Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:29 PM GMT

PDB ID	:	4OYF
Title	:	Crystal structure of GLTPH R397A IN Sodium-bound state
Authors	:	Boudker, O.; Oh, S.; Verdon, G.; Serio, R.
Deposited on	:	2014-02-11
Resolution	:	3.41 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

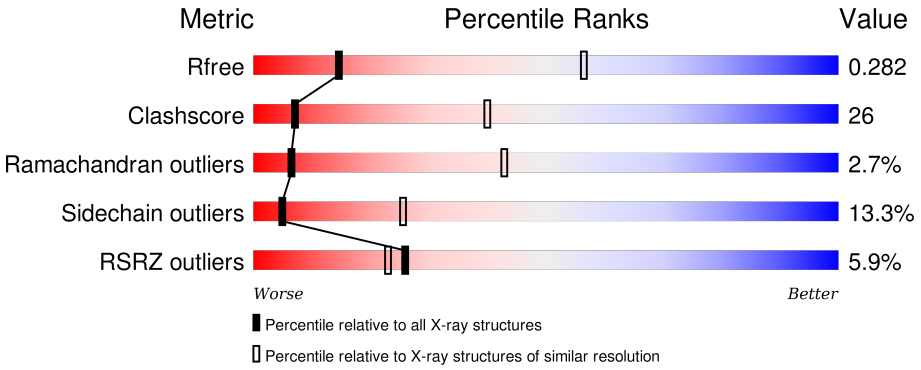
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.41 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}	91344	1049 (3.52-3.32)
Clashscore	102246	1032 (3.50-3.34)
Ramachandran outliers	100387	1002 (3.50-3.34)
Sidechain outliers	100360	1003 (3.50-3.34)
RSRZ outliers	91569	1054 (3.52-3.32)

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	9% 52% 36% 6% 5%
1	B	422	4% 49% 39% 6% 5%
1	C	422	5% 51% 37% 5% 5%
1	D	422	5% 53% 35% 6% 5%
1	E	422	9% 51% 37% 6% 5%

Continued on next page...

Continued from previous page...

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	NA	A	501	-	-	-	X
2	NA	B	501	-	-	-	X
2	NA	C	501	-	-	-	X
2	NA	D	501	-	-	-	X
2	NA	E	501	-	-	-	X
2	NA	F	501	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17592 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 GLUTAMATE SYMPORT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			2930	1926	470	517	17			
1	B	399	Total	C	N	O	S	0	0	0
			2930	1926	470	517	17			
1	C	399	Total	C	N	O	S	0	0	0
			2930	1926	470	517	17			
1	D	399	Total	C	N	O	S	0	0	0
			2930	1926	470	517	17			
1	E	399	Total	C	N	O	S	0	0	0
			2930	1926	470	517	17			
1	F	399	Total	C	N	O	S	0	0	0
			2930	1926	470	517	17			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	F	1	Total	Na	0	0
			1	1		

- Molecule 3 is water.

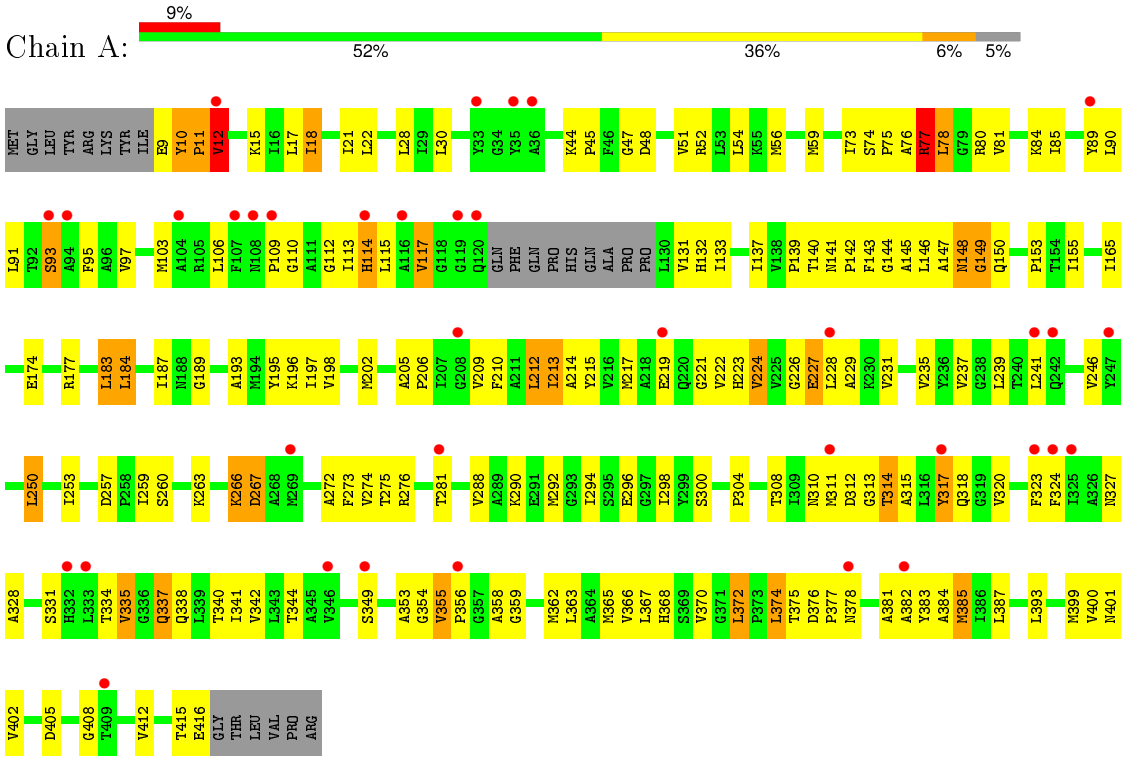
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

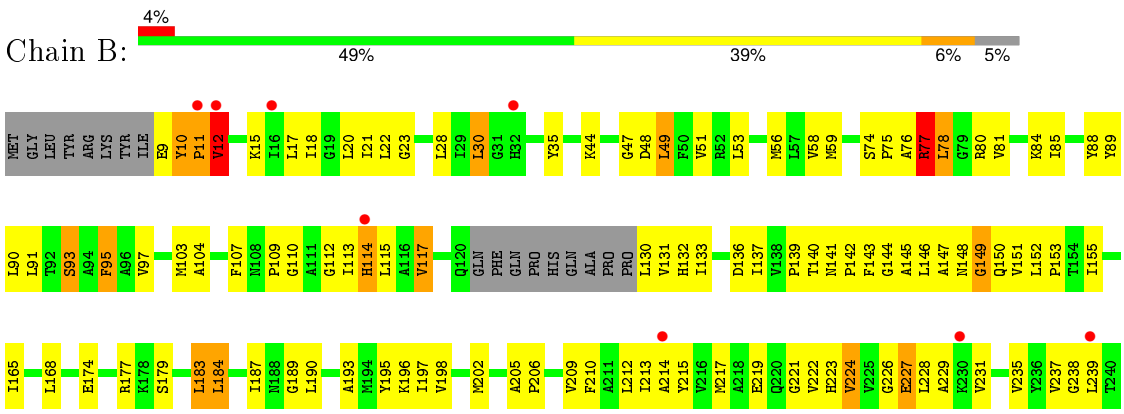
- Molecule 1: GLUTAMATE SYMPORT PROTEIN

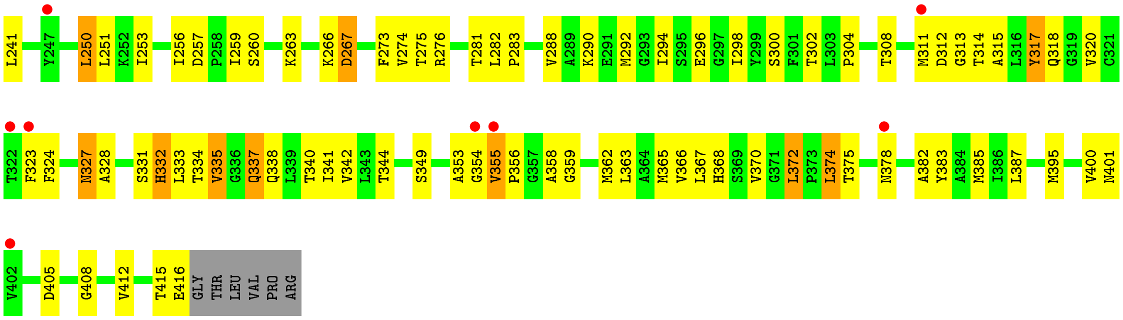
Chain A:



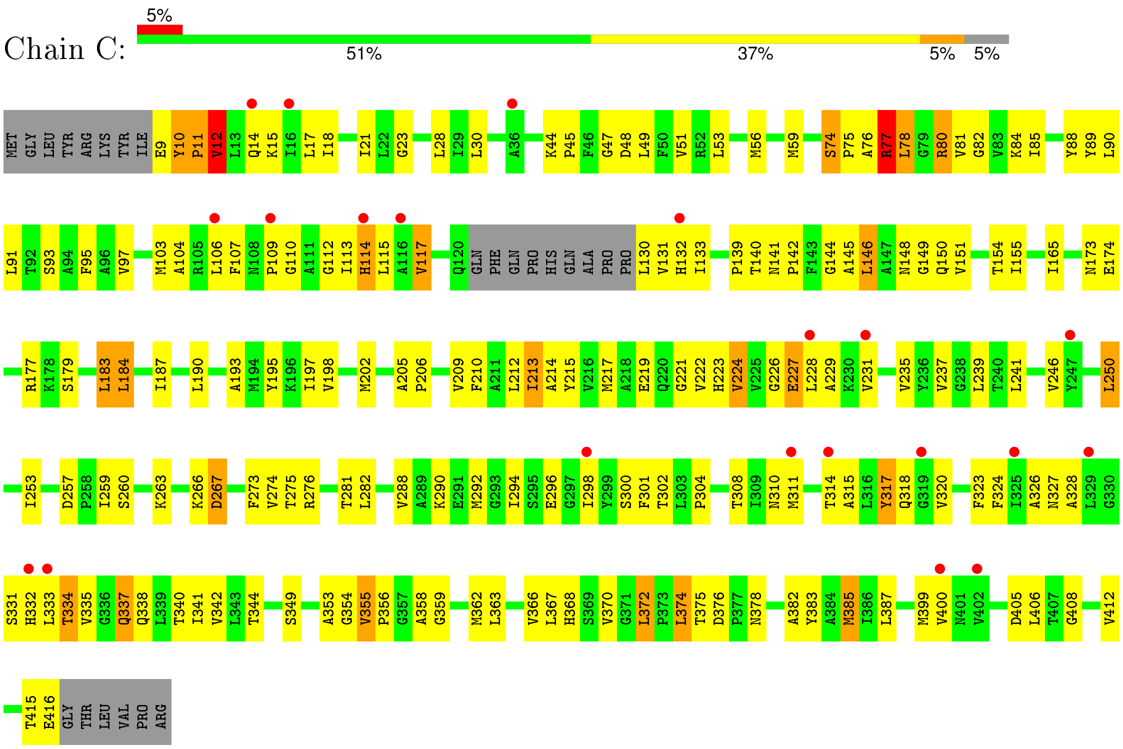
- Molecule 1: GLUTAMATE SYMPORT PROTEIN

Chain B:

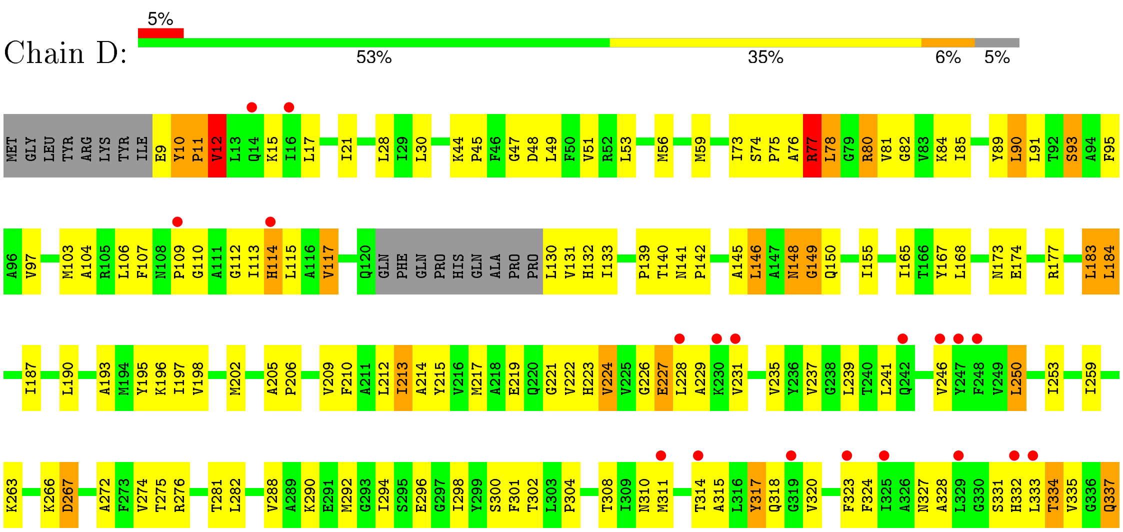


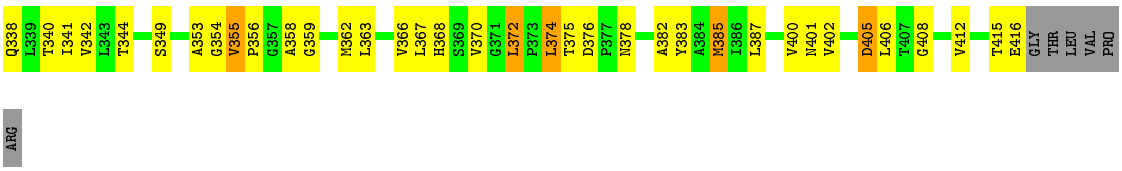


• Molecule 1: GLUTAMATE SYMPORT PROTEIN



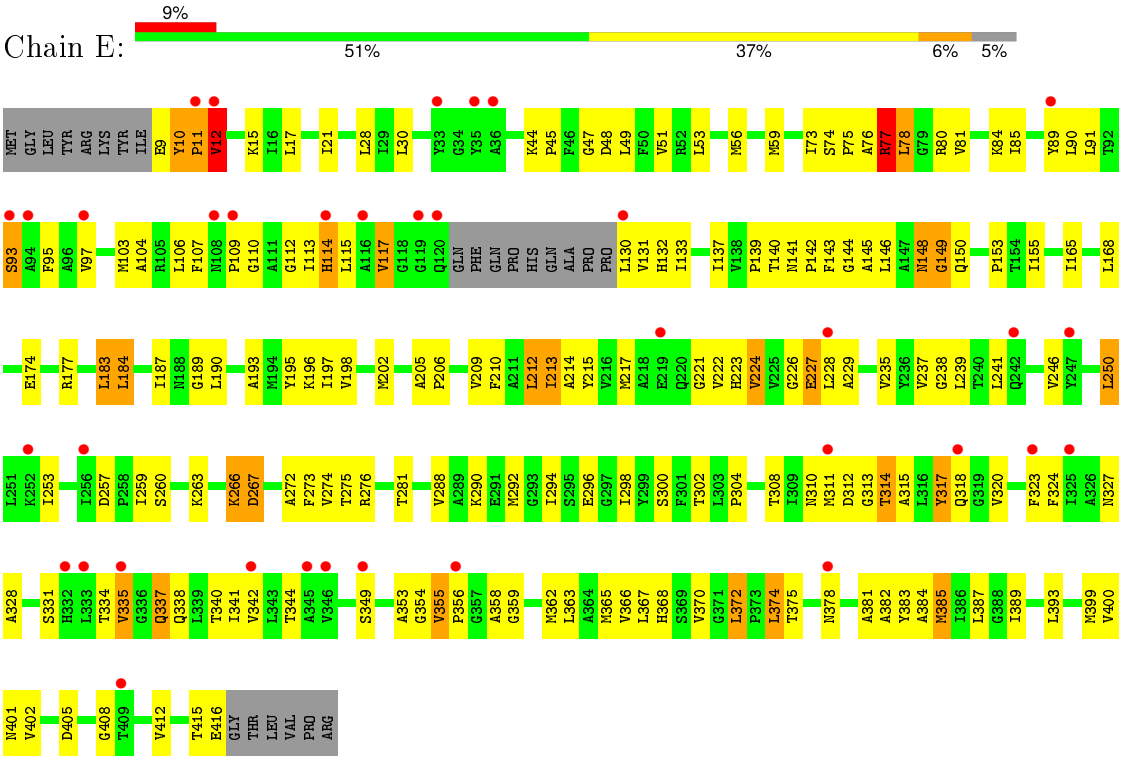
• Molecule 1: GLUTAMATE SYMPORT PROTEIN





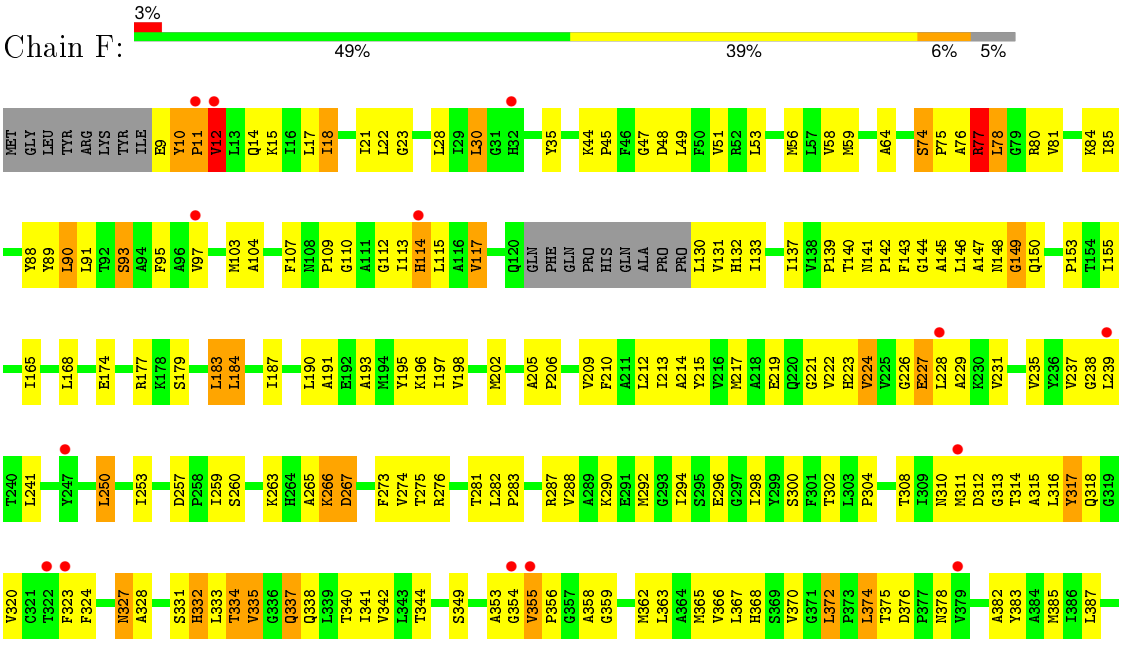
• Molecule 1: GLUTAMATE SYMPORT PROTEIN

Chain E:



• Molecule 1: GLUTAMATE SYMPORT PROTEIN

Chain F:




M395
V400
N401
D405
G408
V412
T415
E416
GLY
THR
LEU
VAL
PRO
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	110.58Å 110.58Å 306.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	12.00 – 3.41 11.99 – 3.41	Depositor EDS
% Data completeness (in resolution range)	88.7 (12.00-3.41) 88.7 (11.99-3.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.75 (at 3.43Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.284 , 0.293 0.272 , 0.282	Depositor DCC
R_{free} test set	2506 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	69.2	Xtriage
Anisotropy	0.609	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 136.3	EDS
Estimated twinning fraction	0.064 for -h,-k,l 0.359 for h,-h-k,-l 0.064 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 49670 reflections	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	17592	wwPDB-VP
Average B, all atoms (Å^2)	152.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.48	0/2983	0.68	0/4067
1	B	0.55	0/2983	0.71	0/4067
1	C	0.54	0/2983	0.70	0/4067
1	D	0.54	0/2983	0.71	0/4067
1	E	0.47	0/2983	0.67	0/4067
1	F	0.56	0/2983	0.72	0/4067
All	All	0.52	0/17898	0.70	0/24402

