W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:52 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)

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

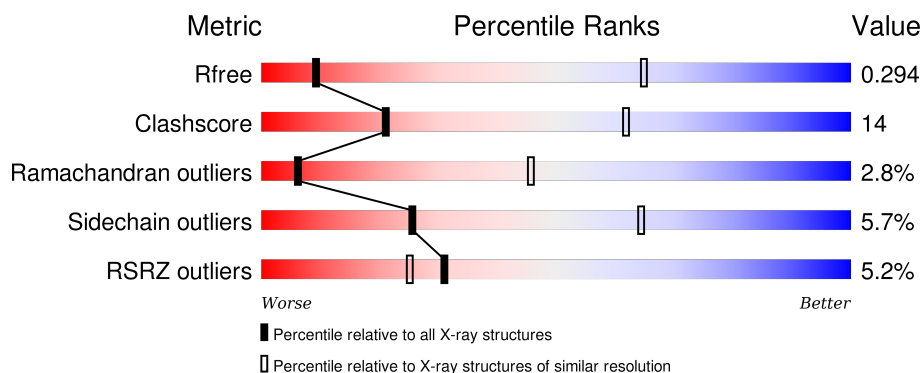|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	Percentile Ranks	Value
Rfree		0.294
Clashscore		14
Ramachandran outliers		2.8%
Sidechain outliers		5.7%
RSRZ outliers		5.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
❘ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1093 (5.70-3.60)
Clashscore	102246	1007 (5.66-3.64)
Ramachandran outliers	100387	1135 (5.70-3.60)
Sidechain outliers	100360	1116 (5.70-3.60)
RSRZ outliers	91569	1096 (5.70-3.60)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	422	7% 68% 27% • •
1	B	422	10% 67% 27% • •
1	C	422	2% 52% 37% 6% 5%
1	D	422	7% 68% 27% • •
1	E	422	2% 68% 26% • 5%

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Mol	Chain	Length	Quality of chain
1	F	422	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ASP	A	501	-	-	-	X
2	ASP	B	501	-	-	-	X
2	ASP	C	501	-	-	-	X
2	ASP	D	501	-	-	-	X
2	ASP	F	501	-	-	-	X
3	NA	A	503	-	-	-	X
3	NA	B	503	-	-	-	X
3	NA	C	502	-	-	-	X
3	NA	D	502	-	-	-	X
3	NA	E	502	-	-	-	X
3	NA	F	502	-	-	-	X

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

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: $C_4H_7NO_4$).
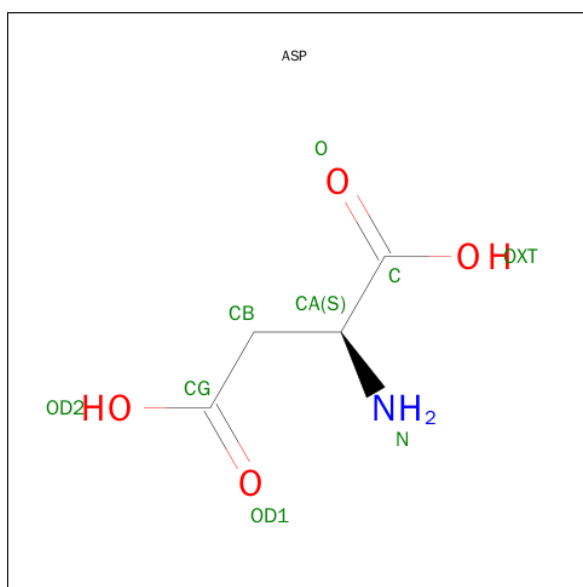
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		
2	C	1	Total	C	N	O	0	0
			9	4	1	4		
2	D	1	Total	C	N	O	0	0
			9	4	1	4		
2	E	1	Total	C	N	O	0	0
			9	4	1	4		
2	F	1	Total	C	N	O	0	0
			9	4	1	4		

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

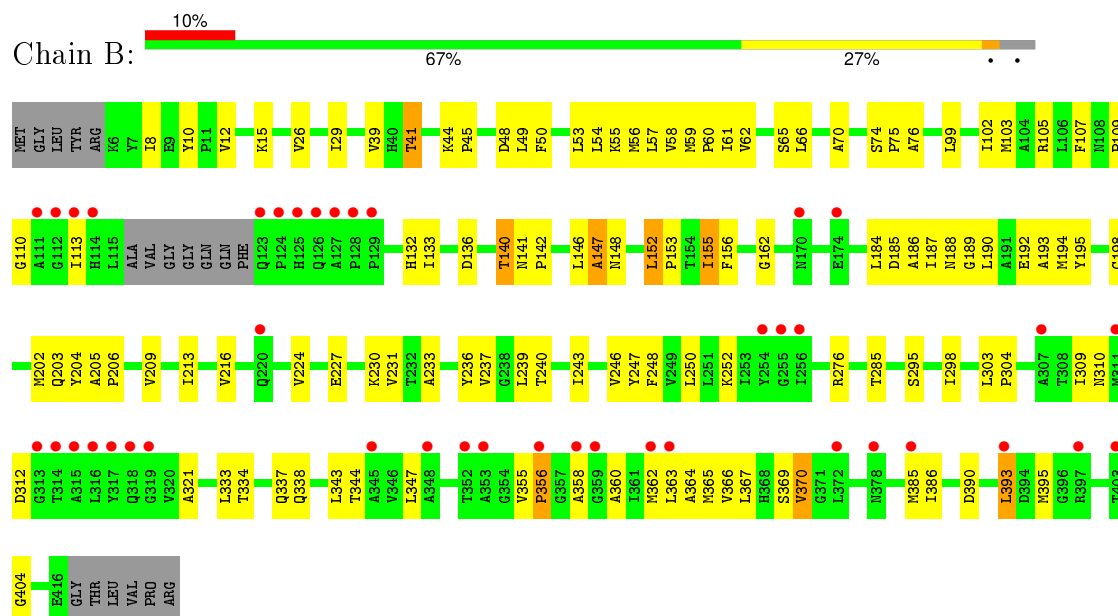| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	Na	0	0
			2	2		
3	E	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	A	2	Total	Na	0	0
			2	2		
3	F	2	Total	Na	0	0
			2	2		

