



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 2, 2023 – 04:17 PM EDT

PDB ID : 3R6Q
Title : A triclinic-lattice structure of aspartase from Bacillus sp. YM55-1
Authors : Fibriansah, G.; Puthan Veetil, V.; Poelarends, G.J.; Thunnissen, A.-M.W.H.
Deposited on : 2011-03-22
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

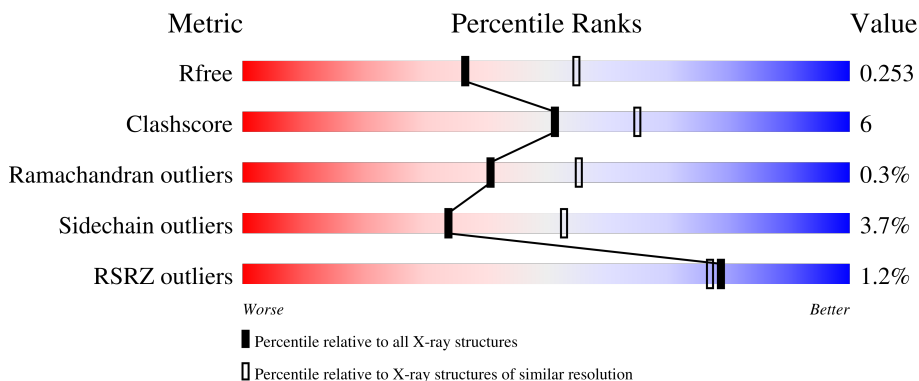
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	468	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">3% 82% 15% ..</p>
1	B	468	<div style="display: flex; align-items: center;"> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 11%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">87% 11% .</p>
1	C	468	<div style="display: flex; align-items: center;"> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 83% 14% ..</p>
1	D	468	<div style="display: flex; align-items: center;"> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">% 85% 12% ..</p>
1	E	468	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">2% 85% 13% ..</p>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	468	 86% 13% ..
1	G	468	%  85% 13% ..
1	H	468	%  82% 16% .

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 29459 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 Aspartase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	462	3583	2262	605	694	22	0	2	0
1	B	462	3568	2253	604	689	22	0	0	0
1	C	462	3568	2253	604	689	22	0	0	0
1	D	462	3568	2253	604	689	22	0	0	0
1	E	462	3568	2253	604	689	22	0	0	0
1	F	463	3576	2257	605	692	22	0	0	0
1	G	462	3568	2253	604	689	22	0	0	0
1	H	462	3568	2253	604	689	22	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	460	ILE	THR	conflict	UNP Q9LCC6
B	460	ILE	THR	conflict	UNP Q9LCC6
C	460	ILE	THR	conflict	UNP Q9LCC6
D	460	ILE	THR	conflict	UNP Q9LCC6
E	460	ILE	THR	conflict	UNP Q9LCC6
F	460	ILE	THR	conflict	UNP Q9LCC6
G	460	ILE	THR	conflict	UNP Q9LCC6
H	460	ILE	THR	conflict	UNP Q9LCC6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	E	1	Total Ca 1 1	0	0
2	H	1	Total Ca 1 1	0	0

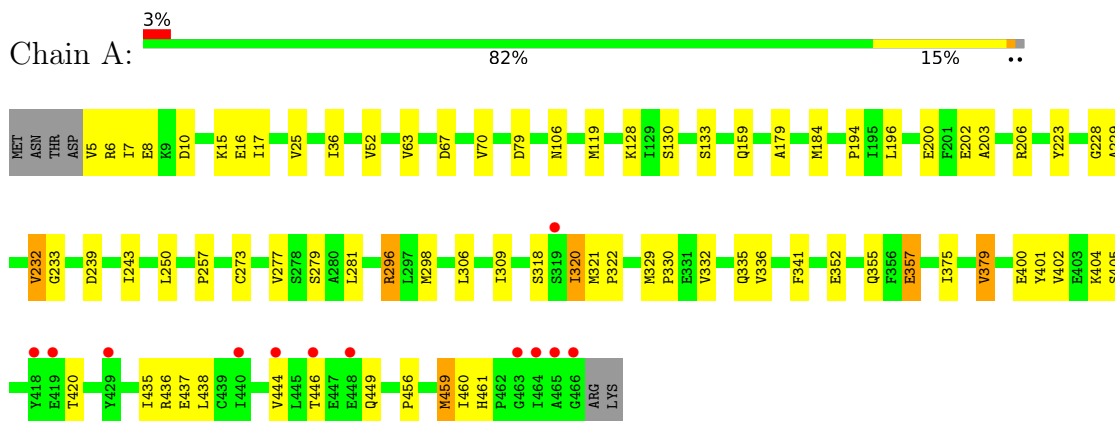
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	128	Total O 128 128	0	0
3	B	104	Total O 104 104	0	0
3	C	103	Total O 103 103	0	0
3	D	128	Total O 128 128	0	0
3	E	109	Total O 109 109	0	0
3	F	113	Total O 113 113	0	0
3	G	90	Total O 90 90	0	0
3	H	113	Total O 113 113	0	0