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2930	0	3077	165	0
1	B	2930	0	3077	161	0
1	C	2930	0	3077	168	0
1	D	2930	0	3077	169	0
1	E	2930	0	3077	163	0
1	F	2930	0	3077	171	0
2	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
All	All	17592	0	18462	949	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (949) 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:113:ILE:HG21	1:D:328:ALA:CA	1.63	1.28
1:C:113:ILE:HG21	1:C:328:ALA:CA	1.65	1.25
1:B:113:ILE:HG21	1:B:328:ALA:CA	1.64	1.24
1:A:113:ILE:HG21	1:A:328:ALA:CA	1.67	1.24
1:F:113:ILE:HG21	1:F:328:ALA:CA	1.65	1.23
1:E:113:ILE:HG21	1:E:328:ALA:CA	1.67	1.23
1:D:113:ILE:CG2	1:D:328:ALA:HA	1.70	1.22
1:C:113:ILE:CG2	1:C:328:ALA:HA	1.72	1.20
1:E:165:ILE:HG21	1:E:184:LEU:HD23	1.23	1.20
1:B:113:ILE:CG2	1:B:328:ALA:HA	1.72	1.18
1:A:113:ILE:CG2	1:A:328:ALA:HA	1.73	1.17
1:F:113:ILE:CG2	1:F:328:ALA:HA	1.73	1.17
1:E:113:ILE:CG2	1:E:328:ALA:HA	1.75	1.15
1:B:165:ILE:HG21	1:B:184:LEU:HD23	1.19	1.14
1:A:165:ILE:HG21	1:A:184:LEU:HD23	1.28	1.13
1:C:165:ILE:HG21	1:C:184:LEU:HD23	1.22	1.09
1:F:165:ILE:HG21	1:F:184:LEU:HD23	1.20	1.08
1:D:165:ILE:HG21	1:D:184:LEU:HD23	1.14	1.06
1:A:209:VAL:HG13	1:A:274:VAL:HG21	1.49	0.95
1:E:209:VAL:HG13	1:E:274:VAL:HG21	1.49	0.94
1:F:209:VAL:HG13	1:F:274:VAL:HG21	1.51	0.92
1:B:209:VAL:HG13	1:B:274:VAL:HG21	1.53	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:VAL:HG13	1:D:274:VAL:HG21	1.54	0.89
1:C:209:VAL:HG13	1:C:274:VAL:HG21	1.54	0.88
1:E:113:ILE:HG21	1:E:328:ALA:HA	0.91	0.87
1:C:112:GLY:O	1:F:114:HIS:NE2	2.08	0.87
1:D:288:VAL:O	1:D:292:MET:HG3	1.76	0.86
1:A:113:ILE:HG21	1:A:328:ALA:HA	0.89	0.85
1:B:114:HIS:NE2	1:D:112:GLY:O	2.09	0.85
1:E:114:HIS:CD2	1:E:114:HIS:H	1.96	0.84
1:A:114:HIS:H	1:A:114:HIS:CD2	1.96	0.84
1:F:113:ILE:HG21	1:F:328:ALA:HA	0.88	0.82
1:C:288:VAL:O	1:C:292:MET:HG3	1.80	0.82
1:B:113:ILE:HG21	1:B:328:ALA:HA	0.87	0.81
1:C:354:GLY:O	1:C:356:PRO:HD2	1.80	0.81
1:B:113:ILE:CG2	1:B:328:ALA:CA	2.45	0.81
1:F:81:VAL:HG21	1:F:298:ILE:HD12	1.62	0.81
1:D:114:HIS:H	1:D:114:HIS:CD2	1.96	0.81
1:D:113:ILE:HG21	1:D:328:ALA:HA	0.86	0.80
1:F:113:ILE:CG2	1:F:328:ALA:CA	2.46	0.80
1:B:81:VAL:HG21	1:B:298:ILE:HD12	1.62	0.80
1:C:113:ILE:HG21	1:C:328:ALA:HA	0.87	0.80
1:B:239:LEU:HB3	1:B:400:VAL:HG21	1.63	0.80
1:B:114:HIS:H	1:B:114:HIS:CD2	1.97	0.80
1:F:114:HIS:CD2	1:F:114:HIS:H	1.98	0.80
1:F:239:LEU:HB3	1:F:400:VAL:HG21	1.63	0.80
1:C:114:HIS:H	1:C:114:HIS:CD2	1.97	0.80
1:C:114:HIS:NE2	1:F:112:GLY:O	2.14	0.79
1:B:288:VAL:O	1:B:292:MET:HG3	1.83	0.79
1:A:112:GLY:O	1:E:114:HIS:NE2	2.15	0.79
1:D:113:ILE:CG2	1:D:328:ALA:CA	2.43	0.78
1:B:112:GLY:O	1:D:114:HIS:NE2	2.15	0.78
1:A:114:HIS:NE2	1:E:112:GLY:O	2.17	0.77
1:D:354:GLY:O	1:D:356:PRO:HD2	1.84	0.77
1:E:9:GLU:HG3	1:E:10:TYR:CD1	2.20	0.77
1:D:165:ILE:HG21	1:D:184:LEU:CD2	2.07	0.76
1:C:84:LYS:HZ2	1:C:415:THR:HG21	1.50	0.76
1:A:113:ILE:CG2	1:A:328:ALA:CA	2.47	0.76
1:A:9:GLU:HG3	1:A:10:TYR:CD1	2.21	0.76
1:F:288:VAL:O	1:F:292:MET:HG3	1.86	0.76
1:A:81:VAL:HG21	1:A:298:ILE:HD12	1.68	0.76
1:C:113:ILE:CG2	1:C:328:ALA:CA	2.46	0.76
1:E:81:VAL:HG21	1:E:298:ILE:HD12	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:LEU:HB3	1:E:400:VAL:HG21	1.67	0.75
1:E:113:ILE:CG2	1:E:328:ALA:CA	2.48	0.75
1:D:84:LYS:HZ2	1:D:415:THR:HG21	1.51	0.75
1:B:354:GLY:O	1:B:356:PRO:HD2	1.86	0.75
1:C:239:LEU:HB3	1:C:400:VAL:HG21	1.68	0.75
1:B:165:ILE:HG21	1:B:184:LEU:CD2	2.11	0.74
1:D:113:ILE:HG21	1:D:328:ALA:CB	2.17	0.74
1:C:81:VAL:HG21	1:C:298:ILE:HD12	1.69	0.74
1:D:239:LEU:HB3	1:D:400:VAL:HG21	1.68	0.74
1:B:195:TYR:O	1:B:198:VAL:HG12	1.87	0.74
1:B:113:ILE:HG21	1:B:328:ALA:CB	2.18	0.74
1:F:113:ILE:HG21	1:F:328:ALA:CB	2.18	0.73
1:D:81:VAL:HG21	1:D:298:ILE:HD12	1.71	0.73
1:D:9:GLU:HG3	1:D:10:TYR:CD1	2.23	0.73
1:A:195:TYR:O	1:A:198:VAL:HG12	1.88	0.73
1:D:12:VAL:H	1:D:15:LYS:HB2	1.54	0.72
1:D:195:TYR:O	1:D:198:VAL:HG12	1.88	0.72
1:C:9:GLU:HG3	1:C:10:TYR:CD1	2.23	0.72
1:E:84:LYS:HZ2	1:E:415:THR:HG21	1.54	0.72
1:F:12:VAL:H	1:F:15:LYS:HB2	1.53	0.72
1:B:112:GLY:HA2	1:B:113:ILE:C	2.09	0.72
1:B:9:GLU:HG3	1:B:10:TYR:CD1	2.23	0.72
1:D:113:ILE:O	1:D:113:ILE:HG22	1.88	0.72
1:C:113:ILE:HG21	1:C:328:ALA:CB	2.20	0.72
1:B:12:VAL:H	1:B:15:LYS:HB2	1.53	0.72
1:C:113:ILE:O	1:C:113:ILE:HG22	1.89	0.71
1:A:84:LYS:HZ2	1:A:415:THR:HG21	1.54	0.71
1:F:112:GLY:HA2	1:F:113:ILE:C	2.09	0.71
1:A:239:LEU:HB3	1:A:400:VAL:HG21	1.71	0.71
1:E:113:ILE:HG21	1:E:328:ALA:CB	2.19	0.71
1:E:195:TYR:O	1:E:198:VAL:HG12	1.90	0.71
1:C:12:VAL:H	1:C:15:LYS:HB2	1.55	0.71
1:F:110:GLY:HA3	1:F:327:ASN:HB3	1.72	0.71
1:B:110:GLY:HA3	1:B:327:ASN:HB3	1.72	0.71
1:D:354:GLY:C	1:D:356:PRO:HD2	2.11	0.71
1:B:77:ARG:HE	1:B:416:GLU:HG2	1.56	0.71
1:A:112:GLY:HA2	1:A:113:ILE:C	2.12	0.70
1:C:112:GLY:HA2	1:C:113:ILE:C	2.12	0.70
1:C:354:GLY:C	1:C:356:PRO:HD2	2.11	0.70
1:A:113:ILE:HG21	1:A:328:ALA:CB	2.20	0.70
1:E:112:GLY:HA2	1:E:113:ILE:C	2.12	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:354:GLY:O	1:F:356:PRO:HD2	1.91	0.70
1:E:78:LEU:HA	1:E:81:VAL:HG12	1.72	0.70
1:F:9:GLU:HG3	1:F:10:TYR:CD1	2.25	0.70
1:A:12:VAL:H	1:A:15:LYS:HB2	1.55	0.70
1:C:81:VAL:HG23	1:C:412:VAL:CG1	2.22	0.69
1:E:12:VAL:H	1:E:15:LYS:HB2	1.56	0.69
1:B:81:VAL:HG23	1:B:412:VAL:CG1	2.23	0.69
1:B:354:GLY:C	1:B:356:PRO:HD2	2.13	0.69
1:C:131:VAL:HG13	1:C:132:HIS:N	2.06	0.69
1:A:224:VAL:O	1:A:229:ALA:HB2	1.93	0.69
1:B:113:ILE:O	1:B:113:ILE:HG22	1.91	0.69
1:E:113:ILE:O	1:E:113:ILE:HG22	1.93	0.69
1:A:78:LEU:HA	1:A:81:VAL:HG12	1.73	0.69
1:B:78:LEU:HA	1:B:81:VAL:HG12	1.75	0.69
1:F:113:ILE:HG22	1:F:113:ILE:O	1.92	0.68
1:B:110:GLY:HA3	1:B:327:ASN:CB	2.24	0.68
1:C:84:LYS:NZ	1:C:415:THR:CG2	2.56	0.68
1:E:288:VAL:O	1:E:292:MET:HG3	1.92	0.68
1:F:81:VAL:HG23	1:F:412:VAL:CG1	2.24	0.68
1:E:81:VAL:HG23	1:E:412:VAL:CG1	2.23	0.68
1:B:76:ALA:O	1:B:77:ARG:HB2	1.92	0.68
1:A:354:GLY:O	1:A:356:PRO:HD2	1.93	0.68
1:F:77:ARG:HE	1:F:416:GLU:HG2	1.59	0.68
1:E:250:LEU:HA	1:E:253:ILE:HG22	1.74	0.68
1:E:224:VAL:O	1:E:229:ALA:HB2	1.94	0.68
1:A:81:VAL:HG23	1:A:412:VAL:CG1	2.23	0.68
1:A:113:ILE:HG22	1:A:113:ILE:O	1.93	0.68
1:A:354:GLY:C	1:A:356:PRO:HD2	2.14	0.68
1:D:193:ALA:O	1:D:197:ILE:HG13	1.93	0.68
1:F:110:GLY:HA3	1:F:327:ASN:CB	2.24	0.68
1:D:112:GLY:HA2	1:D:113:ILE:C	2.15	0.68
1:F:76:ALA:O	1:F:77:ARG:HB2	1.92	0.68
1:E:354:GLY:C	1:E:356:PRO:HD2	2.15	0.68
1:F:354:GLY:C	1:F:356:PRO:HD2	2.15	0.67
1:E:354:GLY:O	1:E:356:PRO:HD2	1.94	0.67
1:E:47:GLY:HA3	1:E:212:LEU:HD23	1.77	0.67
1:D:84:LYS:NZ	1:D:415:THR:CG2	2.58	0.67
1:B:250:LEU:HA	1:B:253:ILE:HG22	1.75	0.67
1:B:131:VAL:HG13	1:B:132:HIS:N	2.10	0.67
1:D:131:VAL:HG13	1:D:132:HIS:N	2.08	0.67
1:D:81:VAL:HG23	1:D:412:VAL:CG1	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:LYS:HZ2	1:F:415:THR:HG21	1.58	0.66
1:F:131:VAL:HG13	1:F:132:HIS:N	2.11	0.66
1:A:250:LEU:HA	1:A:253:ILE:HG22	1.76	0.66
1:F:165:ILE:HG21	1:F:184:LEU:CD2	2.13	0.66
1:A:141:ASN:HD22	1:A:144:GLY:H	1.44	0.65
1:C:195:TYR:O	1:C:198:VAL:HG12	1.95	0.65
1:D:77:ARG:HE	1:D:416:GLU:HG2	1.60	0.65
1:C:193:ALA:O	1:C:197:ILE:HG13	1.95	0.65
1:B:84:LYS:HZ2	1:B:415:THR:HG21	1.60	0.65
1:C:250:LEU:HA	1:C:253:ILE:HG22	1.78	0.65
1:D:250:LEU:HA	1:D:253:ILE:HG22	1.78	0.65
1:F:47:GLY:HA3	1:F:212:LEU:HD23	1.79	0.65
1:F:193:ALA:O	1:F:197:ILE:HG13	1.97	0.64
1:B:47:GLY:HA3	1:B:212:LEU:HD23	1.78	0.64
1:C:110:GLY:HA3	1:C:327:ASN:CB	2.27	0.64
1:B:183:LEU:O	1:B:187:ILE:HG13	1.97	0.64
1:E:110:GLY:HA3	1:E:327:ASN:HB3	1.78	0.64
1:F:250:LEU:HA	1:F:253:ILE:HG22	1.78	0.64
1:B:358:ALA:O	1:B:362:MET:HG3	1.96	0.64
1:B:193:ALA:O	1:B:197:ILE:HG13	1.97	0.64
1:E:110:GLY:HA3	1:E:327:ASN:CB	2.28	0.64
1:F:195:TYR:O	1:F:198:VAL:HG12	1.98	0.64
1:C:76:ALA:O	1:C:77:ARG:HB2	1.96	0.64
1:A:288:VAL:O	1:A:292:MET:HG3	1.97	0.64
1:D:110:GLY:HA3	1:D:327:ASN:HB3	1.78	0.64
1:E:131:VAL:HG13	1:E:132:HIS:N	2.13	0.64
1:F:78:LEU:HA	1:F:81:VAL:HG12	1.78	0.64
1:E:213:ILE:HD12	1:E:214:ALA:H	1.63	0.64
1:E:317:TYR:HD1	1:E:317:TYR:C	2.01	0.64
1:C:110:GLY:HA3	1:C:327:ASN:HB3	1.78	0.64
1:A:317:TYR:HD1	1:A:317:TYR:C	2.02	0.63
1:C:47:GLY:HA3	1:C:212:LEU:HD23	1.79	0.63
1:D:110:GLY:HA3	1:D:327:ASN:CB	2.28	0.63
1:F:183:LEU:O	1:F:187:ILE:HG13	1.98	0.63
1:C:84:LYS:NZ	1:C:415:THR:HG21	2.11	0.63
1:D:84:LYS:NZ	1:D:415:THR:HG21	2.12	0.63
1:D:198:VAL:O	1:D:202:MET:HG2	1.98	0.63
1:C:77:ARG:HE	1:C:416:GLU:HG2	1.62	0.63
1:F:141:ASN:HD22	1:F:144:GLY:H	1.47	0.63
1:A:110:GLY:HA3	1:A:327:ASN:HB3	1.80	0.63
1:A:77:ARG:HE	1:A:416:GLU:HG2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:358:ALA:O	1:F:362:MET:HG3	1.98	0.62
1:A:47:GLY:HA3	1:A:212:LEU:HD23	1.81	0.62
1:B:275:THR:O	1:B:276:ARG:HB2	1.99	0.62
1:F:275:THR:O	1:F:276:ARG:HB2	1.99	0.62
1:C:78:LEU:HA	1:C:81:VAL:HG12	1.81	0.62
1:A:131:VAL:HG13	1:A:132:HIS:N	2.15	0.62
1:D:76:ALA:O	1:D:77:ARG:HB2	1.98	0.62
1:C:221:GLY:O	1:C:224:VAL:HG23	1.99	0.62
1:A:110:GLY:HA3	1:A:327:ASN:CB	2.30	0.62
1:C:317:TYR:C	1:C:317:TYR:HD1	2.03	0.62
1:D:56:MET:HB2	1:E:139:PRO:O	1.99	0.62
1:C:77:ARG:HH21	1:C:416:GLU:HG3	1.65	0.61
1:A:221:GLY:O	1:A:223:HIS:N	2.34	0.61
1:D:47:GLY:HA3	1:D:212:LEU:HD23	1.82	0.61
1:D:78:LEU:HA	1:D:81:VAL:HG12	1.82	0.61
1:E:358:ALA:O	1:E:362:MET:HG3	1.99	0.61
1:F:224:VAL:O	1:F:229:ALA:HB2	2.00	0.60
1:C:84:LYS:HZ1	1:C:415:THR:CG2	2.14	0.60
1:E:221:GLY:O	1:E:223:HIS:N	2.35	0.60
1:E:317:TYR:CD1	1:E:317:TYR:C	2.75	0.60
1:C:114:HIS:CD2	1:F:112:GLY:O	2.54	0.60
1:D:224:VAL:O	1:D:229:ALA:HB2	2.00	0.60
1:A:317:TYR:C	1:A:317:TYR:CD1	2.75	0.60
1:C:224:VAL:O	1:C:229:ALA:HB2	2.00	0.60
1:D:317:TYR:C	1:D:317:TYR:HD1	2.05	0.60
1:B:221:GLY:O	1:B:223:HIS:N	2.35	0.60
1:C:165:ILE:HG21	1:C:184:LEU:CD2	2.15	0.60
1:A:44:LYS:HD2	1:A:215:TYR:CE1	2.37	0.60
1:A:141:ASN:ND2	1:A:144:GLY:H	2.00	0.60
1:E:77:ARG:HE	1:E:416:GLU:HG2	1.67	0.60
1:F:81:VAL:HG23	1:F:412:VAL:HG12	1.83	0.60
1:D:44:LYS:HD2	1:D:215:TYR:CE1	2.37	0.60
1:C:81:VAL:HG23	1:C:412:VAL:HG12	1.82	0.59
1:C:131:VAL:CG1	1:C:132:HIS:N	2.65	0.59
1:B:224:VAL:O	1:B:229:ALA:HB2	2.01	0.59
1:B:317:TYR:C	1:B:317:TYR:HD1	2.05	0.59
1:E:275:THR:O	1:E:276:ARG:HB2	2.02	0.59
1:C:317:TYR:C	1:C:317:TYR:CD1	2.76	0.59
1:A:213:ILE:HD12	1:A:214:ALA:H	1.67	0.59
1:D:213:ILE:HD12	1:D:214:ALA:H	1.67	0.59
1:A:317:TYR:OH	1:A:359:GLY:HA3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG23	1:A:412:VAL:HG11	1.85	0.59
1:C:198:VAL:O	1:C:202:MET:HG2	2.02	0.59
1:B:84:LYS:NZ	1:B:415:THR:CG2	2.66	0.59
1:D:221:GLY:O	1:D:224:VAL:HG23	2.02	0.59
1:D:84:LYS:HZ1	1:D:415:THR:CG2	2.16	0.59