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
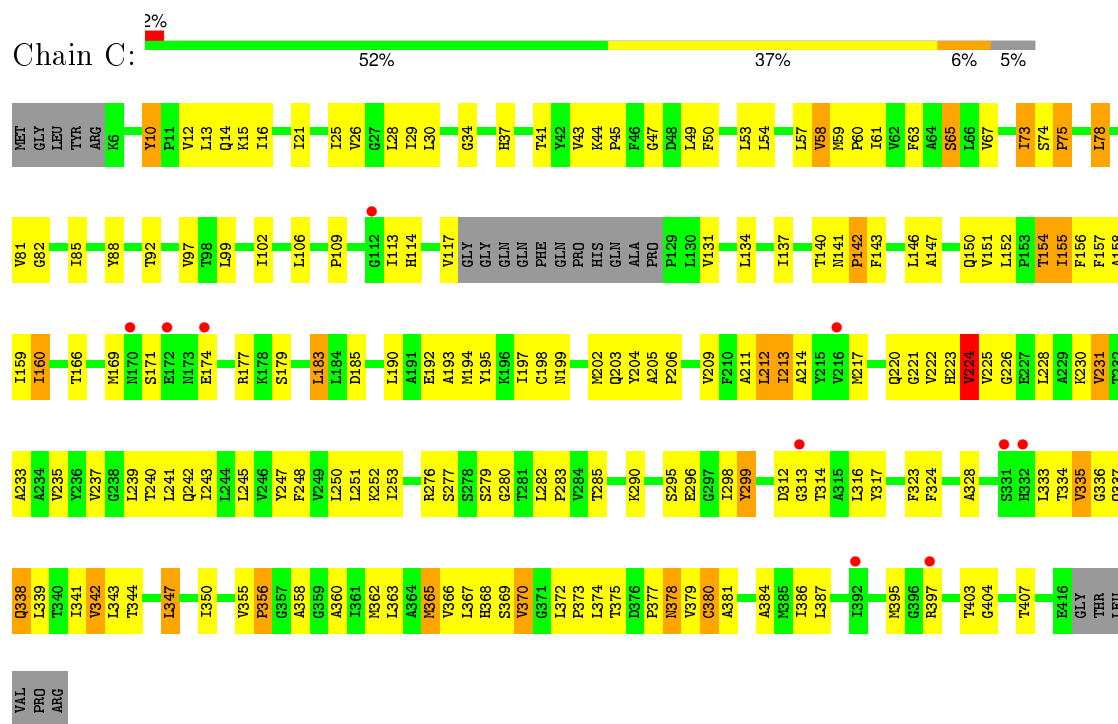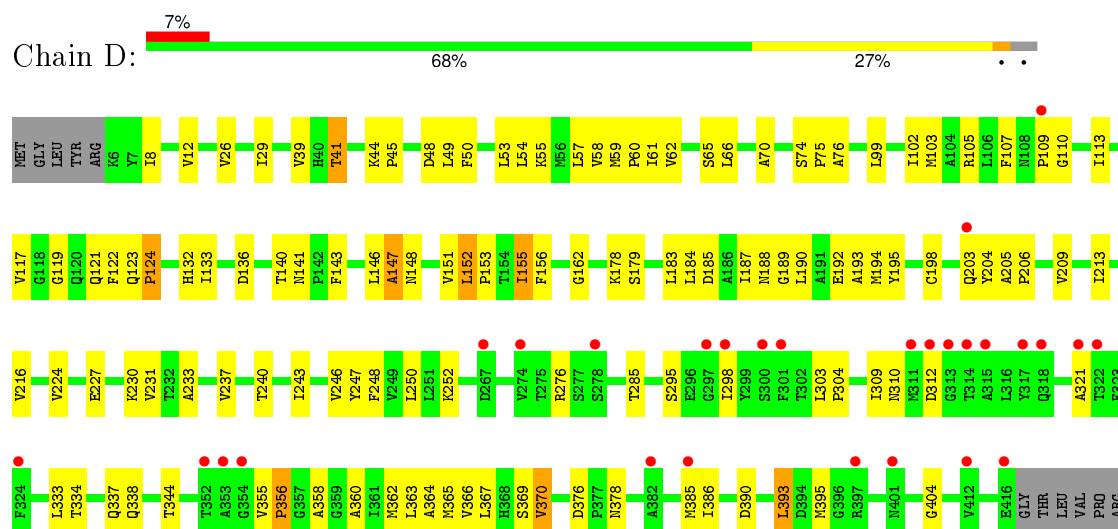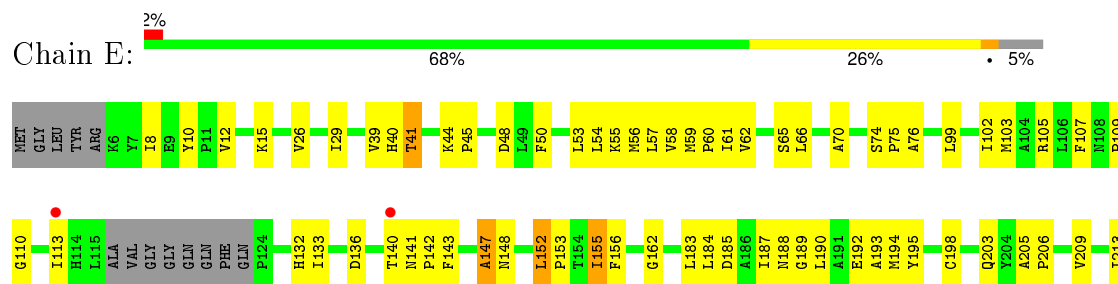
• Molecule 1: sodium-coupled L-aspartate transporter
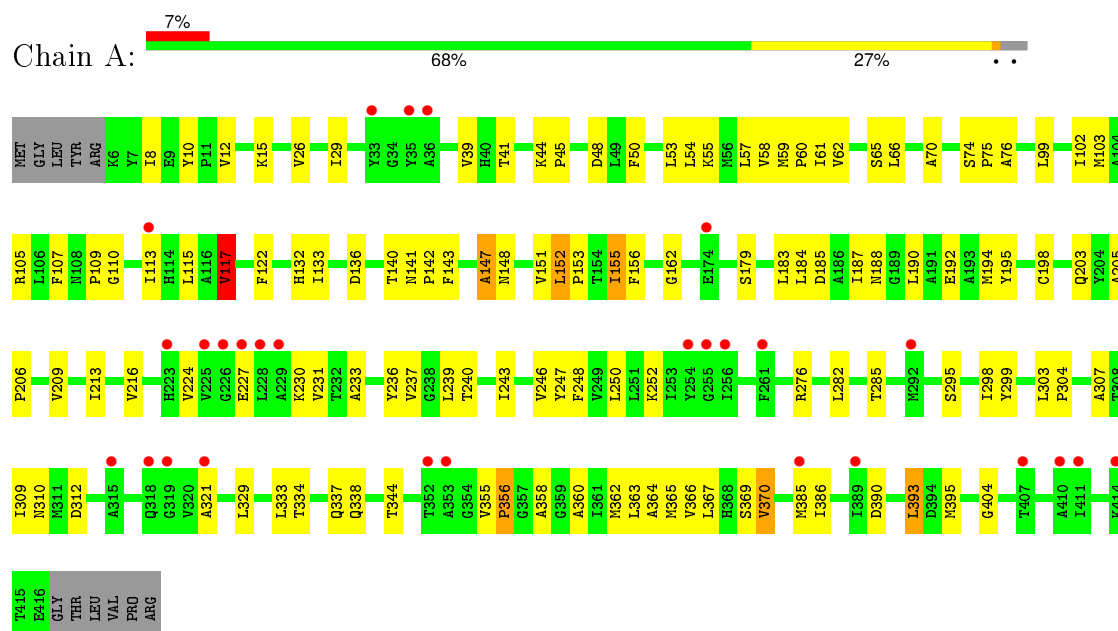
• Molecule 1: sodium-coupled L-aspartate transporter