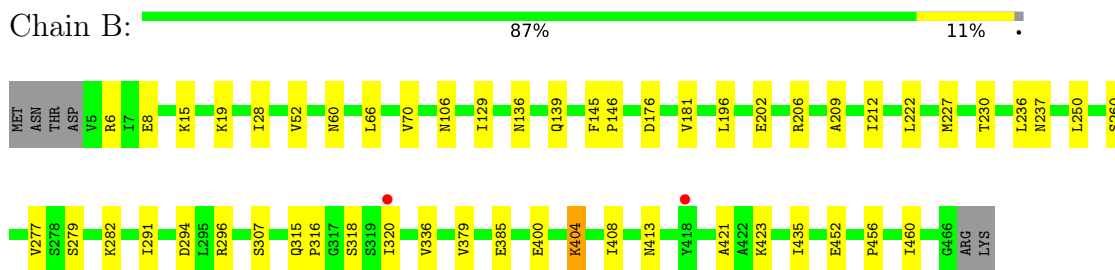
3 Residue-property plots [i](#)

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

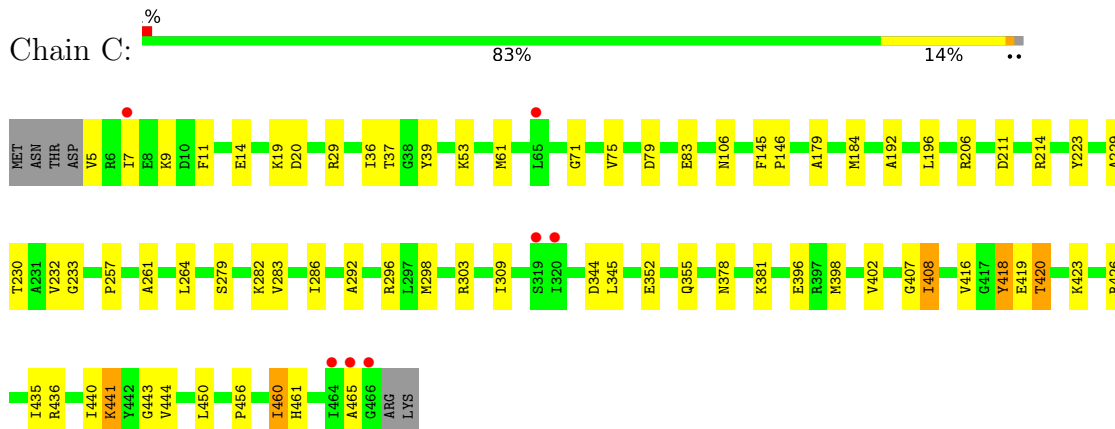
- Molecule 1: Aspartase



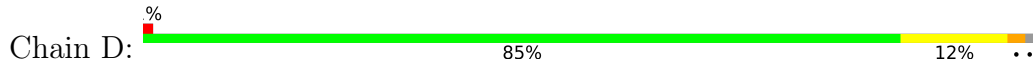
- Molecule 1: Aspartase



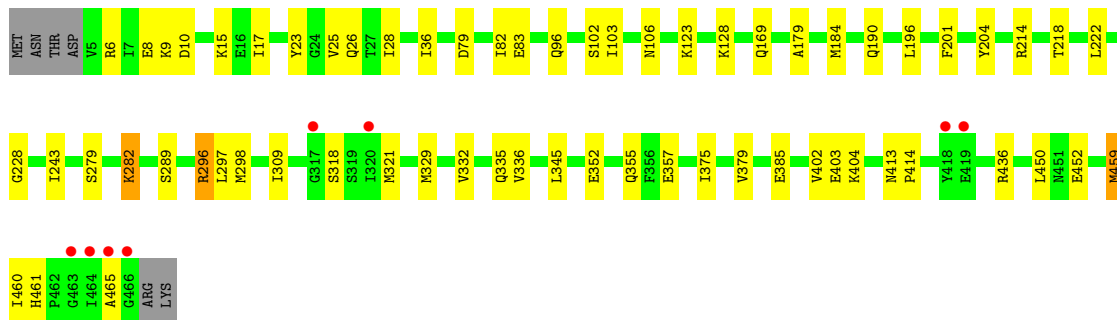
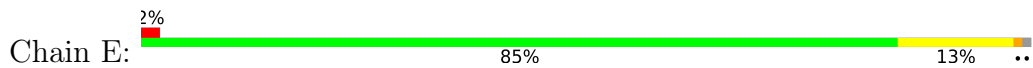
- Molecule 1: Aspartase