1:D:77:ARG:HH21	1:D:416:GLU:HG3	1.67	0.59
1:F:317:TYR:HD1	1:F:317:TYR:C	2.06	0.59
1:E:76:ALA:O	1:E:77:ARG:HB2	2.00	0.59
1:B:317:TYR:OH	1:B:359:GLY:HA3	2.03	0.59
1:E:81:VAL:HG23	1:E:412:VAL:HG11	1.85	0.59
1:F:84:LYS:NZ	1:F:415:THR:CG2	2.66	0.58
1:B:81:VAL:HG23	1:B:412:VAL:HG11	1.85	0.58
1:B:334:THR:OG1	1:B:337:GLN:HB2	2.03	0.58
1:B:112:GLY:O	1:D:114:HIS:CD2	2.56	0.58
1:C:81:VAL:HG23	1:C:412:VAL:HG11	1.85	0.58
1:A:76:ALA:O	1:A:77:ARG:HB2	2.01	0.58
1:C:44:LYS:HD2	1:C:215:TYR:CE1	2.39	0.58
1:B:48:ASP:O	1:B:51:VAL:N	2.37	0.58
1:E:81:VAL:HG23	1:E:412:VAL:HG12	1.85	0.58
1:D:408:GLY:O	1:D:412:VAL:HG23	2.02	0.58
1:B:213:ILE:HD12	1:B:214:ALA:H	1.67	0.58
1:B:221:GLY:O	1:B:224:VAL:HG23	2.04	0.58
1:B:81:VAL:HG23	1:B:412:VAL:HG12	1.85	0.58
1:A:81:VAL:HG23	1:A:412:VAL:HG12	1.85	0.58
1:D:131:VAL:CG1	1:D:132:HIS:N	2.67	0.58
1:A:358:ALA:O	1:A:362:MET:HG3	2.02	0.58
1:E:15:LYS:HE3	1:E:206:PRO:HG3	1.85	0.58
1:B:198:VAL:O	1:B:202:MET:HG2	2.02	0.58
1:F:221:GLY:O	1:F:224:VAL:HG23	2.04	0.58
1:A:275:THR:O	1:A:276:ARG:HB2	2.03	0.58
1:D:317:TYR:C	1:D:317:TYR:CD1	2.77	0.57
1:A:408:GLY:O	1:A:412:VAL:HG23	2.04	0.57
1:B:317:TYR:C	1:B:317:TYR:CD1	2.78	0.57
1:E:198:VAL:O	1:E:202:MET:HG2	2.04	0.57
1:B:80:ARG:NH1	1:B:416:GLU:OE2	2.38	0.57
1:F:141:ASN:ND2	1:F:144:GLY:H	2.02	0.57
1:B:408:GLY:O	1:B:412:VAL:HG23	2.04	0.57
1:F:317:TYR:OH	1:F:359:GLY:HA3	2.04	0.57
1:F:221:GLY:O	1:F:223:HIS:N	2.38	0.57
1:E:317:TYR:OH	1:E:359:GLY:HA3	2.03	0.57
1:C:112:GLY:O	1:F:114:HIS:CD2	2.57	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:ILE:HD12	1:C:214:ALA:H	1.70	0.57
1:F:48:ASP:O	1:F:51:VAL:N	2.38	0.57
1:C:334:THR:OG1	1:C:337:GLN:HB2	2.04	0.57
1:C:275:THR:O	1:C:276:ARG:HB2	2.04	0.57
1:E:408:GLY:O	1:E:412:VAL:HG23	2.05	0.56
1:F:317:TYR:CD1	1:F:317:TYR:C	2.79	0.56
1:E:80:ARG:NH1	1:E:416:GLU:OE2	2.38	0.56
1:E:56:MET:HB2	1:F:139:PRO:O	2.04	0.56
1:B:131:VAL:CG1	1:B:132:HIS:N	2.68	0.56
1:E:44:LYS:HD2	1:E:215:TYR:CE1	2.40	0.56
1:D:275:THR:O	1:D:276:ARG:HB2	2.04	0.56
1:B:239:LEU:HB3	1:B:400:VAL:CG2	2.33	0.56
1:E:239:LEU:HB3	1:E:400:VAL:CG2	2.36	0.56
1:D:334:THR:OG1	1:D:337:GLN:HB2	2.05	0.56
1:B:114:HIS:CD2	1:D:112:GLY:O	2.59	0.56
1:F:239:LEU:HB3	1:F:400:VAL:CG2	2.33	0.56
1:E:84:LYS:NZ	1:E:415:THR:CG2	2.69	0.56
1:D:358:ALA:O	1:D:362:MET:HG3	2.05	0.56
1:C:296:GLU:O	1:C:300:SER:HB2	2.05	0.56
1:D:205:ALA:N	1:D:206:PRO:HD2	2.20	0.56
1:F:334:THR:OG1	1:F:337:GLN:HB2	2.06	0.56
1:D:221:GLY:O	1:D:223:HIS:N	2.39	0.56
1:E:334:THR:OG1	1:E:337:GLN:HB2	2.06	0.55
1:D:80:ARG:NH1	1:D:416:GLU:OE2	2.39	0.55
1:A:84:LYS:NZ	1:A:415:THR:CG2	2.70	0.55
1:F:131:VAL:CG1	1:F:132:HIS:N	2.69	0.55
1:C:221:GLY:O	1:C:223:HIS:N	2.39	0.55
1:D:174:GLU:OE1	1:D:177:ARG:NE	2.40	0.55
1:F:81:VAL:HG23	1:F:412:VAL:HG11	1.89	0.55
1:D:81:VAL:HG23	1:D:412:VAL:HG11	1.86	0.55
1:A:141:ASN:HD22	1:A:144:GLY:N	2.04	0.55
1:D:85:ILE:HG13	1:D:89:TYR:CE1	2.41	0.55
1:E:155:ILE:HD11	1:E:304:PRO:HB2	1.89	0.55
1:A:334:THR:OG1	1:A:337:GLN:HB2	2.07	0.55
1:A:139:PRO:O	1:C:56:MET:HB2	2.07	0.55
1:A:15:LYS:HE3	1:A:206:PRO:HG3	1.89	0.55
1:B:141:ASN:ND2	1:B:144:GLY:H	2.05	0.55
1:F:84:LYS:NZ	1:F:415:THR:HG21	2.21	0.55
1:F:205:ALA:N	1:F:206:PRO:HD2	2.22	0.55
1:C:59:MET:CE	1:C:146:LEU:HD23	2.37	0.55
1:B:141:ASN:HD22	1:B:144:GLY:H	1.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:ARG:NH1	1:F:416:GLU:OE2	2.40	0.54
1:A:77:ARG:HH21	1:A:416:GLU:HG3	1.72	0.54
1:C:226:GLY:O	1:C:228:LEU:N	2.40	0.54
1:B:205:ALA:N	1:B:206:PRO:HD2	2.22	0.54
1:F:198:VAL:O	1:F:202:MET:HG2	2.07	0.54
1:F:97:VAL:HB	1:F:342:VAL:HG13	1.88	0.54
1:C:358:ALA:O	1:C:362:MET:HG3	2.07	0.54
1:C:281:THR:HG22	1:C:281:THR:O	2.06	0.54
1:C:354:GLY:C	1:C:356:PRO:CD	2.75	0.54
1:D:81:VAL:HG23	1:D:412:VAL:HG12	1.88	0.54
1:E:221:GLY:O	1:E:224:VAL:HG23	2.08	0.54
1:E:109:PRO:O	1:E:227:GLU:OE1	2.26	0.54
1:F:213:ILE:HD12	1:F:214:ALA:H	1.71	0.54
1:A:221:GLY:O	1:A:224:VAL:HG23	2.07	0.54
1:B:84:LYS:NZ	1:B:415:THR:HG21	2.22	0.54
1:D:49:LEU:O	1:D:53:LEU:HD12	2.08	0.54
1:A:80:ARG:NH1	1:A:416:GLU:OE2	2.41	0.54
1:D:308:THR:HB	1:D:353:ALA:HB1	1.89	0.54
1:C:174:GLU:OE1	1:C:177:ARG:NE	2.41	0.54
1:C:80:ARG:NH1	1:C:416:GLU:OE2	2.40	0.53
1:B:97:VAL:HB	1:B:342:VAL:HG13	1.90	0.53
1:A:56:MET:HB2	1:B:139:PRO:O	2.08	0.53
1:D:281:THR:HG22	1:D:281:THR:O	2.07	0.53
1:F:317:TYR:HA	1:F:320:VAL:HG12	1.90	0.53
1:E:84:LYS:HZ2	1:E:415:THR:CG2	2.21	0.53
1:D:226:GLY:O	1:D:228:LEU:N	2.41	0.53
1:A:103:MET:HE1	1:A:237:VAL:CG1	2.39	0.53
1:E:131:VAL:CG1	1:E:132:HIS:N	2.72	0.53
1:D:317:TYR:OH	1:D:359:GLY:HA3	2.09	0.53
1:D:165:ILE:HD11	1:D:183:LEU:CD2	2.39	0.53
1:C:84:LYS:HZ1	1:C:415:THR:HG22	1.74	0.53
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.90	0.53
1:A:281:THR:O	1:A:281:THR:HG22	2.09	0.53
1:D:9:GLU:HB3	1:D:15:LYS:NZ	2.24	0.53
1:C:115:LEU:C	1:C:115:LEU:HD12	2.28	0.53
1:A:84:LYS:HZ2	1:A:415:THR:CG2	2.21	0.52
1:C:85:ILE:HG13	1:C:89:TYR:CE1	2.44	0.52
1:C:335:VAL:HA	1:C:338:GLN:NE2	2.24	0.52
1:A:165:ILE:HD11	1:A:183:LEU:CD2	2.38	0.52
1:B:115:LEU:C	1:B:115:LEU:HD12	2.30	0.52
1:B:213:ILE:HD12	1:B:214:ALA:N	2.23	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:GLY:C	1:D:356:PRO:CD	2.77	0.52
1:B:56:MET:HB2	1:C:139:PRO:O	2.09	0.52
1:A:205:ALA:N	1:A:206:PRO:HD2	2.25	0.52
1:B:81:VAL:CG2	1:B:298:ILE:HD12	2.37	0.52
1:A:198:VAL:O	1:A:202:MET:HG2	2.09	0.52
1:B:226:GLY:O	1:B:228:LEU:N	2.42	0.52
1:C:49:LEU:O	1:C:53:LEU:HD12	2.10	0.52
1:E:338:GLN:O	1:E:341:ILE:HB	2.09	0.52
1:A:239:LEU:HB3	1:A:400:VAL:CG2	2.40	0.52
1:A:131:VAL:CG1	1:A:132:HIS:N	2.73	0.52
1:D:89:TYR:CD2	1:D:310:ASN:HB2	2.44	0.52
1:D:213:ILE:HD12	1:D:214:ALA:N	2.25	0.52
1:C:77:ARG:HE	1:C:416:GLU:CG	2.22	0.52
1:D:115:LEU:C	1:D:115:LEU:HD12	2.29	0.52
1:B:103:MET:HE1	1:B:237:VAL:CG1	2.39	0.52
1:D:146:LEU:HD22	1:E:143:PHE:CE1	2.45	0.52
1:E:141:ASN:HD22	1:E:144:GLY:H	1.57	0.52
1:E:103:MET:HE1	1:E:237:VAL:CG1	2.40	0.52
1:F:81:VAL:CG2	1:F:298:ILE:HD12	2.38	0.52
1:C:317:TYR:OH	1:C:359:GLY:HA3	2.10	0.52
1:D:318:GLN:OE1	1:D:363:LEU:N	2.43	0.52
1:B:113:ILE:HG22	1:B:328:ALA:O	2.11	0.51
1:D:292:MET:HE2	1:D:294:ILE:HD11	1.91	0.51
1:C:174:GLU:OE1	1:C:177:ARG:CZ	2.58	0.51
1:B:109:PRO:O	1:B:227:GLU:OE1	2.27	0.51
1:F:142:PRO:O	1:F:145:ALA:HB3	2.10	0.51
1:F:115:LEU:HD12	1:F:115:LEU:C	2.31	0.51
1:C:183:LEU:O	1:C:187:ILE:HG13	2.10	0.51
1:A:10:TYR:HB3	1:A:11:PRO:CD	2.40	0.51
1:B:44:LYS:HD2	1:B:215:TYR:CE1	2.46	0.51
1:F:113:ILE:HG22	1:F:328:ALA:O	2.11	0.51
1:C:15:LYS:HE3	1:C:206:PRO:HG3	1.91	0.51
1:C:317:TYR:HA	1:C:320:VAL:HG12	1.93	0.51
1:B:317:TYR:HA	1:B:320:VAL:HG12	1.92	0.51
1:A:59:MET:CE	1:A:146:LEU:HD23	2.40	0.51
1:A:382:ALA:HA	1:A:385:MET:HG3	1.92	0.51
1:F:226:GLY:O	1:F:228:LEU:N	2.43	0.51
1:E:281:THR:O	1:E:281:THR:HG22	2.11	0.51
1:E:165:ILE:HD11	1:E:183:LEU:CD2	2.40	0.51
1:C:205:ALA:N	1:C:206:PRO:HD2	2.25	0.51
1:D:174:GLU:OE1	1:D:177:ARG:CZ	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ILE:HD11	1:F:304:PRO:HB2	1.93	0.51
1:F:281:THR:O	1:F:281:THR:HG22	2.08	0.51
1:D:183:LEU:O	1:D:187:ILE:HG13	2.10	0.51
1:B:354:GLY:C	1:B:356:PRO:CD	2.79	0.51
1:E:221:GLY:C	1:E:223:HIS:H	2.14	0.51
1:B:338:GLN:O	1:B:341:ILE:HB	2.10	0.51
1:D:142:PRO:O	1:D:145:ALA:HB3	2.11	0.51
1:A:48:ASP:O	1:A:51:VAL:N	2.44	0.51
1:A:109:PRO:O	1:A:227:GLU:OE1	2.29	0.51
1:C:10:TYR:HB3	1:C:11:PRO:CD	2.41	0.51
1:B:15:LYS:HE3	1:B:206:PRO:HG3	1.92	0.51
1:C:89:TYR:CD2	1:C:310:ASN:HB2	2.45	0.51
1:D:296:GLU:O	1:D:300:SER:HB2	2.10	0.51
1:F:382:ALA:HA	1:F:385:MET:HG3	1.93	0.51
1:C:213:ILE:HD12	1:C:214:ALA:N	2.26	0.51
1:B:221:GLY:C	1:B:223:HIS:H	2.15	0.51
1:F:213:ILE:HD12	1:F:214:ALA:N	2.25	0.51
1:F:103:MET:HE1	1:F:237:VAL:CG1	2.40	0.51
1:D:335:VAL:HA	1:D:338:GLN:NE2	2.26	0.51
1:B:281:THR:HG22	1:B:281:THR:O	2.09	0.51
1:F:298:ILE:O	1:F:302:THR:HG23	2.11	0.51
1:D:10:TYR:HB3	1:D:11:PRO:CD	2.41	0.51
1:E:77:ARG:HH21	1:E:416:GLU:HG3	1.76	0.51
1:E:146:LEU:HD22	1:F:143:PHE:CE1	2.46	0.51
1:B:113:ILE:CG2	1:B:328:ALA:O	2.59	0.50
1:E:10:TYR:HB3	1:E:11:PRO:CD	2.41	0.50
1:C:9:GLU:HB3	1:C:15:LYS:NZ	2.26	0.50
1:F:408:GLY:O	1:F:412:VAL:HG23	2.11	0.50
1:C:97:VAL:HB	1:C:342:VAL:HG13	1.93	0.50
1:D:113:ILE:HG22	1:D:328:ALA:O	2.11	0.50
1:E:205:ALA:N	1:E:206:PRO:HD2	2.27	0.50
1:D:84:LYS:HZ1	1:D:415:THR:HG22	1.76	0.50
1:F:10:TYR:HB3	1:F:11:PRO:CD	2.41	0.50
1:A:221:GLY:C	1:A:223:HIS:H	2.14	0.50
1:A:338:GLN:O	1:A:341:ILE:HB	2.11	0.50
1:E:273:PHE:HB2	1:E:399:MET:HB2	1.94	0.50
1:D:266:LYS:HG2	1:D:267:ASP:N	2.26	0.50
1:F:113:ILE:CG2	1:F:328:ALA:O	2.60	0.50
1:F:15:LYS:HE3	1:F:206:PRO:HG3	1.93	0.50
1:D:77:ARG:HE	1:D:416:GLU:CG	2.23	0.50
1:B:266:LYS:HG2	1:B:267:ASP:N	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ALA:O	1:A:197:ILE:HG13	2.11	0.50
1:F:109:PRO:O	1:F:227:GLU:OE1	2.28	0.50
1:C:239:LEU:HB3	1:C:400:VAL:CG2	2.38	0.50
1:D:15:LYS:HE3	1:D:206:PRO:HG3	1.92	0.50
1:E:84:LYS:NZ	1:E:415:THR:HG21	2.25	0.50
1:C:318:GLN:OE1	1:C:363:LEU:N	2.44	0.50
1:F:76:ALA:O	1:F:77:ARG:CB	2.58	0.50
1:B:335:VAL:HA	1:B:338:GLN:NE2	2.27	0.50
1:D:338:GLN:O	1:D:341:ILE:HB	2.11	0.50
1:A:133:ILE:N	1:A:133:ILE:HD12	2.27	0.50
1:D:239:LEU:HB3	1:D:400:VAL:CG2	2.38	0.50
1:A:362:MET:O	1:A:365:MET:HB2	2.11	0.50
1:A:226:GLY:O	1:A:228:LEU:N	2.45	0.50
1:A:10:TYR:HB3	1:A:11:PRO:HD2	1.94	0.50
1:D:317:TYR:HA	1:D:320:VAL:HG12	1.94	0.50
1:B:84:LYS:HZ1	1:B:415:THR:CG2	2.25	0.50
1:E:115:LEU:HD12	1:E:115:LEU:C	2.32	0.50
1:D:113:ILE:CG2	1:D:328:ALA:O	2.60	0.49
1:A:143:PHE:CE1	1:C:146:LEU:HD22	2.47	0.49
1:E:382:ALA:HA	1:E:385:MET:HG3	1.93	0.49
1:D:97:VAL:HB	1:D:342:VAL:HG13	1.94	0.49
1:B:298:ILE:O	1:B:302:THR:HG23	2.12	0.49
1:B:77:ARG:HH21	1:B:416:GLU:HG3	1.77	0.49
1:C:308:THR:HB	1:C:353:ALA:HB1	1.94	0.49
1:E:97:VAL:HB	1:E:342:VAL:HG13	1.92	0.49
1:A:273:PHE:HB2	1:A:399:MET:HB2	1.95	0.49
1:D:109:PRO:O	1:D:227:GLU:OE1	2.30	0.49
1:E:272:ALA:HB2	1:E:402:VAL:HG21	1.92	0.49
1:E:213:ILE:HD12	1:E:214:ALA:N	2.27	0.49
1:B:209:VAL:HG22	1:B:274:VAL:HG11	1.94	0.49
1:C:235:VAL:O	1:C:239:LEU:HG	2.13	0.49
1:B:10:TYR:HB3	1:B:11:PRO:CD	2.42	0.49
1:A:374:LEU:HD11	1:A:383:TYR:CD1	2.48	0.49
1:C:165:ILE:HD11	1:C:183:LEU:CD2	2.42	0.49
1:E:292:MET:CE	1:E:294:ILE:HD11	2.43	0.49
1:A:354:GLY:C	1:A:356:PRO:CD	2.81	0.49
1:C:266:LYS:HG2	1:C:267:ASP:N	2.28	0.49
1:A:381:ALA:O	1:A:384:ALA:HB3	2.12	0.49
1:F:354:GLY:C	1:F:356:PRO:CD	2.81	0.49
1:B:366:VAL:O	1:B:370:VAL:N	2.45	0.49
1:F:95:PHE:CD2	1:F:95:PHE:C	2.86	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:VAL:O	1:D:239:LEU:HG	2.13	0.49
1:F:77:ARG:HH21	1:F:416:GLU:HG3	1.77	0.49