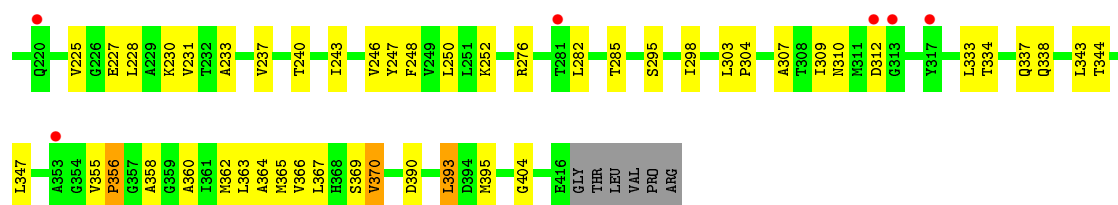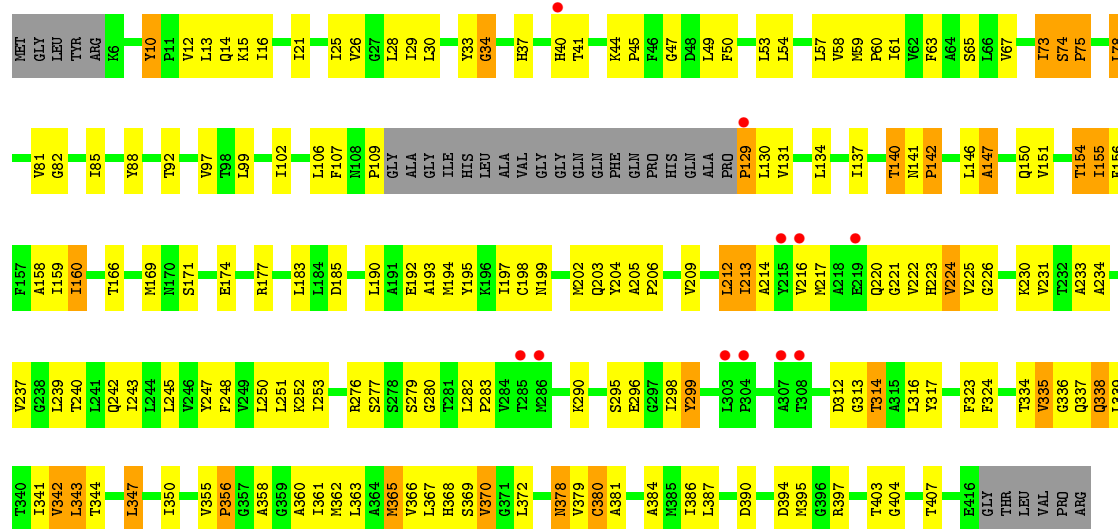- Molecule 1: sodium-coupled L-aspartate transporter

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:

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) 73.5 (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 0.255 , 0.294	Depositor DCC
R_{free} test set	997 reflections (5.62%)	DCC
Wilson B-factor (Å^2)	255.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.15 , 114.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.39, < L^2 > = 0.22$	Xtriage
Outliers	0 of 19459 reflections	Xtriage
F_o,F_c correlation	0.80	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.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	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: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:243:ILE:HA	1:B:247:TYR:CD2	2.18	0.75
1:B:152:LEU:HD12	1:B:152:LEU:H	1.51	0.75
1:D:121:GLN:HG3	1:D:378:ASN:ND2	2.02	0.75
1:C:113:ILE:HA	1:F:40:HIS:HE1	1.50	0.75
1:A:152:LEU:HD12	1:A:152:LEU:H	1.51	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:334:THR:O	1:D:337:GLN:HG2	1.96	0.65
1:D:122:PHE:HB2	1:D:376:ASP:OD1	1.95	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:C:360:ALA:O	1:C:363:LEU:HB3	1.97	0.64
1:B:369:SER:O	1:B:370:VAL:HB	1.96	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:F:61:ILE:HD11	1:F:279:SER:HB2	1.80	0.63
1:E:152:LEU:HB2	1:E:153:PRO:HD3	1.81	0.63
1:D:55:LYS:O	1:D:58:VAL:HG12	1.99	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:E:192:GLU:HA	1:E:195:TYR:CD2	2.35	0.62
1:C:61:ILE:HG22	1:C:194:MET:HB3	1.79	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:E:55:LYS:O	1:E:58:VAL:HG12	2.00	0.61
1:C:339:LEU:O	1:C:342: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:D:141:ASN:ND2	1:F:147:ALA:O	2.33	0.60
1:C:369:SER:O	1:C:370:VAL:HB	2.00	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:F:344:THR:HB	1:F:366:VAL:HG23	1.83	0.60
1:C:61:ILE:HD11	1:C:279:SER:HB2	1.82	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:E:99:LEU:HA	1:E:102:ILE:HD12	1.85	0.58
1:B:44:LYS:N	1:B:45:PRO:HD2	2.19	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:E:195:TYR:HA	1:E:198:CYS:SG	2.44	0.57
1:C:159:ILE:HG22	1:C:160:ILE:N	2.19	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:C:150:GLN:O	1:C:154:THR:OG1	2.22	0.57
1:A:99:LEU:HA	1:A:102:ILE:HD12	1.86	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:E:103:MET:CE	1:E:237:VAL:HG23	2.35	0.57
1:A:44:LYS:N	1:A:45:PRO:HD2	2.20	0.57
1:F:250:LEU:HA	1:F:253:ILE:HG22	1.87	0.56
1:E:44:LYS:N	1:E:45:PRO:HD2	2.20	0.56
1:A:141:ASN:ND2	1:C:147:ALA:O	2.38	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:B:190:LEU:O	1:B:194:MET:HG2	2.06	0.56
1:D:190:LEU:O	1:D:194:MET:HG2	2.05	0.56
1:F:384:ALA:HA	1:F:387:LEU:HB3	1.88	0.56
1:F:339:LEU:O	1:F:342:VAL:HG12	2.05	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:C:282:LEU:H	1:C:283:PRO:HD2	1.70	0.55
1:B:227:GLU:O	1:B:231:VAL:HG23	2.06	0.55
1:C:282:LEU:N	1:C:283:PRO:HD2	2.22	0.55
1:B:195:TYR:HA	1:B:198:CYS:SG	2.46	0.55
1:F:67:VAL:HG22	1:F:158:ALA:HB1	1.87	0.55
1:F:338:GLN:HA	1:F:341:ILE:HD12	1.88	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:282:LEU:N	1:F:283:PRO:HD2	2.22	0.55
1:C:67:VAL:HG22	1:C:158:ALA:HB1	1.87	0.55
1:F:97:VAL:HG21	1:F:342:VAL:HA	1.89	0.55
1:F:282:LEU:H	1:F:283:PRO:HD2	1.71	0.55
1:D:103:MET:CE	1:D:237:VAL:HG23	2.37	0.55
1:F:379:VAL:C	1:F:381:ALA:H	2.07	0.54
1:D:103:MET:HE2	1:D:237:VAL:HG23	1.90	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:C:377:PRO:HG3	1:F:361:ILE:HG12	1.91	0.53
1:A:53:LEU:O	1:A:57:LEU:HG	2.07	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:F:54:LEU:HD23	1:F:277:SER:HB2	1.92	0.52
1:D:227:GLU:O	1:D:231:VAL:HG23	2.10	0.52
1:D:146:LEU:HD11	1:E:143:PHE:CE1	2.45	0.52
1:A:26:VAL:HA	1:A:29:ILE:HG12	1.91	0.52
1:F:47:GLY:O	1:F:50:PHE:HB3	2.10	0.52
1:D:26:VAL:HA	1:D:29:ILE:HG12	1.92	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: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:D:184:LEU:HA	1:D:187:ILE:HD12	1.92	0.51
1:C:224:VAL:N	1:C:228:LEU:HD12	2.26	0.51
1:C:205:ALA:N	1:C:206:PRO:HD2	2.26	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:D:190:LEU:CA	1:E:183:LEU:HD11	2.40	0.51
1:B:246:VAL:O	1:B:250:LEU:HG	2.11	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:D:147:ALA:O	1:E:141:ASN:ND2	2.44	0.50
1:C:82:GLY:HA2	1:C:85:ILE:HG22	1.92	0.50
1:B:390:ASP:HA	1:B:393:LEU:HD12	1.93	0.50
1:D:132:HIS:O	1:D:136:ASP:N	2.40	0.50
1:C:29:ILE:HG13	1:C:30:LEU:N	2.26	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:B:360:ALA:O	1:B:363:LEU:HB3	2.12	0.50
1:A:133:ILE:HA	1:A:136:ASP:HB2	1.94	0.50
1:A:132:HIS:O	1:A:136:ASP:N	2.42	0.50
1:D:190:LEU:N	1:E:183:LEU:HD11	2.26	0.50
1:F:75:PRO:HA	1:F:78:LEU:N	2.27	0.50
1:E:56:MET:HA	1:F:140:THR:O	2.11	0.50
1:D:246:VAL:O	1:D:250:LEU:HG	2.12	0.50
1:C:380:CYS:CB	1:F:380:CYS:CB	2.89	0.50
1:E:26:VAL:HA	1:E:29:ILE:HG12	1.92	0.50
1:E:390:ASP:HA	1:E:393:LEU:HD12	1.93	0.50
1:F:199:ASN:HA	1:F:202:MET:HG2	1.93	0.50