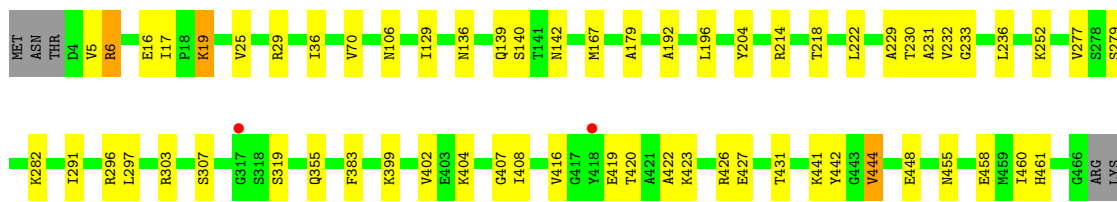
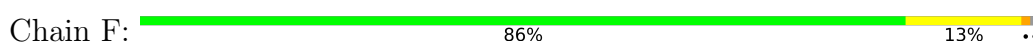
• Molecule 1: Aspartase



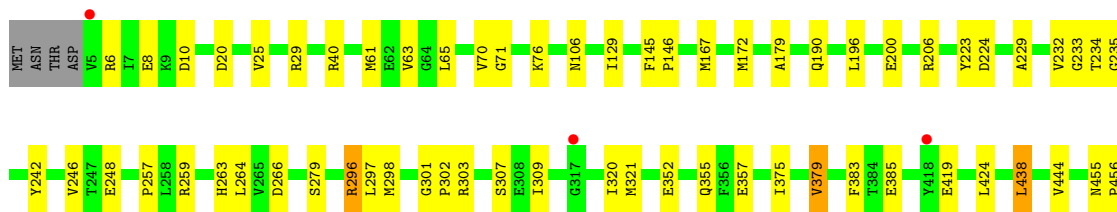
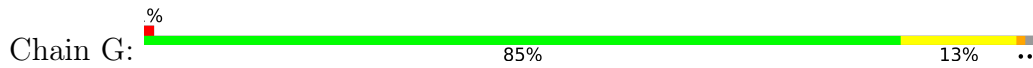
• Molecule 1: Aspartase

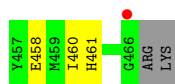


• Molecule 1: Aspartase

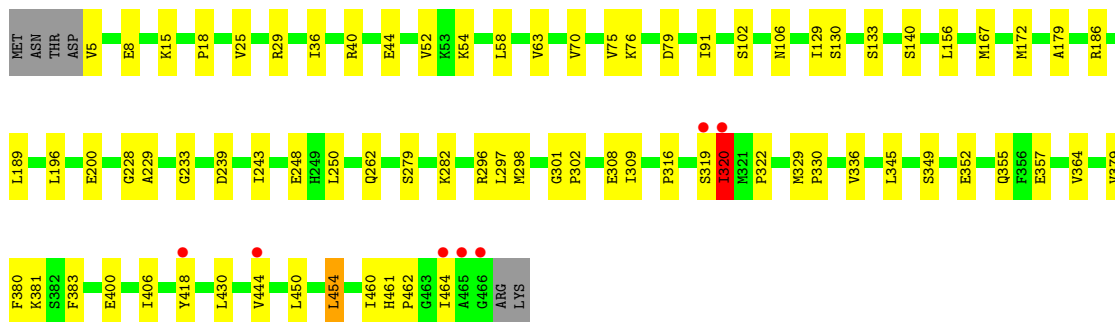
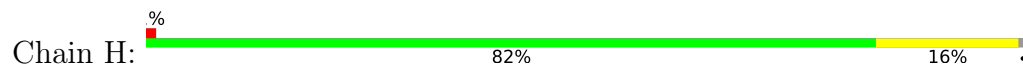


