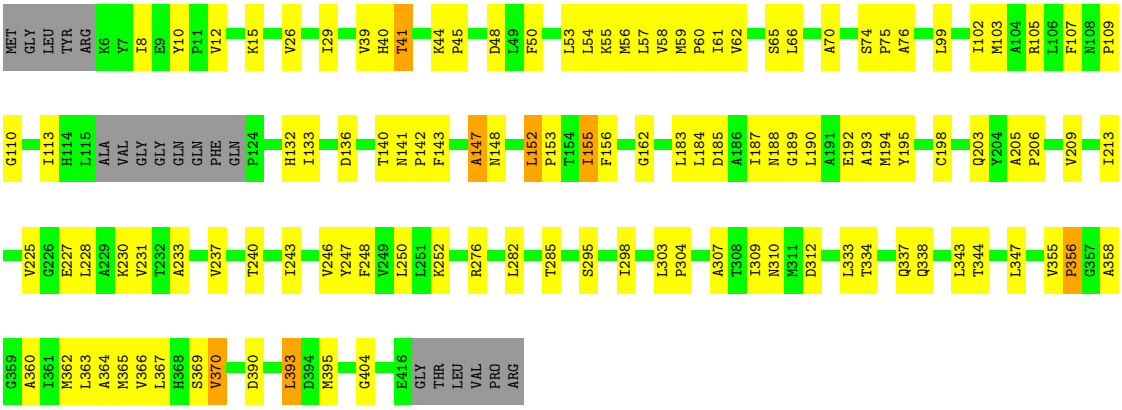
• Molecule 1: sodium-coupled L-aspartate transporter

Chain D:



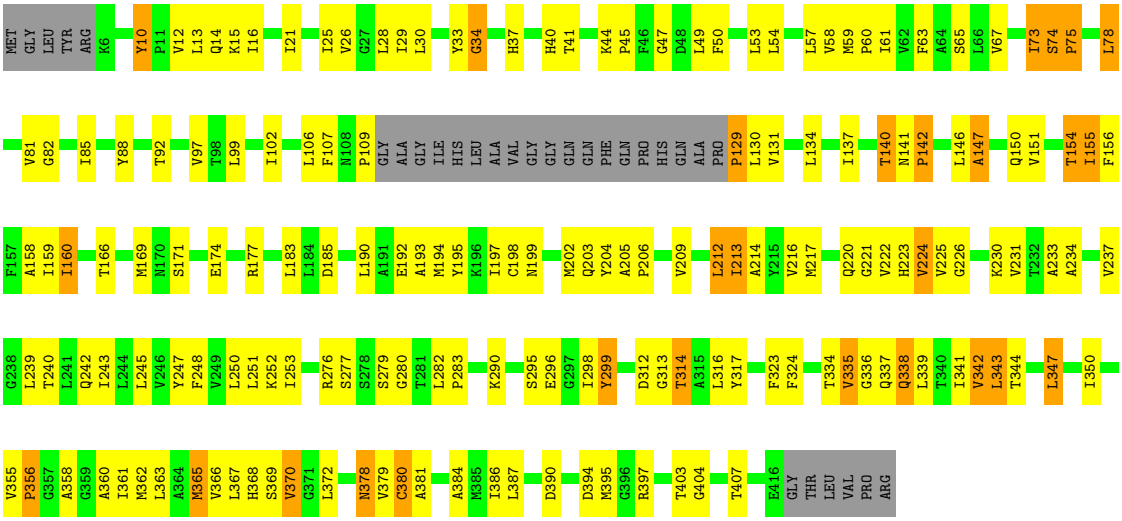
• Molecule 1: sodium-coupled L-aspartate transporter

Chain E:



• Molecule 1: sodium-coupled L-aspartate transporter

Chain F:


MET GLY LEU TYR ARG K6 Y10 P11 V12 L13 Q14 K15 I16 I21 I25 V26 G27 L28 I29 L30 Y33 G34 H37 H40 T41 K44 P45 F46 G47 D48 L49 F50 L53 L54 L57 V58 M59 P60 I61 V62 F63 A64 S65 L66 V67 I73 S74 P75 L78
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
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
G238 L239 T240 L241 Q242 I243 L244 L245 V246 Y247 F248 V249 L250 L251 K252 I253 R276 S277 S278 S279 G280 T281 L282 P283 K290 S295 E296 G297 I298 Y299 D312 G313 T314 A315 L316 Y317 F323 F324 T334 V335 G336 Q337 Q338 L339 T340 I341 V342 L343 T344 L347 I350
V355 P356 G357 A358 G359 A360 I361 M362 L363 A364 M365 V366 L367 H368 S369 V370 G371 L372 N378 V379 C380 A381 A384 M385 I386 L387 D390 D394 M395 G396 R397 T403 G404 T407 E416 GLY THR LEU VAL PRO ARG