1:D:219:GLU:OE2	1:D:219:GLU:HA	2.13	0.49
1:F:174:GLU:OE1	1:F:177:ARG:NE	2.46	0.49
1:E:48:ASP:O	1:E:51:VAL:N	2.46	0.49
1:B:95:PHE:CD2	1:B:95:PHE:C	2.86	0.49
1:E:141:ASN:ND2	1:E:144:GLY:H	2.11	0.49
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.95	0.49
1:F:59:MET:CE	1:F:146:LEU:HD23	2.43	0.49
1:E:10:TYR:HB3	1:E:11:PRO:HD2	1.95	0.49
1:E:354:GLY:C	1:E:356:PRO:CD	2.82	0.49
1:C:44:LYS:N	1:C:45:PRO:HD2	2.28	0.49
1:C:113:ILE:HG22	1:C:328:ALA:O	2.13	0.48
1:A:114:HIS:CD2	1:A:114:HIS:N	2.73	0.48
1:E:226:GLY:O	1:E:228:LEU:N	2.46	0.48
1:E:317:TYR:HA	1:E:320:VAL:HG12	1.95	0.48
1:B:85:ILE:HG13	1:B:89:TYR:CE1	2.48	0.48
1:E:259:ILE:HD12	1:E:259:ILE:N	2.28	0.48
1:E:174:GLU:OE1	1:E:177:ARG:NE	2.45	0.48
1:B:165:ILE:HD11	1:B:183:LEU:CD2	2.43	0.48
1:C:77:ARG:HG2	1:C:80:ARG:NH2	2.29	0.48
1:B:59:MET:CE	1:B:146:LEU:HD23	2.44	0.48
1:B:137:ILE:O	1:B:153:PRO:HA	2.13	0.48
1:C:109:PRO:O	1:C:227:GLU:OE1	2.31	0.48
1:B:210:PHE:O	1:B:213:ILE:HD12	2.13	0.48
1:D:10:TYR:HB3	1:D:11:PRO:HD2	1.96	0.48
1:C:10:TYR:HB3	1:C:11:PRO:HD2	1.96	0.48
1:E:17:LEU:O	1:E:21:ILE:HG12	2.13	0.48
1:A:112:GLY:O	1:E:114:HIS:CD2	2.67	0.48
1:F:110:GLY:CA	1:F:327:ASN:HB3	2.41	0.48
1:D:17:LEU:O	1:D:21:ILE:HG12	2.13	0.48
1:F:335:VAL:HA	1:F:338:GLN:NE2	2.29	0.48
1:D:282:LEU:HD21	1:D:304:PRO:HA	1.96	0.48
1:B:17:LEU:O	1:B:21:ILE:HG12	2.13	0.48
1:A:213:ILE:HD12	1:A:214:ALA:N	2.28	0.48
1:F:209:VAL:HG22	1:F:274:VAL:HG11	1.96	0.48
1:F:266:LYS:HG2	1:F:267:ASP:N	2.28	0.48
1:E:296:GLU:O	1:E:300:SER:HB2	2.14	0.48
1:B:367:LEU:HD22	1:B:372:LEU:HD12	1.96	0.48
1:A:113:ILE:HG22	1:A:328:ALA:O	2.14	0.48
1:F:165:ILE:HD11	1:F:183:LEU:CD2	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LEU:HD11	1:B:383:TYR:CD1	2.49	0.48
1:A:115:LEU:C	1:A:115:LEU:HD12	2.34	0.48
1:C:113:ILE:CG2	1:C:328:ALA:O	2.62	0.48
1:E:174:GLU:OE1	1:E:177:ARG:CZ	2.61	0.48
1:B:382:ALA:HA	1:B:385:MET:HG3	1.96	0.48
1:F:317:TYR:HA	1:F:320:VAL:CG1	2.44	0.48
1:A:81:VAL:CG2	1:A:298:ILE:HD12	2.42	0.48
1:F:84:LYS:HZ1	1:F:415:THR:CG2	2.26	0.48
1:F:174:GLU:OE1	1:F:177:ARG:CZ	2.62	0.48
1:E:311:MET:HB2	1:E:349:SER:HB2	1.95	0.48
1:E:81:VAL:CG2	1:E:298:ILE:HD12	2.42	0.47
1:E:292:MET:HE2	1:E:294:ILE:HD11	1.96	0.47
1:C:74:SER:HB3	1:C:77:ARG:HG3	1.96	0.47
1:F:221:GLY:C	1:F:223:HIS:H	2.18	0.47
1:D:103:MET:HE1	1:D:237:VAL:CG1	2.44	0.47
1:D:374:LEU:HD11	1:D:383:TYR:CD1	2.49	0.47
1:A:183:LEU:O	1:A:187:ILE:HG13	2.14	0.47
1:B:110:GLY:CA	1:B:327:ASN:HB3	2.41	0.47
1:E:193:ALA:O	1:E:197:ILE:HG13	2.14	0.47
1:A:17:LEU:O	1:A:21:ILE:HG12	2.13	0.47
1:F:366:VAL:O	1:F:370:VAL:N	2.46	0.47
1:E:113:ILE:HG22	1:E:328:ALA:O	2.14	0.47
1:F:44:LYS:HD2	1:F:215:TYR:CE1	2.50	0.47
1:C:374:LEU:HD11	1:C:383:TYR:CD1	2.50	0.47
1:A:311:MET:HB2	1:A:349:SER:HB2	1.96	0.47
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.96	0.47
1:B:308:THR:HB	1:B:353:ALA:HB1	1.96	0.47
1:F:17:LEU:O	1:F:21:ILE:HG12	2.14	0.47
1:E:110:GLY:HA3	1:E:327:ASN:HB2	1.96	0.47
1:A:77:ARG:HE	1:A:416:GLU:CG	2.26	0.47
1:B:89:TYR:O	1:B:93:SER:HB2	2.15	0.47
1:D:130:LEU:CB	1:D:133:ILE:HD13	2.44	0.47
1:E:113:ILE:CG2	1:E:328:ALA:CB	2.89	0.47
1:F:85:ILE:HG13	1:F:89:TYR:CE1	2.49	0.47
1:C:415:THR:HG22	1:C:415:THR:O	2.15	0.47
1:D:9:GLU:HB3	1:D:15:LYS:HZ3	1.79	0.47
1:A:131:VAL:HG21	1:C:45:PRO:HB3	1.96	0.47
1:A:335:VAL:HA	1:A:338:GLN:NE2	2.30	0.47
1:C:142:PRO:O	1:C:145:ALA:HB3	2.15	0.47
1:F:367:LEU:HD22	1:F:372:LEU:HD12	1.97	0.47
1:A:113:ILE:CG2	1:A:328:ALA:CB	2.89	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:HIS:CD2	1:E:112:GLY:O	2.68	0.47
1:A:9:GLU:HB3	1:A:15:LYS:NZ	2.30	0.47
1:C:81:VAL:CG2	1:C:298:ILE:HD12	2.43	0.47
1:A:141:ASN:ND2	1:A:143:PHE:HB2	2.30	0.47
1:E:59:MET:CE	1:E:146:LEU:HD23	2.45	0.47
1:B:263:LYS:O	1:B:266:LYS:HD3	2.15	0.47
1:C:363:LEU:O	1:C:366:VAL:HG22	2.15	0.47
1:C:366:VAL:O	1:C:370:VAL:N	2.46	0.47
1:F:59:MET:SD	1:F:149:GLY:O	2.72	0.47
1:D:155:ILE:HD11	1:D:304:PRO:HB2	1.96	0.47
1:F:374:LEU:HD11	1:F:383:TYR:CD1	2.50	0.47
1:A:174:GLU:OE1	1:A:177:ARG:NE	2.47	0.47
1:A:174:GLU:OE1	1:A:177:ARG:CZ	2.62	0.47
1:D:382:ALA:HA	1:D:385:MET:HG3	1.95	0.47
1:B:113:ILE:CG2	1:B:328:ALA:CB	2.88	0.47
1:B:77:ARG:HE	1:B:416:GLU:CG	2.25	0.47
1:F:362:MET:O	1:F:365:MET:HB2	2.15	0.47
1:E:133:ILE:HD12	1:E:133:ILE:N	2.30	0.47
1:F:81:VAL:CG2	1:F:412:VAL:HG11	2.45	0.47
1:E:235:VAL:O	1:E:239:LEU:HG	2.15	0.47
1:D:77:ARG:HG2	1:D:80:ARG:NH2	2.30	0.47
1:B:317:TYR:HA	1:B:320:VAL:CG1	2.45	0.47
1:B:174:GLU:OE1	1:B:177:ARG:NE	2.48	0.47
1:F:308:THR:HB	1:F:353:ALA:HB1	1.97	0.47
1:B:117:VAL:HG21	1:B:378:ASN:HB2	1.97	0.47
1:B:117:VAL:HG23	1:B:378:ASN:HD22	1.79	0.47
1:C:110:GLY:HA3	1:C:327:ASN:HB2	1.97	0.47
1:F:9:GLU:HB3	1:F:15:LYS:NZ	2.31	0.46
1:D:383:TYR:CE2	1:D:387:LEU:CD1	2.99	0.46
1:D:139:PRO:O	1:F:56:MET:HB2	2.15	0.46
1:A:93:SER:HA	1:A:312:ASP:OD1	2.16	0.46
1:F:113:ILE:CG2	1:F:328:ALA:CB	2.88	0.46
1:C:81:VAL:CG2	1:C:412:VAL:HG11	2.45	0.46
1:F:77:ARG:HE	1:F:416:GLU:CG	2.25	0.46
1:C:17:LEU:O	1:C:21:ILE:HG12	2.15	0.46
1:A:113:ILE:CG2	1:A:328:ALA:O	2.63	0.46
1:C:221:GLY:C	1:C:223:HIS:H	2.18	0.46
1:F:273:PHE:CE1	1:F:395:MET:HB3	2.50	0.46
1:E:257:ASP:OD2	1:E:260:SER:N	2.43	0.46
1:D:113:ILE:CG2	1:D:328:ALA:CB	2.86	0.46
1:E:113:ILE:CG2	1:E:328:ALA:O	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:383:TYR:CE2	1:A:387:LEU:CD1	2.98	0.46
1:B:47:GLY:HA3	1:B:212:LEU:CD2	2.43	0.46
1:D:263:LYS:O	1:D:266:LYS:HD3	2.16	0.46
1:E:374:LEU:HD11	1:E:383:TYR:CD1	2.51	0.46
1:A:308:THR:HB	1:A:353:ALA:HB1	1.96	0.46
1:C:130:LEU:CB	1:C:133:ILE:HD13	2.45	0.46
1:B:231:VAL:O	1:B:235:VAL:HG23	2.15	0.46
1:C:76:ALA:O	1:C:77:ARG:CB	2.63	0.46
1:A:296:GLU:O	1:A:300:SER:HB2	2.16	0.46
1:F:117:VAL:HG23	1:F:378:ASN:HD22	1.79	0.46
1:A:97:VAL:HB	1:A:342:VAL:HG13	1.96	0.46
1:A:142:PRO:O	1:A:145:ALA:HB3	2.16	0.46
1:F:93:SER:HA	1:F:312:ASP:OD1	2.16	0.46
1:A:257:ASP:OD2	1:A:260:SER:N	2.44	0.46
1:B:318:GLN:OE1	1:B:363:LEU:N	2.49	0.46
1:B:81:VAL:CG2	1:B:412:VAL:HG11	2.46	0.46
1:D:415:THR:O	1:D:415:THR:HG22	2.16	0.46
1:A:317:TYR:HA	1:A:320:VAL:HG12	1.98	0.46
1:C:338:GLN:O	1:C:341:ILE:HB	2.16	0.46
1:E:335:VAL:HA	1:E:338:GLN:NE2	2.31	0.46
1:A:73:ILE:HD12	1:A:73:ILE:HA	1.86	0.46
1:C:47:GLY:HA3	1:C:212:LEU:CD2	2.46	0.45
1:B:78:LEU:CA	1:B:81:VAL:HG12	2.44	0.45
1:E:89:TYR:CD2	1:E:310:ASN:HB2	2.51	0.45
1:D:183:LEU:HD13	1:F:190:LEU:N	2.32	0.45
1:E:130:LEU:CB	1:E:133:ILE:HD13	2.46	0.45
1:B:110:GLY:HA3	1:B:327:ASN:HB2	1.95	0.45
1:C:110:GLY:CA	1:C:327:ASN:HB3	2.46	0.45
1:A:131:VAL:HG21	1:C:45:PRO:CB	2.46	0.45
1:E:318:GLN:OE1	1:E:363:LEU:N	2.49	0.45
1:D:168:LEU:HD11	1:F:193:ALA:N	2.31	0.45
1:C:97:VAL:HG22	1:C:315:ALA:O	2.16	0.45
1:B:259:ILE:HD12	1:B:259:ILE:N	2.30	0.45
1:D:209:VAL:HG22	1:D:274:VAL:HG11	1.98	0.45
1:F:10:TYR:HB3	1:F:11:PRO:HD2	1.97	0.45
1:E:317:TYR:CD2	1:E:393:LEU:HB3	2.52	0.45
1:D:317:TYR:HA	1:D:320:VAL:CG1	2.47	0.45
1:D:117:VAL:HG21	1:D:378:ASN:HB2	1.97	0.45
1:C:103:MET:HE1	1:C:237:VAL:CG1	2.47	0.45
1:B:104:ALA:O	1:B:107:PHE:O	2.33	0.45
1:F:231:VAL:O	1:F:235:VAL:HG23	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:408:GLY:O	1:C:412:VAL:HG23	2.16	0.45
1:D:81:VAL:CG2	1:D:298:ILE:HD12	2.45	0.45
1:B:10:TYR:HB3	1:B:11:PRO:HD2	1.97	0.45
1:B:9:GLU:HB3	1:B:15:LYS:NZ	2.32	0.45
1:D:110:GLY:CA	1:D:327:ASN:HB3	2.47	0.45
1:D:221:GLY:C	1:D:223:HIS:H	2.19	0.45
1:F:383:TYR:CE2	1:F:387:LEU:CD1	3.00	0.45
1:B:142:PRO:O	1:B:145:ALA:HB3	2.17	0.45
1:B:257:ASP:OD2	1:B:260:SER:N	2.44	0.45
1:F:259:ILE:HD12	1:F:259:ILE:N	2.30	0.45
1:E:266:LYS:HG2	1:E:267:ASP:N	2.32	0.45
1:A:89:TYR:CD2	1:A:310:ASN:HB2	2.52	0.45
1:A:110:GLY:HA3	1:A:327:ASN:HB2	1.99	0.45
1:A:327:ASN:HA	1:A:327:ASN:HD22	1.63	0.45
1:E:141:ASN:HD22	1:E:144:GLY:N	2.15	0.45
1:B:296:GLU:O	1:B:300:SER:HB2	2.17	0.45
1:D:110:GLY:HA3	1:D:327:ASN:HB2	1.98	0.45
1:D:45:PRO:HB3	1:E:131:VAL:HG21	1.98	0.45
1:D:59:MET:CE	1:D:146:LEU:HD23	2.46	0.45
1:C:219:GLU:OE2	1:C:219:GLU:HA	2.17	0.45
1:F:338:GLN:O	1:F:341:ILE:HB	2.17	0.45
1:E:383:TYR:CE2	1:E:387:LEU:CD1	2.99	0.45
1:E:9:GLU:HB3	1:E:15:LYS:NZ	2.32	0.45
1:F:235:VAL:O	1:F:239:LEU:HG	2.17	0.45
1:D:366:VAL:O	1:D:370:VAL:N	2.48	0.45
1:D:97:VAL:HG22	1:D:315:ALA:O	2.17	0.45
1:E:130:LEU:HB2	1:E:133:ILE:HD13	1.98	0.45
1:B:174:GLU:OE1	1:B:177:ARG:CZ	2.65	0.45
1:F:117:VAL:HG21	1:F:378:ASN:HB2	1.98	0.45
1:F:104:ALA:O	1:F:107:PHE:O	2.34	0.45
1:D:367:LEU:HD22	1:D:372:LEU:HD12	1.97	0.45
1:E:183:LEU:O	1:E:187:ILE:HG13	2.17	0.44
1:D:209:VAL:O	1:D:213:ILE:HG13	2.16	0.44
1:F:292:MET:HE2	1:F:294:ILE:HD11	1.99	0.44
1:E:77:ARG:HE	1:E:416:GLU:CG	2.28	0.44
1:B:147:ALA:O	1:C:141:ASN:ND2	2.50	0.44
1:F:296:GLU:O	1:F:300:SER:HB2	2.18	0.44
1:C:382:ALA:HA	1:C:385:MET:HG3	1.98	0.44
1:E:308:THR:HB	1:E:353:ALA:HB1	1.98	0.44
1:C:246:VAL:O	1:C:250:LEU:HB2	2.18	0.44
1:F:47:GLY:HA3	1:F:212:LEU:CD2	2.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLY:C	1:C:228:LEU:N	2.71	0.44
1:C:263:LYS:O	1:C:266:LYS:HD3	2.17	0.44
1:B:93:SER:HA	1:B:312:ASP:OD1	2.18	0.44
1:C:95:PHE:C	1:C:95:PHE:CD2	2.90	0.44
1:A:9:GLU:HB3	1:A:15:LYS:HZ3	1.83	0.44
1:C:292:MET:HE2	1:C:294:ILE:HD11	1.98	0.44
1:B:292:MET:HE2	1:B:294:ILE:HD11	1.99	0.44
1:E:314:THR:HG21	1:E:362:MET:CE	2.47	0.44
1:A:146:LEU:HD22	1:B:143:PHE:CE1	2.52	0.44
1:D:17:LEU:HD13	1:D:17:LEU:HA	1.80	0.44
1:E:389:ILE:HD12	1:E:389:ILE:HA	1.91	0.44
1:C:48:ASP:O	1:C:51:VAL:N	2.50	0.44
1:E:327:ASN:HD22	1:E:327:ASN:HA	1.63	0.44
1:C:296:GLU:O	1:C:300:SER:CB	2.65	0.44
1:D:363:LEU:O	1:D:366:VAL:HG22	2.18	0.44
1:A:193:ALA:N	1:B:168:LEU:HD11	2.32	0.44
1:E:367:LEU:HD22	1:E:372:LEU:HD12	1.99	0.44
1:B:18:ILE:O	1:B:22:LEU:HB3	2.17	0.44
1:A:367:LEU:HD22	1:A:372:LEU:HD12	1.99	0.44
1:C:104:ALA:O	1:C:107:PHE:O	2.36	0.44
1:F:333:LEU:HD23	1:F:333:LEU:HA	1.89	0.44
1:F:18:ILE:O	1:F:22:LEU:HB3	2.18	0.44
1:C:113:ILE:CG2	1:C:328:ALA:CB	2.88	0.44
1:E:45:PRO:CB	1:F:131:VAL:HG21	2.47	0.44
1:D:130:LEU:HB2	1:D:133:ILE:HD13	2.00	0.44
1:C:367:LEU:HD22	1:C:372:LEU:HD12	1.98	0.44
1:E:93:SER:HA	1:E:312:ASP:OD1	2.18	0.44
1:F:332:HIS:CD2	1:F:332:HIS:H	2.36	0.44
1:F:137:ILE:O	1:F:153:PRO:HA	2.18	0.44
1:B:190:LEU:N	1:C:183:LEU:HD13	2.33	0.44
1:D:76:ALA:O	1:D:77:ARG:CB	2.65	0.44
1:B:362:MET:O	1:B:365:MET:HB2	2.18	0.44
1:A:76:ALA:O	1:A:77:ARG:CB	2.66	0.44
1:B:103:MET:HG3	1:B:238:GLY:HA2	2.00	0.44
1:F:282:LEU:HD21	1:F:304:PRO:HA	1.99	0.44
1:C:117:VAL:HG21	1:C:378:ASN:HB2	1.98	0.44
1:A:272:ALA:HB2	1:A:402:VAL:HG21	1.98	0.44
1:D:272:ALA:HB2	1:D:402:VAL:HG21	1.99	0.44
1:E:73:ILE:HD12	1:E:73:ILE:HA	1.88	0.44