• Molecule 1: Aspartase





- Molecule 1: Aspartase



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.59Å 118.19Å 140.23Å 89.85° 89.59° 76.51°	Depositor
Resolution (Å)	39.56 – 2.40 39.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	87.7 (39.56-2.40) 85.9 (39.28-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.39Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.199 , 0.253 0.200 , 0.253	Depositor DCC
R_{free} test set	8118 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtrriage
Anisotropy	0.193	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 4.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.438 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29459	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/3645	0.58	1/4932 (0.0%)
1	B	0.49	0/3627	0.58	0/4908
1	C	0.48	0/3627	0.58	0/4908
1	D	0.49	0/3627	0.59	3/4908 (0.1%)
1	E	0.49	0/3627	0.59	1/4908 (0.0%)
1	F	0.49	0/3635	0.58	0/4919
1	G	0.47	0/3627	0.60	2/4908 (0.0%)
1	H	0.50	0/3627	0.59	0/4908
All	All	0.49	0/29042	0.59	7/39299 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	296	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	296	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	296	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	D	345	LEU	CA-CB-CG	5.60	128.19	115.30
1	G	296	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	296	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	E	296	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3583	0	3596	49	0
1	B	3568	0	3585	34	0
1	C	3568	0	3585	48	0
1	D	3568	0	3585	47	0
1	E	3568	0	3585	49	0
1	F	3576	0	3589	41	0
1	G	3568	0	3585	38	0
1	H	3568	0	3585	62	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	H	1	0	0	0	0
3	A	128	0	0	0	0
3	B	104	0	0	0	0
3	C	103	0	0	2	0
3	D	128	0	0	1	0
3	E	109	0	0	0	0
3	F	113	0	0	1	0
3	G	90	0	0	1	0
3	H	113	0	0	1	0
All	All	29459	0	28695	320	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 6.