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:HD12	1:D:152:LEU:H	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:H	1:E:152:LEU:HD12	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:44:LYS:N	1:F:45:PRO:HD2	2.14	0.62
1:F:169:MET:O	1:F:177:ARG:HG2	2.00	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:62:VAL:O	1:A:66:LEU:HG	2.00	0.61
1:A:334:THR:O	1:A:337:GLN:HG2	2.01	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:62:VAL:O	1:B:66:LEU:HG	2.01	0.59
1:B:192:GLU:HA	1:B:195:TYR:CD2	2.36	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: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:E:44:LYS:N	1:E:45:PRO:HD2	2.20	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:53:LEU:O	1:A:57:LEU:HG	2.07	0.53
1:A:155:ILE:HG22	1:A:156:PHE:N	2.23	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:61:ILE:HG13	1:D:62:VAL:H	1.73	0.52
1:D:209:VAL:O	1:D:213:ILE:HG13	2.10	0.52
1:F:75:PRO:HG3	1:F:78:LEU:HD23	1.92	0.51
1:F:159:ILE:HG22	1:F:160:ILE:N	2.25	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:50:PHE:O	1:D:54:LEU:HD12	2.11	0.51
1:D:360:ALA:O	1:D:363:LEU:HB3	2.10	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:58:VAL:HG13	1:D:59:MET:N	2.27	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: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:56:MET:HE2	1:C:157:PHE:HD1	1.78	0.49
1:B:103:MET:HE2	1:B:237:VAL:HG23	1.93	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:A:183:LEU:HD11	1:C:190:LEU:N	2.29	0.48
1:B:309:ILE:HG22	1:B:310:ASN: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:105:ARG:HH21	1:A:338:GLN:HE22	1.62	0.47
1:A:115:LEU:HD12	1:A:117:VAL:HG13	1.96	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:C	1:C:299:TYR:CD2	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:39:VAL:C	1:E:41:THR:H	2.18	0.47
1:E:333:LEU:HA	1:E:337:GLN:NE2	2.30	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:50:PHE:HB2	1:C:204:TYR:HE2	1.80	0.46
1:C:247:TYR:OH	1:C:404:GLY:HA3	2.16	0.46
1:C:378:ASN:OD1	1:C:378:ASN:N	2.42	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:8:ILE:O	1:D:8:ILE:HG23	2.17	0.45
1:D:295:SER:HB3	1:D:298:ILE:HD13	1.97	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:8:ILE:HG23	1:A:8:ILE:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASP:O	1:A:188:ASN:O	2.35	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:39:VAL:C	1:D:41:THR:H	2.20	0.45
1:D:369:SER:O	1:D:370:VAL:CB	2.64	0.45
1:F:99:LEU:HD22	1:F:316:LEU:HD11	1.99	0.45
1:F:282:LEU:H	1:F:283:PRO:HD3	1.81	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:C	1:F:299:TYR:CD2	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:276:ARG:HD3	1:A:395:MET:HG2	1.99	0.45
1:A:295:SER:HB3	1:A:298:ILE:HD13	1.98	0.45
1:A:39:VAL:C	1:A:41:THR:H	2.20	0.44
1:F:88:TYR:CZ	1:F:92:THR:HG21	2.52	0.44
1:F:355:VAL:HG12	1:F:356:PRO:HD2	1.99	0.44
1:C:73:ILE:HG23	1:C:73:ILE:O	2.17	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:F:12:VAL:O	1:F:13:LEU:C	2.55	0.44
1:D:216:VAL:HG11	1:D:385:MET:HG2	2.00	0.44
1:D:362:MET:O	1:D:365:MET:HB3	2.17	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:53:LEU:O	1:F:57:LEU:HG	2.17	0.44
1:F:334:THR:HG22	1:F:337:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ILE:O	1:C:65:SER:HB3	2.18	0.44
1:C:212:LEU:C	1:C:214:ALA:H	2.21	0.44
1:E:8:ILE:HG23	1:E:8:ILE:O	2.17	0.44
1:E:75:PRO:HA	1:E:76:ALA:HA	1.63	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:75:PRO:HA	1:A:76:ALA:HA	1.61	0.43
1:A:187:ILE:O	1:A:190:LEU:HB3	2.19	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:60:PRO:HB2	1:F:194:MET:HE2	2.01	0.42
1:F:107:PHE:HB2	1:F:234:ALA:HB2	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:A:183:LEU:CD1	1:C:190:LEU:H	2.32	0.42
1:B:140:THR:HG23	1:B:141:ASN:H	1.84	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:59:MET:HB2	1:E:60:PRO:HD3	2.00	0.42
1:E:282:LEU:HD13	1:E:307:ALA:HB2	2.02	0.42
1:E:303:LEU:N	1:E:304:PRO:HD2	2.34	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:HD12	1:F:54:LEU:N	2.35	0.42
1:C:16:ILE:HG23	1:C:206:PRO:HA	2.01	0.41
1:C:61:ILE:HG22	1:C:194:MET:CB	2.46	0.41
1:C:243:ILE:H	1:C:243:ILE:HG13	1.61	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:HG23	1:F:73:ILE:O	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:70:ALA:HB3	1:B:162:GLY:HA3	2.03	0.41
1:B:185:ASP:O	1:B:188:ASN:O	2.38	0.41
1:B:236:TYR:HA	1:B:239:LEU:HD12	2.03	0.41
1:C:43:VAL:O	1:C:211:ALA:HB1	2.21	0.41
1:C:75:PRO:HA	1:C:78:LEU:H	1.84	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:D:49:LEU:HD23	1:D:204:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:343:LEU:O	1:E:347:LEU:HD13	2.21	0.41
1:F:63:PHE:O	1:F:67:VAL:HG23	2.21	0.41
1:F:213:ILE:HA	1:F:216:VAL:HB	2.03	0.41
1:F:341:ILE:C	1:F:343:LEU:N	2.73	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:H	1:B:393:LEU:HG	1.73	0.40
1:D:123:GLN:HA	1:D:124:PRO:HD2	1.79	0.40
1:F:74:SER:O	1:F:75:PRO:C	2.59	0.40
1:F:239:LEU:O	1:F:242:GLN:HB3	2.22	0.40
1:A:216:VAL:HG11	1:A:385:MET:HG2	2.02	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: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 (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	409/422 (97%)	357 (87%)	44 (11%)	8 (2%)	7 40
1	B	400/422 (95%)	350 (88%)	44 (11%)	6 (2%)	10 46
1	C	396/422 (94%)	302 (76%)	75 (19%)	19 (5%)	2 23
1	D	409/422 (97%)	356 (87%)	44 (11%)	9 (2%)	6 37
1	E	399/422 (94%)	350 (88%)	42 (10%)	7 (2%)	8 42
1	F	388/422 (92%)	296 (76%)	73 (19%)	19 (5%)	2 23
All	All	2401/2532 (95%)	2011 (84%)	322 (13%)	68 (3%)	5 33