1:F:213:ILE:HG13	1:F:213:ILE:H	1.62	0.44
1:E:298:ILE:O	1:E:302:THR:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LYS:N	1:A:45:PRO:HD2	2.33	0.44
1:E:193:ALA:N	1:F:168:LEU:HD11	2.32	0.44
1:A:209:VAL:O	1:A:213:ILE:HG13	2.17	0.43
1:D:210:PHE:HA	1:D:213:ILE:HD11	2.00	0.43
1:F:89:TYR:CD2	1:F:310:ASN:HB2	2.53	0.43
1:C:298:ILE:O	1:C:302:THR:HG23	2.18	0.43
1:E:110:GLY:CA	1:E:327:ASN:HB3	2.47	0.43
1:C:215:TYR:O	1:C:219:GLU:HG2	2.18	0.43
1:C:141:ASN:ND2	1:C:144:GLY:H	2.16	0.43
1:C:117:VAL:HG23	1:C:378:ASN:HD22	1.82	0.43
1:D:173:ASN:OD1	1:D:173:ASN:C	2.56	0.43
1:C:210:PHE:HA	1:C:213:ILE:HD11	2.00	0.43
1:A:235:VAL:O	1:A:239:LEU:HG	2.18	0.43
1:D:215:TYR:O	1:D:219:GLU:HG2	2.18	0.43
1:D:44:LYS:N	1:D:45:PRO:HD2	2.33	0.43
1:C:282:LEU:HD21	1:C:304:PRO:HA	2.00	0.43
1:E:366:VAL:O	1:E:370:VAL:N	2.50	0.43
1:D:117:VAL:HG23	1:D:378:ASN:HD22	1.82	0.43
1:D:104:ALA:O	1:D:107:PHE:O	2.36	0.43
1:A:266:LYS:HG2	1:A:267:ASP:N	2.33	0.43
1:A:366:VAL:O	1:A:370:VAL:N	2.50	0.43
1:F:110:GLY:HA3	1:F:327:ASN:HB2	1.97	0.43
1:A:292:MET:HE2	1:A:294:ILE:HD11	2.01	0.43
1:C:317:TYR:HA	1:C:320:VAL:CG1	2.49	0.43
1:F:263:LYS:O	1:F:266:LYS:HD3	2.19	0.43
1:C:17:LEU:HA	1:C:17:LEU:HD13	1.80	0.43
1:B:332:HIS:H	1:B:332:HIS:CD2	2.37	0.43
1:E:209:VAL:O	1:E:213:ILE:HG13	2.18	0.43
1:D:226:GLY:C	1:D:228:LEU:N	2.72	0.43
1:B:59:MET:SD	1:B:149:GLY:O	2.76	0.43
1:F:318:GLN:OE1	1:F:363:LEU:N	2.51	0.43
1:D:95:PHE:C	1:D:95:PHE:CD2	2.91	0.43
1:D:47:GLY:HA3	1:D:212:LEU:CD2	2.49	0.43
1:E:45:PRO:HB3	1:F:131:VAL:HG21	1.99	0.43
1:D:73:ILE:HG13	1:D:77:ARG:HD2	2.01	0.43
1:A:97:VAL:HG22	1:A:315:ALA:O	2.18	0.43
1:C:141:ASN:HD22	1:C:144:GLY:H	1.65	0.43
1:B:210:PHE:HA	1:B:213:ILE:HD11	2.00	0.43
1:D:318:GLN:OE1	1:D:363:LEU:CA	2.66	0.43
1:B:324:PHE:C	1:B:324:PHE:CD2	2.91	0.43
1:B:49:LEU:O	1:B:53:LEU:HD12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:311:MET:HB2	1:F:349:SER:HB2	2.00	0.43
1:F:49:LEU:O	1:F:53:LEU:HD12	2.17	0.43
1:A:263:LYS:O	1:A:266:LYS:HD3	2.19	0.43
1:F:53:LEU:O	1:F:56:MET:HB3	2.19	0.43
1:A:95:PHE:C	1:A:95:PHE:CD2	2.91	0.43
1:B:213:ILE:H	1:B:213:ILE:HG13	1.64	0.43
1:D:193:ALA:N	1:E:168:LEU:HD11	2.34	0.43
1:E:47:GLY:HA3	1:E:212:LEU:CD2	2.46	0.43
1:A:77:ARG:NE	1:A:416:GLU:HG2	2.33	0.43
1:B:383:TYR:CE2	1:B:387:LEU:CD1	3.02	0.43
1:E:381:ALA:O	1:E:384:ALA:HB3	2.19	0.43
1:B:209:VAL:O	1:B:213:ILE:HG13	2.19	0.42
1:F:103:MET:HG3	1:F:238:GLY:HA2	2.01	0.42
1:D:259:ILE:N	1:D:259:ILE:HD12	2.34	0.42
1:A:317:TYR:CD2	1:A:393:LEU:HB3	2.54	0.42
1:B:226:GLY:C	1:B:228:LEU:N	2.72	0.42
1:F:313:GLY:N	1:F:401:ASN:OD1	2.52	0.42
1:F:130:LEU:CB	1:F:133:ILE:HD13	2.49	0.42
1:F:324:PHE:CD2	1:F:324:PHE:C	2.92	0.42
1:B:333:LEU:HA	1:B:333:LEU:HD23	1.92	0.42
1:D:246:VAL:O	1:D:250:LEU:HB2	2.20	0.42
1:C:318:GLN:OE1	1:C:363:LEU:CA	2.67	0.42
1:A:259:ILE:N	1:A:259:ILE:HD12	2.35	0.42
1:C:209:VAL:O	1:C:213:ILE:HG13	2.18	0.42
1:A:110:GLY:CA	1:A:327:ASN:HB3	2.48	0.42
1:B:97:VAL:HG22	1:B:315:ALA:O	2.18	0.42
1:C:88:TYR:CD1	1:C:89:TYR:N	2.87	0.42
1:F:30:LEU:O	1:F:35:TYR:HB2	2.19	0.42
1:F:257:ASP:OD2	1:F:260:SER:N	2.47	0.42
1:D:112:GLY:O	1:D:227:GLU:HG3	2.20	0.42
1:B:77:ARG:NE	1:B:416:GLU:HG2	2.29	0.42
1:F:74:SER:HB3	1:F:77:ARG:HG3	2.02	0.42
1:B:221:GLY:C	1:B:223:HIS:N	2.73	0.42
1:E:318:GLN:OE1	1:E:363:LEU:CA	2.68	0.42
1:E:263:LYS:O	1:E:266:LYS:HD3	2.20	0.42
1:E:313:GLY:N	1:E:401:ASN:OD1	2.52	0.42
1:B:235:VAL:O	1:B:239:LEU:HG	2.20	0.42
1:E:78:LEU:CA	1:E:81:VAL:HG12	2.43	0.42
1:A:314:THR:HG21	1:A:362:MET:CE	2.50	0.42
1:F:219:GLU:OE2	1:F:219:GLU:HA	2.20	0.42
1:E:49:LEU:O	1:E:53:LEU:HD12	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:PHE:C	1:E:95:PHE:CD2	2.92	0.42
1:D:212:LEU:HD12	1:D:274:VAL:HG13	2.00	0.42
1:E:81:VAL:CG2	1:E:412:VAL:HG11	2.48	0.42
1:E:85:ILE:HG13	1:E:89:TYR:CE1	2.55	0.42
1:A:137:ILE:O	1:A:153:PRO:HA	2.20	0.42
1:C:333:LEU:HA	1:C:333:LEU:HD23	1.88	0.42
1:C:406:LEU:HD23	1:C:406:LEU:HA	1.88	0.42
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.86	0.42
1:F:88:TYR:C	1:F:88:TYR:CD1	2.92	0.42
1:A:114:HIS:O	1:E:226:GLY:HA3	2.19	0.42
1:A:183:LEU:HD13	1:C:190:LEU:N	2.35	0.42
1:A:81:VAL:CG2	1:A:412:VAL:HG11	2.49	0.42
1:A:231:VAL:O	1:A:235:VAL:HG23	2.20	0.42
1:D:174:GLU:OE1	1:D:177:ARG:HD2	2.20	0.42
1:E:117:VAL:HG21	1:E:378:ASN:HB2	2.01	0.42
1:D:311:MET:HB2	1:D:349:SER:HB2	2.00	0.42
1:D:141:ASN:ND2	1:F:147:ALA:O	2.52	0.42
1:D:210:PHE:O	1:D:213:ILE:HD12	2.18	0.42
1:D:12:VAL:N	1:D:15:LYS:HB2	2.30	0.42
1:A:45:PRO:CB	1:B:131:VAL:HG21	2.49	0.42
1:A:141:ASN:HD21	1:A:143:PHE:HB2	1.84	0.42
1:F:117:VAL:HG21	1:F:376:ASP:OD2	2.20	0.42
1:C:117:VAL:HG21	1:C:376:ASP:OD2	2.19	0.42
1:E:189:GLY:N	1:F:179:SER:HB3	2.35	0.42
1:D:324:PHE:C	1:D:324:PHE:CD2	2.93	0.42
1:A:205:ALA:O	1:A:209:VAL:HG23	2.20	0.41
1:C:212:LEU:HD12	1:C:274:VAL:HG13	2.00	0.41
1:C:231:VAL:O	1:C:235:VAL:HG23	2.19	0.41
1:D:45:PRO:CB	1:E:131:VAL:HG21	2.50	0.41
1:A:17:LEU:HD13	1:A:17:LEU:HA	1.76	0.41
1:D:117:VAL:HG21	1:D:376:ASP:OD2	2.20	0.41
1:E:142:PRO:O	1:E:145:ALA:HB3	2.20	0.41
1:D:333:LEU:HD23	1:D:333:LEU:HA	1.88	0.41
1:B:23:GLY:HA2	1:B:210:PHE:CE2	2.55	0.41
1:F:97:VAL:HG22	1:F:315:ALA:O	2.19	0.41
1:C:259:ILE:HD12	1:C:259:ILE:N	2.35	0.41
1:D:113:ILE:CG2	1:D:328:ALA:C	2.89	0.41
1:E:210:PHE:HA	1:E:213:ILE:HD11	2.02	0.41
1:A:85:ILE:HD13	1:A:412:VAL:HG21	2.02	0.41
1:A:292:MET:CE	1:A:294:ILE:HD11	2.51	0.41
1:E:141:ASN:ND2	1:E:143:PHE:HB2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:296:GLU:O	1:D:300:SER:CB	2.68	0.41
1:A:133:ILE:N	1:A:133:ILE:CD1	2.84	0.41
1:D:103:MET:CE	1:D:237:VAL:HB	2.50	0.41
1:B:282:LEU:HD21	1:B:304:PRO:HA	2.01	0.41
1:F:58:VAL:HG22	1:F:283:PRO:HD3	2.02	0.41
1:D:82:GLY:HA2	1:D:301:PHE:HE2	1.85	0.41
1:D:401:ASN:O	1:D:405:ASP:OD1	2.38	0.41
1:B:30:LEU:O	1:B:35:TYR:HB2	2.19	0.41
1:B:88:TYR:CD1	1:B:88:TYR:C	2.93	0.41
1:D:90:LEU:HA	1:D:90:LEU:HD12	1.89	0.41
1:E:324:PHE:C	1:E:324:PHE:CD2	2.93	0.41
1:A:148:ASN:O	1:A:149:GLY:C	2.57	0.41
1:E:190:LEU:N	1:F:183:LEU:HD13	2.34	0.41
1:E:205:ALA:O	1:E:209:VAL:HG23	2.20	0.41
1:E:210:PHE:O	1:E:213:ILE:HD12	2.20	0.41
1:F:85:ILE:HD13	1:F:412:VAL:HG21	2.02	0.41
1:C:84:LYS:NZ	1:C:415:THR:HG22	2.30	0.41
1:A:85:ILE:HG13	1:A:89:TYR:CE1	2.56	0.41
1:E:292:MET:HE2	1:E:294:ILE:CD1	2.50	0.41
1:C:311:MET:HB2	1:C:349:SER:HB2	2.01	0.41
1:E:148:ASN:O	1:E:149:GLY:C	2.57	0.41
1:A:324:PHE:C	1:A:324:PHE:CD2	2.93	0.41
1:B:311:MET:HB2	1:B:349:SER:HB2	2.02	0.41
1:C:130:LEU:HB2	1:C:133:ILE:HD13	2.02	0.41
1:C:133:ILE:N	1:C:133:ILE:HD12	2.34	0.41
1:C:326:ALA:HB1	1:C:333:LEU:HG	2.01	0.41
1:A:318:GLN:OE1	1:A:363:LEU:N	2.53	0.41
1:D:48:ASP:O	1:D:51:VAL:N	2.53	0.41
1:C:23:GLY:HA2	1:C:210:PHE:CE2	2.56	0.41
1:E:78:LEU:HA	1:E:81:VAL:CG1	2.48	0.41
1:D:298:ILE:O	1:D:302:THR:HG23	2.20	0.41
1:C:131:VAL:CG1	1:C:132:HIS:H	2.33	0.41
1:A:147:ALA:O	1:B:141:ASN:ND2	2.54	0.41
1:E:363:LEU:O	1:E:366:VAL:HG22	2.21	0.41
1:E:104:ALA:O	1:E:107:PHE:O	2.39	0.41
1:C:151:VAL:O	1:C:154:THR:HB	2.20	0.41
1:A:189:GLY:N	1:B:179:SER:HB3	2.36	0.41
1:A:117:VAL:HG21	1:A:378:ASN:HB2	2.02	0.41
1:B:58:VAL:HG22	1:B:283:PRO:HD3	2.02	0.41
1:F:210:PHE:O	1:F:213:ILE:HD12	2.20	0.41
1:D:292:MET:CE	1:D:294:ILE:HD11	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:VAL:O	1:E:250:LEU:HB2	2.20	0.41
1:E:362:MET:O	1:E:365:MET:HB2	2.20	0.41
1:E:97:VAL:HG22	1:E:315:ALA:O	2.21	0.41
1:A:383:TYR:CE2	1:A:387:LEU:HD13	2.56	0.41
1:B:251:LEU:HD22	1:B:256:ILE:HG23	2.01	0.41
1:D:406:LEU:HD23	1:D:406:LEU:HA	1.91	0.41
1:A:246:VAL:O	1:A:250:LEU:HB2	2.20	0.41
1:E:103:MET:HG3	1:E:238:GLY:HA2	2.01	0.41
1:F:226:GLY:C	1:F:228:LEU:N	2.74	0.41
1:D:148:ASN:O	1:D:149:GLY:C	2.58	0.41
1:C:332:HIS:CD2	1:C:332:HIS:H	2.38	0.41
1:F:210:PHE:HA	1:F:213:ILE:HD11	2.02	0.41
1:F:239:LEU:HD23	1:F:316:LEU:HD13	2.03	0.41
1:A:78:LEU:CA	1:A:81:VAL:HG12	2.45	0.41
1:D:231:VAL:O	1:D:235:VAL:HG23	2.20	0.41
1:D:89:TYR:O	1:D:93:SER:HB2	2.21	0.41
1:A:103:MET:CE	1:A:237:VAL:HB	2.51	0.41
1:A:193:ALA:CA	1:B:168:LEU:HD11	2.50	0.41
1:F:14:GLN:O	1:F:17:LEU:N	2.54	0.41
1:A:117:VAL:HG21	1:A:376:ASP:OD2	2.20	0.41
1:C:324:PHE:C	1:C:324:PHE:CD2	2.94	0.41
1:B:273:PHE:CE1	1:B:395:MET:HB3	2.56	0.41
1:B:313:GLY:N	1:B:401:ASN:OD1	2.54	0.41
1:A:209:VAL:HG22	1:A:274:VAL:HG11	2.03	0.41
1:A:210:PHE:O	1:A:213:ILE:HD12	2.20	0.41
1:F:89:TYR:O	1:F:93:SER:HB2	2.21	0.41
1:F:198:VAL:CG1	1:F:287:ARG:HD3	2.50	0.41
1:E:137:ILE:O	1:E:153:PRO:HA	2.21	0.41
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.36	0.41
1:F:90:LEU:HD12	1:F:90:LEU:HA	1.95	0.41
1:B:20:LEU:C	1:B:20:LEU:HD23	2.41	0.41
1:C:112:GLY:O	1:C:227:GLU:HG3	2.22	0.40
1:A:226:GLY:HA3	1:E:114:HIS:O	2.21	0.40
1:F:209:VAL:O	1:F:213:ILE:HG13	2.22	0.40
1:F:265:ALA:HA	1:F:288:VAL:HG11	2.03	0.40
1:C:88:TYR:HD1	1:C:89:TYR:N	2.20	0.40
1:C:383:TYR:CE2	1:C:387:LEU:CD1	3.05	0.40
1:F:130:LEU:HB2	1:F:133:ILE:HD13	2.03	0.40
1:A:376:ASP:HA	1:A:377:PRO:HD3	1.95	0.40
1:B:130:LEU:CB	1:B:133:ILE:HD13	2.51	0.40
1:F:64:ALA:HB1	1:F:191:ALA:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:235:VAL:HG22	1:F:320:VAL:HG11	2.04	0.40
1:B:9:GLU:HB3	1:B:15:LYS:HZ3	1.86	0.40
1:C:14:GLN:O	1:C:17:LEU:N	2.54	0.40
1:F:259:ILE:HD12	1:F:259:ILE:H	1.86	0.40
1:C:82:GLY:HA2	1:C:301:PHE:HE2	1.86	0.40
1:C:257:ASP:OD2	1:C:260:SER:N	2.42	0.40
1:F:23:GLY:HA2	1:F:210:PHE:CE2	2.56	0.40
1:F:44:LYS:N	1:F:45:PRO:HD2	2.37	0.40
1:E:383:TYR:CE2	1:E:387:LEU:HD13	2.56	0.40
1:C:141:ASN:HD22	1:C:144:GLY:N	2.18	0.40
1:D:332:HIS:H	1:D:332:HIS:CD2	2.39	0.40
1:C:273:PHE:HB2	1:C:399:MET:HB2	2.02	0.40
1:F:221:GLY:C	1:F:223:HIS:N	2.75	0.40
1:A:18:ILE:O	1:A:22:LEU:HB3	2.21	0.40
1:B:189:GLY:N	1:C:179:SER:HB3	2.37	0.40
1:A:313:GLY:N	1:A:401:ASN:OD1	2.54	0.40
1:D:190:LEU:N	1:E:183:LEU:HD13	2.37	0.40
1:D:292:MET:HE2	1:D:294:ILE:CD1	2.51	0.40
1:D:44:LYS:HD2	1:D:215:TYR:CD1	2.57	0.40
1:E:317:TYR:HA	1:E:320:VAL:CG1	2.51	0.40
1:C:226:GLY:O	1:C:229:ALA:N	2.40	0.40
1:A:219:GLU:OE2	1:A:219:GLU:HA	2.22	0.40
1:B:219:GLU:HA	1:B:219:GLU:OE2	2.22	0.40
1:C:173:ASN:C	1:C:173:ASN:OD1	2.60	0.40
1:D:167:TYR:N	1:D:167:TYR:CD1	2.89	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	395/422 (94%)	352 (89%)	33 (8%)	10 (2%)	7 44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	395/422 (94%)	353 (89%)	31 (8%)	11 (3%)	6	42
1	C	395/422 (94%)	356 (90%)	27 (7%)	12 (3%)	5	40
1	D	395/422 (94%)	356 (90%)	27 (7%)	12 (3%)	5	40
1	E	395/422 (94%)	358 (91%)	27 (7%)	10 (2%)	7	44
1	F	395/422 (94%)	355 (90%)	30 (8%)	10 (2%)	7	44
All	All	2370/2532 (94%)	2130 (90%)	175 (7%)	65 (3%)	6	43