1:E:184:LEU:HA	1:E:187:ILE:HD12	1.93	0.50
1:C:384:ALA:HA	1:C:387:LEU:HB3	1.93	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: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:E:133:ILE:HA	1:E:136:ASP:HB2	1.94	0.50
1:E:58:VAL:HG13	1:E:59:MET:N	2.27	0.49
1:B:26:VAL:HA	1:B:29:ILE:HG12	1.93	0.49
1:D:247:TYR:CE1	1:D:404:GLY:HA2	2.47	0.49
1:D:105:ARG:HH21	1:D:338:GLN:HE22	1.61	0.49
1:A:205:ALA:N	1:A:206:PRO:HD2	2.27	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:195:TYR:HA	1:D:198:CYS:SG	2.51	0.49
1:D:183:LEU:CD1	1:F:190:LEU:N	2.75	0.49
1:A:247:TYR:CE1	1:A:404:GLY:HA2	2.48	0.49
1:C:97:VAL:HG21	1:C:342:VAL:HA	1.95	0.49
1:E:50:PHE:O	1:E:54:LEU:HD12	2.13	0.49
1:C:13:LEU:HD22	1:C:14:GLN:NE2	2.28	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:247:TYR:CE1	1:E:404:GLY:HA2	2.48	0.49
1:A:362:MET:O	1:A:365:MET:HB3	2.13	0.49
1:F:344:THR:HA	1:F:347:LEU:HD22	1.95	0.49
1:B:103:MET:HE2	1:B:237:VAL:HG23	1.93	0.49
1:E:103:MET:HE2	1:E:237:VAL:HG23	1.94	0.49
1:A:61:ILE:O	1:A:65:SER:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:MET:HE2	1:C:157:PHE:HD1	1.78	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:F:347:LEU:HA	1:F:350:ILE:HD12	1.95	0.48
1:E:205:ALA:N	1:E:206:PRO:HD2	2.28	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:50:PHE:O	1:B:54:LEU:HD12	2.13	0.48
1:C:347:LEU:HA	1:C:350:ILE:HD12	1.95	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:B:209:VAL:O	1:B:213:ILE:HG13	2.13	0.48
1:E:189:GLY:O	1:E:193:ALA:N	2.27	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:C:344:THR:HA	1:C:347:LEU:HD22	1.95	0.48
1:B:61:ILE:HG13	1:B:62:VAL:H	1.79	0.48
1:E:309:ILE:HG22	1:E:310:ASN:N	2.29	0.48
1:F:102:ILE:O	1:F:106:LEU:HG	2.14	0.47
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: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:333:LEU:HA	1:B:337:GLN:NE2	2.29	0.47
1:B:155:ILE:HG22	1:B:156:PHE:N	2.29	0.47
1:B:247:TYR:CE1	1:B:404:GLY:HA2	2.49	0.47
1:C:299:TYR:CD2	1:C:299:TYR:C	2.87	0.47
1:A:333:LEU:HA	1:A:337:GLN:NE2	2.29	0.47
1:C:240:THR:HA	1:C:243:ILE:HD12	1.96	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:D:61:ILE:O	1:D:65:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:50:PHE:HB2	1:F:204:TYR:HE2	1.79	0.47
1:B:295:SER:HB3	1:B:298:ILE:HD13	1.97	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:F:61:ILE:CG2	1:F:194:MET:HB3	2.45	0.47
1:E:333:LEU:HA	1:E:337:GLN:NE2	2.30	0.47
1:C:54:LEU:HD23	1:C:277:SER:HB2	1.96	0.47
1:A:309:ILE:HG22	1:A:310:ASN:N	2.30	0.47
1:B:362:MET:O	1:B:365:MET:HB3	2.14	0.47
1:B:107:PHE:O	1:B:109:PRO:HD3	2.15	0.47
1:E:39:VAL:C	1:E:41:THR:H	2.18	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:F:75:PRO:HA	1:F:78:LEU:H	1.81	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:A:209:VAL:O	1:A:213:ILE:HG13	2.15	0.46
1:D:143:PHE:CE2	1:F:146:LEU:HD21	2.50	0.46
1:A:107:PHE:O	1:A:109:PRO:HD3	2.16	0.46
1:F:192:GLU:CA	1:F:195:TYR:HD2	2.20	0.46
1:B:189:GLY:O	1:B:193:ALA:N	2.26	0.46
1:F:193:ALA:O	1:F:197:ILE:HG13	2.16	0.46
1:E:187:ILE:O	1:E:190:LEU:HB3	2.15	0.46
1:A:364:ALA:HA	1:A:367:LEU:HD12	1.97	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:N	1:C:378:ASN:OD1	2.42	0.46
1:C:194:MET:HA	1:C:197:ILE:HD12	1.97	0.46
1:B:105:ARG:HH21	1:B:338:GLN:HE22	1.63	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:E:61:ILE:O	1:E:65:SER:HB3	2.17	0.45
1:D:8:ILE:HG23	1:D:8:ILE:O	2.17	0.45
1:D:295:SER:HB3	1:D:298:ILE:HD13	1.97	0.45
1:F:151:VAL:O	1:F:154:THR:OG1	2.28	0.45
1:C:282:LEU:H	1:C:283:PRO:HD3	1.79	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:A:8:ILE:HG23	1:A:8:ILE:O	2.16	0.45
1:F:282:LEU:H	1:F:283:PRO:HD3	1.81	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:D:39:VAL:C	1:D:41:THR:H	2.20	0.45
1:F:299:TYR:CD2	1:F:299:TYR:C	2.89	0.45
1:B:61:ILE:O	1:B:65:SER:HB3	2.17	0.45
1:E:276:ARG:HD3	1:E:395:MET:HG2	1.98	0.45
1:D:276:ARG:HD3	1:D:395:MET:HG2	1.99	0.45
1:F:379:VAL:C	1:F:381:ALA:N	2.69	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: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:186:ALA:O	1:C:183:LEU:HG	2.16	0.45
1:F:363:LEU:O	1:F:367:LEU:HG	2.17	0.45
1:F:355:VAL:CG1	1:F:356:PRO:HD2	2.47	0.45
1:C:313:GLY:C	1:C:397:ARG:HG3	2.37	0.45
1:B:39:VAL:C	1:B:41:THR:H	2.21	0.45
1:F:240:THR:HA	1:F:243:ILE:HD12	1.99	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: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:A:39:VAL:C	1:A:41:THR:H	2.20	0.44
1:F:12:VAL:O	1:F:13:LEU:C	2.55	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:49:LEU:O	1:F:53:LEU:HG	2.17	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:C:290:LYS:HE3	1:C:299:TYR:HH	1.81	0.44
1:C:21:ILE:O	1:C:25:ILE:HD12	2.17	0.44
1:D:364:ALA:HA	1:D:367:LEU:HD12	1.98	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
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