All (320) 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:218:THR:HG23	1:D:277:VAL:HG22	1.27	1.11
1:H:336:VAL:HG21	1:H:379:VAL:HG11	1.35	1.08
1:E:184:MET:CE	1:E:402:VAL:HA	1.93	0.98
1:E:318:SER:HB2	1:E:321:MET:HB3	1.48	0.92
1:D:218:THR:CG2	1:D:277:VAL:HG22	2.01	0.90
1:A:63:VAL:HG11	1:A:239:ASP:OD1	1.70	0.89
1:G:196:LEU:HG	1:G:460:ILE:HD13	1.56	0.88
1:H:336:VAL:HG21	1:H:379:VAL:CG1	2.03	0.87
1:B:336:VAL:HG21	1:B:379:VAL:HG11	1.64	0.79
1:E:36:ILE:HD12	1:H:379:VAL:HG12	1.64	0.78
1:B:421:ALA:HB3	1:D:320:ILE:HD11	1.67	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:336:VAL:CG2	1:H:379:VAL:HG11	2.14	0.76
1:D:464:ILE:HG13	1:D:465:ALA:H	1.50	0.76
1:A:446:THR:H	1:A:449:GLN:HE21	1.33	0.76
1:H:63:VAL:HG11	1:H:239:ASP:OD1	1.86	0.76
1:F:17:ILE:HD11	1:F:25:VAL:HG13	1.72	0.72
1:E:184:MET:HE3	1:E:402:VAL:HA	1.70	0.72
1:G:190:GLN:NE2	3:G:674:HOH:O	2.22	0.71
1:H:229:ALA:HB1	1:H:233:GLY:HA2	1.70	0.71
1:D:460:ILE:HD12	1:D:461:HIS:ND1	2.06	0.71
1:D:23:TYR:HE2	1:D:28:ILE:HD11	1.57	0.70
1:H:345:LEU:O	1:H:345:LEU:HD23	1.92	0.69
1:F:460:ILE:CD1	1:F:461:HIS:CE1	2.76	0.69
1:F:355:GLN:OE1	1:G:296:ARG:NH2	2.26	0.68
1:F:460:ILE:HD12	1:F:461:HIS:CE1	2.28	0.68
1:B:336:VAL:HG21	1:B:379:VAL:CG1	2.22	0.68
1:C:279:SER:HB3	1:D:279:SER:HB3	1.75	0.68
1:E:196:LEU:HD23	1:E:460:ILE:HD13	1.77	0.67
1:H:167:MET:HE3	1:H:380:PHE:HA	1.77	0.66
1:B:296:ARG:NH2	1:C:355:GLN:OE1	2.29	0.66
1:E:318:SER:CB	1:E:321:MET:HB3	2.26	0.65
1:E:336:VAL:HG21	1:E:379:VAL:HG11	1.79	0.65
1:D:229:ALA:HB1	1:D:233:GLY:HA2	1.80	0.64
1:A:5:VAL:CG2	1:A:16:GLU:HB3	2.28	0.64
1:B:136:ASN:O	1:B:139:GLN:HG2	1.98	0.64
1:B:421:ALA:CB	1:D:320:ILE:HD11	2.28	0.63
1:G:167:MET:HE2	1:G:383:PHE:HD1	1.62	0.63
1:G:179:ALA:O	1:G:196:LEU:HD13	1.98	0.63
1:E:460:ILE:HD12	1:E:461:HIS:CE1	2.34	0.62
1:A:279:SER:HB3	1:B:279:SER:HB3	1.82	0.62
1:F:297:LEU:HD21	1:H:297:LEU:HD21	1.80	0.62
1:B:196:LEU:HD23	1:B:460:ILE:HD13	1.82	0.62
1:F:296:ARG:NH2	1:G:355:GLN:OE1	2.33	0.62
1:F:179:ALA:O	1:F:196:LEU:HD13	2.00	0.62
1:F:460:ILE:HD12	1:F:461:HIS:ND1	2.15	0.62
1:H:460:ILE:HD12	1:H:461:HIS:ND1	2.15	0.61
1:D:44:GLU:HG2	1:D:156:LEU:HG	1.83	0.61
1:G:200:GLU:OE2	1:H:357:GLU:OE1	2.18	0.60
1:E:297:LEU:HD21	1:G:297:LEU:HD21	1.83	0.60
1:F:36:ILE:HD12	1:G:379:VAL:HG13	1.82	0.60
1:H:460:ILE:CD1	1:H:461:HIS:CE1	2.84	0.60
1:G:229:ALA:HB1	1:G:233:GLY:HA2	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:345:LEU:HD23	1:H:345:LEU:C	2.22	0.60
1:G:279:SER:HB3	1:H:279:SER:HB3	1.84	0.60
1:E:355:GLN:OE1	1:H:296:ARG:NH2	2.35	0.60
1:H:298:MET:HB3	1:H:309:ILE:HG12	1.83	0.60
1:E:329:MET:O	1:E:332:VAL:HG12	2.02	0.60
1:D:441:LYS:HA	1:D:441:LYS:HE3	1.83	0.59
1:C:211:ASP:OD1	1:C:214:ARG:NH2	2.28	0.59
1:C:418:TYR:HD2	1:C:418:TYR:N	2.00	0.59
1:D:456:PRO:O	1:D:460:ILE:HG13	2.03	0.59
1:H:63:VAL:CG1	1:H:239:ASP:OD1	2.50	0.59
1:A:329:MET:O	1:A:332:VAL:HG12	2.04	0.58