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	12	VAL
1	A	77	ARG
1	B	10	TYR
1	B	12	VAL
1	B	77	ARG
1	C	10	TYR
1	C	12	VAL
1	C	77	ARG
1	C	355	VAL
1	D	10	TYR
1	D	12	VAL
1	D	77	ARG
1	D	355	VAL
1	E	10	TYR
1	E	12	VAL
1	E	77	ARG
1	F	10	TYR
1	F	12	VAL
1	F	77	ARG
1	A	149	GLY
1	A	222	VAL
1	A	227	GLU
1	A	355	VAL
1	B	149	GLY
1	B	222	VAL
1	B	227	GLU
1	B	355	VAL
1	C	149	GLY
1	C	222	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	227	GLU
1	D	149	GLY
1	D	222	VAL
1	D	227	GLU
1	E	149	GLY
1	E	222	VAL
1	E	227	GLU
1	E	355	VAL
1	F	149	GLY
1	F	222	VAL
1	F	227	GLU
1	F	355	VAL
1	A	150	GLN
1	B	150	GLN
1	E	150	GLN
1	A	75	PRO
1	C	80	ARG
1	C	150	GLN
1	D	146	LEU
1	E	75	PRO
1	B	49	LEU
1	C	146	LEU
1	D	80	ARG
1	F	150	GLN
1	A	11	PRO
1	B	11	PRO
1	B	75	PRO
1	C	75	PRO
1	D	75	PRO
1	D	150	GLN
1	F	75	PRO
1	C	11	PRO
1	D	11	PRO
1	E	11	PRO
1	F	11	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	304/330 (92%)	262 (86%)	42 (14%)	4 24
1	B	304/330 (92%)	263 (86%)	41 (14%)	5 25
1	C	304/330 (92%)	265 (87%)	39 (13%)	5 27
1	D	304/330 (92%)	265 (87%)	39 (13%)	5 27
1	E	304/330 (92%)	263 (86%)	41 (14%)	5 25
1	F	304/330 (92%)	263 (86%)	41 (14%)	5 25
All	All	1824/1980 (92%)	1581 (87%)	243 (13%)	5 25