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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: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:E:243:ILE:HG22	1:E:248:PHE:CE1	2.53	0.44
1:D:303:LEU:N	1:D:304:PRO:HD2	2.32	0.44
1:E:355:VAL:HG13	1:E:356:PRO:HD2	2.00	0.44
1:B:303:LEU:N	1:B:304:PRO:HD2	2.33	0.44
1:F:28:LEU:HD22	1:F:217:MET:HB3	2.00	0.43
1:E:107:PHE:O	1:E:109:PRO:HD3	2.17	0.43
1:F:390:ASP:O	1:F:394:ASP:N	2.45	0.43
1:C:334:THR:N	1:C:337:GLN:HE21	2.11	0.43
1:C:28:LEU:HD22	1:C:217:MET:HB3	1.99	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:363:LEU:HA	1:A:366:VAL:HG12	2.00	0.43
1:F:16:ILE:HG23	1:F:206:PRO:HA	2.00	0.43
1:D:143:PHE:CE1	1:F:146:LEU:HD11	2.53	0.43
1:A:216:VAL:HG12	1:A:224:VAL:HG11	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:F:313:GLY:O	1:F:397:ARG:HG3	2.18	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:B:75:PRO:HA	1:B:76:ALA:HA	1.62	0.43
1:F:334:THR:C	1:F:336:GLY:H	2.22	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:F:141:ASN:HA	1:F:142:PRO:HD2	1.76	0.43
1:A:70:ALA:HB3	1:A:162:GLY:HA3	2.01	0.43
1:D:75:PRO:HA	1:D:76:ALA:HA	1.63	0.43
1:B:355:VAL:HG13	1:B:356:PRO:HD2	2.01	0.43
1:E:10:TYR:HB2	1:E:15:LYS:HD2	2.01	0.43
1:A:240:THR:HA	1:A:243:ILE:HD12	2.00	0.43
1:C:334:THR:C	1:C:336:GLY:H	2.21	0.43
1:C:109:PRO:O	1:C:324:PHE:HA	2.19	0.43
1:D:187:ILE:O	1:D:190:LEU:HB3	2.19	0.43
1:C:231:VAL:O	1:C:235:VAL:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:TYR:HB2	1:B:15:LYS:HD2	2.01	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: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:B:364:ALA:HA	1:B:367:LEU:HD12	2.01	0.42
1:A:243:ILE:HG22	1:A:248:PHE:CE1	2.54	0.42
1:D:190:LEU:H	1:E:183:LEU:CD1	2.30	0.42
1:C:379:VAL:C	1:C:381:ALA:N	2.72	0.42
1:B:276:ARG:HD3	1:B:395:MET:HG2	2.01	0.42
1:E:70:ALA:HB3	1:E:162:GLY:HA3	2.00	0.42
1:A:321:ALA:HB1	1:A:386:ILE:HD13	2.00	0.42
1:F:61:ILE:HG22	1:F:194:MET:CB	2.50	0.42
1:D:363:LEU:HA	1:D:366:VAL:HG12	2.00	0.42
1:B:140:THR:HG23	1:B:141:ASN:H	1.84	0.42
1:E:363:LEU:HA	1:E:366:VAL:HG12	2.01	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:E:369:SER:O	1:E:370:VAL:CB	2.66	0.42
1:C:171:SER:O	1:C:177:ARG:HG3	2.20	0.42
1:A:393:LEU:H	1:A:393:LEU:HG	1.72	0.42
1:A:110:GLY:O	1:A:113:ILE:HG22	2.20	0.42
1:F:247:TYR:OH	1:F:404:GLY:HA3	2.19	0.42
1:E:185:ASP:O	1:E:188:ASN:O	2.38	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: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:C:57:LEU:O	1:C:58:VAL:C	2.58	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: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:D:243:ILE:O	1:D:248:PHE:HD1	2.03	0.42
1:C:141:ASN:HA	1:C:142:PRO:HD2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:GLU:HA	1:F:299:TYR:CE1	2.55	0.42
1:B:363:LEU:HA	1:B:366:VAL:HG12	2.02	0.42
1:F:314:THR:HG23	1:F:397:ARG:HD3	2.02	0.42