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	321/330 (97%)	309 (96%)	12 (4%)	34 59
1	B	317/330 (96%)	305 (96%)	12 (4%)	33 58
1	C	312/330 (94%)	281 (90%)	31 (10%)	8 28
1	D	321/330 (97%)	308 (96%)	13 (4%)	31 56
1	E	316/330 (96%)	304 (96%)	12 (4%)	33 58
1	F	308/330 (93%)	279 (91%)	29 (9%)	8 30
All	All	1895/1980 (96%)	1786 (94%)	109 (6%)	20 47

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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	C	501	-	6,8,8	1.32	1 (16%)	8,10,10	1.42	1 (12%)
2	ASP	D	501	-	6,8,8	1.24	1 (16%)	8,10,10	1.42	2 (25%)
2	ASP	E	501	-	6,8,8	1.26	1 (16%)	8,10,10	1.45	2 (25%)
2	ASP	A	501	-	6,8,8	1.24	1 (16%)	8,10,10	1.44	2 (25%)
2	ASP	B	501	-	6,8,8	1.26	1 (16%)	8,10,10	1.41	2 (25%)
2	ASP	F	501	-	6,8,8	1.26	1 (16%)	8,10,10	1.59	2 (25%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ASP	OXT-C	-2.29	1.23	1.30
2	C	501	ASP	OXT-C	-2.28	1.23	1.30
2	E	501	ASP	OXT-C	-2.26	1.23	1.30
2	D	501	ASP	OXT-C	-2.20	1.23	1.30
2	A	501	ASP	OXT-C	-2.19	1.23	1.30
2	F	501	ASP	OXT-C	-2.15	1.23	1.30

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	ASP	OXT-C-O	-3.44	116.28	124.09
2	E	501	ASP	OXT-C-O	-2.92	117.46	124.09
2	A	501	ASP	OXT-C-O	-2.90	117.50	124.09
2	B	501	ASP	OXT-C-O	-2.88	117.54	124.09
2	C	501	ASP	OXT-C-O	-2.86	117.60	124.09
2	D	501	ASP	OXT-C-O	-2.79	117.75	124.09
2	E	501	ASP	OXT-C-CA	2.32	121.28	113.38
2	D	501	ASP	OXT-C-CA	2.29	121.18	113.38
2	A	501	ASP	OXT-C-CA	2.28	121.14	113.38
2	B	501	ASP	OXT-C-CA	2.19	120.83	113.38
2	F	501	ASP	OXT-C-CA	2.10	120.54	113.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	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

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.