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	18	ILE
1	A	28	LEU
1	A	30	LEU
1	A	74	SER
1	A	77	ARG
1	A	78	LEU
1	A	90	LEU
1	A	91	LEU
1	A	93	SER
1	A	106	LEU
1	A	114	HIS
1	A	117	VAL
1	A	140	THR
1	A	148	ASN
1	A	183	LEU
1	A	184	LEU
1	A	196	LYS
1	A	212	LEU
1	A	213	ILE
1	A	217	MET
1	A	224	VAL
1	A	241	LEU
1	A	250	LEU
1	A	266	LYS
1	A	267	ASP
1	A	290	LYS
1	A	314	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	317	TYR
1	A	323	PHE
1	A	331	SER
1	A	335	VAL
1	A	337	GLN
1	A	340	THR
1	A	344	THR
1	A	355	VAL
1	A	368	HIS
1	A	372	LEU
1	A	374	LEU
1	A	375	THR
1	A	385	MET
1	A	405	ASP
1	B	12	VAL
1	B	28	LEU
1	B	30	LEU
1	B	74	SER
1	B	77	ARG
1	B	78	LEU
1	B	90	LEU
1	B	91	LEU
1	B	93	SER
1	B	95	PHE
1	B	114	HIS
1	B	117	VAL
1	B	140	THR
1	B	148	ASN
1	B	151	VAL
1	B	152	LEU
1	B	183	LEU
1	B	184	LEU
1	B	196	LYS
1	B	217	MET
1	B	224	VAL
1	B	241	LEU
1	B	250	LEU
1	B	267	ASP
1	B	290	LYS
1	B	314	THR
1	B	317	TYR
1	B	323	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	ASN
1	B	331	SER
1	B	332	HIS
1	B	335	VAL
1	B	337	GLN
1	B	340	THR
1	B	344	THR
1	B	355	VAL
1	B	368	HIS
1	B	372	LEU
1	B	374	LEU
1	B	375	THR
1	B	405	ASP
1	C	12	VAL
1	C	18	ILE
1	C	28	LEU
1	C	30	LEU
1	C	74	SER
1	C	77	ARG
1	C	78	LEU
1	C	90	LEU
1	C	91	LEU
1	C	93	SER
1	C	106	LEU
1	C	114	HIS
1	C	117	VAL
1	C	140	THR
1	C	148	ASN
1	C	183	LEU
1	C	184	LEU
1	C	213	ILE
1	C	217	MET
1	C	224	VAL
1	C	241	LEU
1	C	250	LEU
1	C	267	ASP
1	C	290	LYS
1	C	314	THR
1	C	317	TYR
1	C	323	PHE
1	C	331	SER
1	C	334	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	337	GLN
1	C	340	THR
1	C	344	THR
1	C	355	VAL
1	C	368	HIS
1	C	372	LEU
1	C	374	LEU
1	C	375	THR
1	C	385	MET
1	C	405	ASP
1	D	12	VAL
1	D	28	LEU
1	D	30	LEU
1	D	74	SER
1	D	77	ARG
1	D	78	LEU
1	D	90	LEU
1	D	91	LEU
1	D	93	SER
1	D	106	LEU
1	D	114	HIS
1	D	117	VAL
1	D	140	THR
1	D	148	ASN
1	D	183	LEU
1	D	184	LEU
1	D	196	LYS
1	D	213	ILE
1	D	217	MET
1	D	224	VAL
1	D	241	LEU
1	D	250	LEU
1	D	267	ASP
1	D	290	LYS
1	D	314	THR
1	D	317	TYR
1	D	323	PHE
1	D	331	SER
1	D	334	THR
1	D	337	GLN
1	D	340	THR
1	D	344	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	355	VAL
1	D	368	HIS
1	D	372	LEU
1	D	374	LEU
1	D	375	THR
1	D	385	MET
1	D	405	ASP
1	E	12	VAL
1	E	28	LEU
1	E	30	LEU
1	E	74	SER
1	E	77	ARG
1	E	78	LEU
1	E	90	LEU
1	E	91	LEU
1	E	93	SER
1	E	106	LEU
1	E	114	HIS
1	E	117	VAL
1	E	140	THR
1	E	148	ASN
1	E	183	LEU
1	E	184	LEU
1	E	196	LYS
1	E	212	LEU
1	E	213	ILE
1	E	217	MET
1	E	224	VAL
1	E	241	LEU
1	E	250	LEU
1	E	266	LYS
1	E	267	ASP
1	E	290	LYS
1	E	314	THR
1	E	317	TYR
1	E	323	PHE
1	E	331	SER
1	E	335	VAL
1	E	337	GLN
1	E	340	THR
1	E	344	THR
1	E	355	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	368	HIS
1	E	372	LEU
1	E	374	LEU
1	E	375	THR
1	E	385	MET
1	E	405	ASP
1	F	12	VAL
1	F	18	ILE
1	F	28	LEU
1	F	30	LEU
1	F	74	SER
1	F	77	ARG
1	F	78	LEU
1	F	90	LEU
1	F	91	LEU
1	F	93	SER
1	F	114	HIS
1	F	117	VAL
1	F	140	THR
1	F	148	ASN
1	F	183	LEU
1	F	184	LEU
1	F	196	LYS
1	F	217	MET
1	F	224	VAL
1	F	241	LEU
1	F	250	LEU
1	F	266	LYS
1	F	267	ASP
1	F	290	LYS
1	F	314	THR
1	F	317	TYR
1	F	323	PHE
1	F	327	ASN
1	F	331	SER
1	F	332	HIS
1	F	334	THR
1	F	335	VAL
1	F	337	GLN
1	F	340	THR
1	F	344	THR
1	F	355	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	368	HIS
1	F	372	LEU
1	F	374	LEU
1	F	375	THR
1	F	405	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	HIS
1	A	114	HIS
1	A	141	ASN
1	A	327	ASN
1	A	332	HIS
1	B	40	HIS
1	B	141	ASN
1	B	327	ASN
1	B	332	HIS
1	C	40	HIS
1	C	114	HIS
1	C	141	ASN
1	C	327	ASN
1	C	332	HIS
1	D	40	HIS
1	D	114	HIS
1	D	141	ASN
1	D	327	ASN
1	D	332	HIS
1	E	40	HIS
1	E	141	ASN
1	E	327	ASN
1	E	332	HIS
1	F	40	HIS
1	F	141	ASN
1	F	327	ASN
1	F	332	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	399/422 (94%)	0.73	36 (9%)	12	12	98, 159, 220, 284	0
1	B	399/422 (94%)	0.59	16 (4%)	42	37	85, 144, 207, 267	0
1	C	399/422 (94%)	0.63	21 (5%)	30	27	90, 146, 205, 266	0
1	D	399/422 (94%)	0.59	19 (4%)	34	30	85, 144, 205, 262	0
1	E	399/422 (94%)	0.77	36 (9%)	12	12	101, 163, 222, 286	0
1	F	399/422 (94%)	0.57	14 (3%)	48	42	84, 144, 207, 266	0
All	All	2394/2532 (94%)	0.65	142 (5%)	26	23	84, 151, 212, 286	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	TYR	5.6
1	E	93	SER	5.0
1	F	114	HIS	4.7
1	E	247	TYR	4.4
1	B	323	PHE	4.1
1	A	120	GLN	4.0
1	E	333	LEU	3.9
1	A	93	SER	3.9
1	A	409	THR	3.8
1	E	323	PHE	3.8
1	C	311	MET	3.7
1	D	311	MET	3.7
1	C	114	HIS	3.6
1	E	345	ALA	3.5
1	E	94	ALA	3.5
1	E	109	PRO	3.5
1	E	311	MET	3.5
1	C	109	PRO	3.5
1	F	323	PHE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	114	HIS	3.3
1	B	354	GLY	3.3
1	E	114	HIS	3.3
1	D	109	PRO	3.3
1	E	409	THR	3.2
1	E	108	ASN	3.2
1	A	332	HIS	3.2
1	B	214	ALA	3.2
1	C	16	ILE	3.2
1	B	355	VAL	3.1
1	A	333	LEU	3.1
1	B	114	HIS	3.1
1	F	247	TYR	3.1
1	A	35	TYR	3.1
1	F	11	PRO	3.1
1	F	311	MET	3.1
1	E	89	TYR	3.1
1	E	97	VAL	3.0
1	A	114	HIS	3.0
1	B	247	TYR	3.0
1	A	116	ALA	3.0
1	A	219	GLU	2.9
1	E	332	HIS	2.9
1	D	14	GLN	2.9
1	C	228	LEU	2.9
1	A	323	PHE	2.9
1	A	242	GLN	2.9
1	C	319	GLY	2.8
1	A	119	GLY	2.8
1	F	322	THR	2.8
1	A	12	VAL	2.8
1	E	116	ALA	2.8
1	A	108	ASN	2.8
1	E	325	ILE	2.7
1	E	12	VAL	2.7
1	A	356	PRO	2.7
1	D	16	ILE	2.7
1	D	319	GLY	2.7
1	A	36	ALA	2.6
1	A	378	ASN	2.6
1	F	354	GLY	2.6
1	A	89	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	322	THR	2.6
1	C	333	LEU	2.6
1	E	342	VAL	2.5
1	C	400	VAL	2.5
1	D	231	VAL	2.5
1	E	378	ASN	2.5
1	C	231	VAL	2.4
1	E	35	TYR	2.4
1	A	311	MET	2.4
1	F	97	VAL	2.4
1	A	325	ILE	2.4
1	B	239	LEU	2.4
1	E	120	GLN	2.4
1	E	242	GLN	2.4
1	E	356	PRO	2.4
1	A	317	TYR	2.4
1	C	132	HIS	2.4
1	F	239	LEU	2.4
1	B	378	ASN	2.4
1	D	248	PHE	2.4
1	E	318	GLN	2.4
1	E	11	PRO	2.4
1	A	382	ALA	2.4
1	A	228	LEU	2.4
1	F	355	VAL	2.3
1	A	241	LEU	2.3
1	D	228	LEU	2.3
1	A	324	PHE	2.3
1	B	311	MET	2.3
1	C	14	GLN	2.3
1	E	252	LYS	2.3
1	B	230	LYS	2.3
1	C	325	ILE	2.3
1	A	107	PHE	2.3
1	A	281	THR	2.3
1	D	332	HIS	2.2
1	C	116	ALA	2.2
1	D	230	LYS	2.2
1	D	247	TYR	2.2
1	B	12	VAL	2.2
1	B	11	PRO	2.2
1	E	346	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	332	HIS	2.2
1	D	333	LEU	2.2
1	C	36	ALA	2.2
1	A	109	PRO	2.2
1	E	119	GLY	2.2
1	F	379	VAL	2.2
1	E	33	TYR	2.2
1	E	228	LEU	2.2
1	D	325	ILE	2.2
1	C	106	LEU	2.1
1	E	219	GLU	2.1
1	D	323	PHE	2.1
1	D	314	THR	2.1
1	C	298	ILE	2.1
1	A	349	SER	2.1
1	A	269	MET	2.1
1	F	228	LEU	2.1
1	A	33	TYR	2.1
1	E	130	LEU	2.1
1	A	94	ALA	2.1
1	E	36	ALA	2.1
1	C	314	THR	2.1
1	A	346	VAL	2.1
1	C	402	VAL	2.1
1	E	349	SER	2.1
1	D	242	GLN	2.1
1	B	32	HIS	2.1
1	F	32	HIS	2.1
1	B	16	ILE	2.1
1	C	329	LEU	2.0
1	E	256	ILE	2.0
1	A	208	GLY	2.0
1	A	104	ALA	2.0
1	F	12	VAL	2.0
1	B	402	VAL	2.0
1	C	247	TYR	2.0
1	D	329	LEU	2.0
1	D	246	VAL	2.0
1	E	335	VAL	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, 95^{th} 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	NA	E	501	1/1	0.96	1.36	9.27	226,226,226,226	0
2	NA	A	501	1/1	0.96	1.04	8.46	247,247,247,247	0
2	NA	D	501	1/1	0.92	0.88	4.37	114,114,114,114	0
2	NA	F	501	1/1	0.95	0.79	4.25	92,92,92,92	0
2	NA	B	501	1/1	0.93	0.56	2.39	91,91,91,91	0
2	NA	C	501	1/1	0.94	0.50	1.28	97,97,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.