1:D:216:VAL:HG12	1:D:224:VAL:HG11	2.02	0.42
1:B:321:ALA:HB1	1:B:386:ILE:HD13	2.01	0.42
1:C:152:LEU:O	1:C:155:ILE:HB	2.20	0.42
1:B:49:LEU:HD23	1:B:204:TYR:OH	2.20	0.42
1:C:373:PRO:C	1:C:375:THR:H	2.23	0.42
1:F:54:LEU:HD12	1:F:54:LEU:N	2.35	0.42
1:B:216:VAL:HG12	1:B:224:VAL:HG11	2.02	0.42
1:C:61:ILE:HG22	1:C:194:MET:CB	2.46	0.41
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:F:334:THR:N	1:F:337:GLN:HE21	2.11	0.41
1:E:225:VAL:HA	1:E:228:LEU:HD12	2.02	0.41
1:C:198:CYS:O	1:C:202:MET:CG	2.63	0.41
1:F:403:THR:O	1:F:407:THR:OG1	2.36	0.41
1:F:155:ILE:O	1:F:156:PHE:C	2.58	0.41
1:C:50:PHE:O	1:C:54:LEU:HD13	2.20	0.41
1:B:216:VAL:HG11	1:B:385:MET:HG2	2.02	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:E:240:THR:HA	1:E:243:ILE:HD12	2.03	0.41
1:B:185:ASP:OD1	1:C:179:SER:HA	2.20	0.41
1:E:141:ASN:HA	1:E:142:PRO:HD2	1.82	0.41
1:B:198:CYS:O	1:B:202:MET:HG2	2.21	0.41
1:A:299:TYR:HB2	1:A:303:LEU:HD23	2.02	0.41
1:D:185:ASP:O	1:D:188:ASN:O	2.39	0.41
1:E:243:ILE:O	1:E:248:PHE:HD1	2.03	0.41
1:B:243:ILE:O	1:B:248:PHE:HD1	2.04	0.41
1:F:85:ILE:O	1:F:88:TYR:HB3	2.21	0.41
1:F:341:ILE:C	1:F:343:LEU:N	2.73	0.41
1:C:193:ALA:O	1:C:197:ILE:HG13	2.21	0.41
1:F:213:ILE:HA	1:F:216:VAL:HB	2.03	0.41
1:F:63:PHE:O	1:F:67:VAL:HG23	2.21	0.41
1:C:75:PRO:HA	1:C:78:LEU:H	1.84	0.41
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:TYR:HA	1:B:239:LEU:HD12	2.03	0.41
1:B:70:ALA:HB3	1:B:162:GLY:HA3	2.03	0.41
1:E:343:LEU:O	1:E:347:LEU:HD13	2.21	0.41
1:D:49:LEU:HD23	1:D:204:TYR:OH	2.21	0.41
1:C:333:LEU:HA	1:C:337:GLN:HE21	1.85	0.41
1:C:276:ARG:HG2	1:C:395:MET:HA	2.03	0.41
1:B:309:ILE:HG22	1:B:310:ASN:H	1.86	0.41
1:E:110:GLY:O	1:E:113:ILE:HG22	2.20	0.41
1:A:282:LEU:HD13	1:A:307:ALA:HB2	2.03	0.41
1:D:240:THR:HA	1:D:243:ILE:HD12	2.02	0.40
1:C:190:LEU:O	1:C:194:MET:HG2	2.21	0.40
1:A:151:VAL:HG12	1:A:155:ILE:HD13	2.03	0.40
1:A:195:TYR:HA	1:A:198:CYS:SG	2.60	0.40
1:A:155:ILE:O	1:A:156:PHE:C	2.59	0.40
1:F:74:SER:O	1:F:75:PRO:C	2.59	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:A:243:ILE:O	1:A:248:PHE:HD1	2.04	0.40
1:D:183:LEU:HD11	1:F:190:LEU:HB2	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:A:355:VAL:HG13	1:A:356:PRO:HD2	2.03	0.40
1:D:151:VAL:HG12	1:D:155:ILE:HD13	2.04	0.40
1:C:155:ILE:HD12	1:C:155:ILE:H	1.87	0.40
1:A:143:PHE:CE2	1:C:146:LEU:HD21	2.56	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:D:309:ILE:HG22	1:D:310:ASN:H	1.87	0.40
1:C:155:ILE:O	1:C:156:PHE:C	2.59	0.40
1:B:343:LEU:O	1:B:347:LEU:HD13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	409/422 (97%)	357 (87%)	44 (11%)	8 (2%)	9	53
1	B	400/422 (95%)	350 (88%)	44 (11%)	6 (2%)	13	58
1	C	396/422 (94%)	302 (76%)	75 (19%)	19 (5%)	3	32
1	D	409/422 (97%)	356 (87%)	44 (11%)	9 (2%)	8	51
1	E	399/422 (94%)	350 (88%)	42 (10%)	7 (2%)	11	54
1	F	388/422 (92%)	296 (76%)	73 (19%)	19 (5%)	3	31
All	All	2401/2532 (95%)	2011 (84%)	322 (13%)	68 (3%)	6	46

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%)	41	74
1	B	317/330 (96%)	305 (96%)	12 (4%)	40	74
1	C	312/330 (94%)	281 (90%)	31 (10%)	10	42
1	D	321/330 (97%)	308 (96%)	13 (4%)	38	72
1	E	316/330 (96%)	304 (96%)	12 (4%)	40	74
1	F	308/330 (93%)	279 (91%)	29 (9%)	11	44
All	All	1895/1980 (96%)	1786 (94%)	109 (6%)	25	63

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 (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 carbohydrates 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	A	501	-	2,8,8	0.20	0	0,10,10	0.00	-
2	ASP	B	501	-	2,8,8	0.22	0	0,10,10	0.00	-
2	ASP	C	501	-	2,8,8	0.15	0	0,10,10	0.00	-
2	ASP	D	501	-	2,8,8	0.19	0	0,10,10	0.00	-
2	ASP	E	501	-	2,8,8	0.19	0	0,10,10	0.00	-
2	ASP	F	501	-	2,8,8	0.16	0	0,10,10	0.00	-

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/422 (97%)	0.10	28 (6%)	20	16	216, 306, 404, 449	0
1	B	404/422 (95%)	0.26	41 (10%)	9	8	198, 281, 385, 436	0
1	C	400/422 (94%)	-0.16	10 (2%)	61	51	192, 246, 347, 443	0
1	D	411/422 (97%)	0.05	28 (6%)	20	16	213, 290, 399, 435	0
1	E	403/422 (95%)	-0.13	8 (1%)	68	59	208, 264, 369, 402	0
1	F	392/422 (92%)	-0.20	11 (2%)	56	47	200, 246, 348, 452	0
All	All	2421/2532 (95%)	-0.01	126 (5%)	31	25	192, 274, 386, 452	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	352	THR	8.5
1	B	317	TYR	6.5
1	B	124	PRO	6.3
1	B	315	ALA	6.1
1	B	112	GLY	5.8
1	F	129	PRO	5.8
1	B	314	THR	5.6
1	D	313	GLY	5.6
1	B	353	ALA	5.3
1	B	318	GLN	5.1
1	D	318	GLN	5.1
1	D	314	THR	4.9
1	D	297	GLY	4.9
1	B	123	GLN	4.6
1	C	216	VAL	4.5
1	B	316	LEU	4.5
1	B	359	GLY	4.4
1	A	226	GLY	4.3
1	B	319	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	313	GLY	4.2
1	C	174	GLU	4.1
1	B	113	ILE	4.0
1	D	352	THR	4.0
1	D	353	ALA	4.0
1	A	228	LEU	4.0
1	A	229	ALA	3.7
1	D	416	GLU	3.7
1	B	127	ALA	3.7
1	D	278	SER	3.6
1	B	397	ARG	3.5
1	D	298	ILE	3.5
1	E	220	GLN	3.5
1	D	385	MET	3.5
1	A	411	ILE	3.4
1	D	317	TYR	3.4
1	A	256	ILE	3.3
1	D	300	SER	3.3
1	B	378	ASN	3.3
1	C	112	GLY	3.2
1	D	382	ALA	3.2
1	A	315	ALA	3.2
1	A	352	THR	3.2
1	A	407	THR	3.2
1	F	304	PRO	3.1
1	B	362	MET	3.1
1	F	216	VAL	3.1
1	A	227	GLU	3.1
1	A	318	GLN	3.1
1	C	172	GLU	3.1
1	A	223	HIS	3.0
1	C	332	HIS	3.0
1	B	128	PRO	3.0
1	C	170	ASN	2.9
1	B	174	GLU	2.9
1	A	174	GLU	2.9
1	A	389	ILE	2.9
1	A	319	GLY	2.8
1	A	33	TYR	2.8
1	A	113	ILE	2.8
1	D	311	MET	2.8
1	B	170	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	354	GLY	2.8
1	B	129	PRO	2.8
1	B	220	GLN	2.8
1	A	36	ALA	2.7
1	B	126	GLN	2.7
1	D	401	ASN	2.7
1	D	322	THR	2.7
1	B	358	ALA	2.7
1	A	225	VAL	2.7
1	A	414	LYS	2.7
1	B	125	HIS	2.7
1	E	353	ALA	2.7
1	D	203	GLN	2.6
1	E	317	TYR	2.6
1	A	255	GLY	2.6
1	A	353	ALA	2.6
1	D	267	ASP	2.6
1	F	285	THR	2.6
1	B	114	HIS	2.6
1	C	392	ILE	2.6
1	B	254	TYR	2.6
1	A	410	ALA	2.6
1	B	255	GLY	2.6
1	B	363	LEU	2.5
1	E	312	ASP	2.5
1	D	109	PRO	2.5
1	F	303	LEU	2.5
1	D	274	VAL	2.4
1	D	315	ALA	2.4
1	D	324	PHE	2.4
1	B	345	ALA	2.4
1	A	35	TYR	2.4
1	F	215	TYR	2.4
1	B	111	ALA	2.4
1	B	311	MET	2.4
1	A	261	PHE	2.3
1	B	393	LEU	2.3
1	B	256	ILE	2.3
1	B	372	LEU	2.3
1	A	254	TYR	2.3
1	F	286	MET	2.3
1	F	40	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	403	THR	2.3
1	C	313	GLY	2.2
1	A	292	MET	2.2
1	F	307	ALA	2.2
1	B	348	ALA	2.2
1	D	312	ASP	2.2
1	D	301	PHE	2.2
1	B	385	MET	2.2
1	E	140	THR	2.2
1	E	281	THR	2.1
1	D	397	ARG	2.1
1	C	331	SER	2.1
1	E	113	ILE	2.1
1	A	385	MET	2.1
1	B	356	PRO	2.1
1	D	412	VAL	2.1
1	F	219	GLU	2.1
1	B	307	ALA	2.1
1	F	308	THR	2.1
1	C	397	ARG	2.1
1	A	321	ALA	2.0
1	E	313	GLY	2.0
1	D	321	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	ASP	D	501	9/9	0.87	1.22	2.21	258,265,274,278	0
2	ASP	F	501	9/9	0.93	0.52	2.13	209,210,213,215	0
2	ASP	C	501	9/9	0.90	0.60	1.69	203,205,206,210	0
3	NA	D	502	1/1	0.98	0.80	1.14	281,281,281,281	0
3	NA	F	502	1/1	0.99	0.58	1.06	206,206,206,206	0
3	NA	C	502	1/1	0.89	0.51	0.89	193,193,193,193	0
3	NA	E	502	1/1	0.97	0.42	0.67	245,245,245,245	0
2	ASP	B	501	9/9	0.74	0.89	0.55	244,250,260,262	0
3	NA	A	503	1/1	0.90	0.66	0.24	270,270,270,270	0
2	ASP	A	501	9/9	0.91	0.42	0.14	263,269,278,280	0
2	ASP	E	501	9/9	0.96	0.34	-0.05	220,226,234,237	0
3	NA	B	503	1/1	0.72	0.60	-0.33	253,253,253,253	0
3	NA	A	502	1/1	0.93	0.24	-0.48	283,283,283,283	0
3	NA	B	502	1/1	0.86	0.36	-0.50	264,264,264,264	0
3	NA	D	503	1/1	0.85	0.32	-0.87	269,269,269,269	0
3	NA	C	503	1/1	0.99	0.17	-1.31	195,195,195,195	0
3	NA	F	503	1/1	0.97	0.25	-1.31	203,203,203,203	0
3	NA	E	503	1/1	0.84	0.16	-1.55	241,241,241,241	0

6.5 Other polymers (i)

There are no such residues in this entry.