1:C:418:TYR:N	1:C:418:TYR:CD2	2.71	0.58
1:E:36:ILE:HD12	1:H:379:VAL:CG1	2.33	0.58
1:E:379:VAL:HG13	1:H:36:ILE:HD12	1.85	0.57
1:D:228:GLY:HA3	1:D:243:ILE:HG12	1.86	0.57
1:F:167:MET:HE2	1:F:383:PHE:HD1	1.70	0.57
1:A:63:VAL:O	1:A:63:VAL:HG12	2.04	0.57
1:B:318:SER:HB3	1:B:320:ILE:HG22	1.87	0.57
1:E:336:VAL:HG21	1:E:379:VAL:CG1	2.35	0.57
1:F:229:ALA:HB1	1:F:233:GLY:HA2	1.87	0.57
1:A:322:PRO:HG3	1:C:426:ARG:HA	1.87	0.57
1:E:184:MET:HE2	1:E:402:VAL:HA	1.83	0.57
1:H:460:ILE:HD12	1:H:461:HIS:CE1	2.40	0.57
1:E:196:LEU:HD23	1:E:460:ILE:HG21	1.87	0.56
1:A:355:GLN:OE1	1:D:296:ARG:NH2	2.38	0.56
1:C:460:ILE:HD12	1:C:461:HIS:CE1	2.41	0.56
1:D:217:ASN:HB3	3:D:505:HOH:O	2.04	0.56
1:H:44:GLU:OE1	3:H:483:HOH:O	2.18	0.56
1:F:426:ARG:HA	1:H:322:PRO:HG3	1.86	0.56
1:A:130:SER:HB3	1:A:133:SER:HB2	1.88	0.56
1:G:196:LEU:CG	1:G:460:ILE:HD13	2.31	0.56
1:E:298:MET:HB3	1:E:309:ILE:HG12	1.88	0.56
1:A:5:VAL:HG21	1:A:16:GLU:HB3	1.88	0.55
1:G:145:PHE:HB3	1:G:146:PRO:HD3	1.89	0.55
1:A:36:ILE:HD12	1:D:379:VAL:HG13	1.88	0.55
1:D:375:ILE:O	1:D:379:VAL:HG22	2.05	0.55
1:D:83:GLU:OE1	1:D:85:LYS:NZ	2.39	0.55
1:E:23:TYR:HE2	1:E:28:ILE:HD11	1.72	0.55
1:C:79:ASP:O	1:C:83:GLU:HG2	2.07	0.54
1:C:345:LEU:C	1:C:345:LEU:HD23	2.26	0.54
1:C:416:VAL:CG1	1:C:420:THR:HB	2.37	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:LYS:NZ	1:F:427:GLU:OE1	2.39	0.54
1:E:8:GLU:HB2	1:E:17:ILE:HD13	1.90	0.54
1:F:5:VAL:HG22	1:F:6:ARG:H	1.71	0.54
1:E:436:ARG:HG3	1:E:450:LEU:HD13	1.90	0.54
1:B:336:VAL:CG2	1:B:379:VAL:HG11	2.34	0.54
1:A:6:ARG:HG2	1:A:7:ILE:H	1.72	0.54
1:B:456:PRO:O	1:B:460:ILE:HG12	2.08	0.54
1:G:320:ILE:HG22	1:G:321:MET:HG3	1.89	0.54
1:G:375:ILE:O	1:G:379:VAL:HG22	2.07	0.54
1:B:236:LEU:O	1:B:237:ASN:HB2	2.09	0.53
1:D:215:ILE:O	1:D:218:THR:HB	2.08	0.53
1:A:202:GLU:O	1:A:206:ARG:HG3	2.08	0.53
1:D:371:GLN:O	1:D:375:ILE:HG12	2.09	0.53
1:G:456:PRO:O	1:G:460:ILE:HG12	2.09	0.53
1:E:379:VAL:CG1	1:H:36:ILE:HD12	2.39	0.53
1:D:23:TYR:CE2	1:D:28:ILE:HD11	2.40	0.53
1:C:145:PHE:HB3	1:C:146:PRO:HD3	1.91	0.52
1:C:196:LEU:HG	1:C:460:ILE:HD13	1.92	0.52
1:D:6:ARG:NH1	1:D:8:GLU:OE2	2.43	0.52
1:C:7:ILE:HD11	1:C:14:GLU:HB3	1.91	0.52
1:C:298:MET:HB3	1:C:309:ILE:HG12	1.91	0.52
1:A:318:SER:OG	1:A:321:MET:HB3	2.09	0.52
1:A:336:VAL:HG21	1:A:379:VAL:HG11	1.92	0.52
1:E:96:GLN:HE22	1:E:103:ILE:HG13	1.73	0.52
1:G:167:MET:CE	1:G:383:PHE:HD1	2.22	0.52
1:A:298:MET:HB3	1:A:309:ILE:HG12	1.92	0.52
1:D:5:VAL:N	1:D:19:LYS:HZ2	2.08	0.52
1:C:184:MET:HE3	1:C:402:VAL:HG13	1.91	0.52
1:E:296:ARG:NH2	1:H:355:GLN:OE1	2.43	0.51
1:C:283:VAL:HA	1:C:286:ILE:HD12	1.92	0.51
1:C:196:LEU:HD11	1:C:460:ILE:HD11	1.92	0.51
1:E:179:ALA:O	1:E:196:LEU:HD12	2.10	0.51
1:G:223:TYR:CE2	1:G:257:PRO:HD2	2.45	0.51
1:B:70:VAL:HG13	1:B:129:ILE:HG12	1.92	0.51
1:E:96:GLN:NE2	1:E:103:ILE:HG13	2.25	0.51
1:B:181:VAL:O	1:B:196:LEU:HD13	2.11	0.51
1:C:61:MET:SD	1:C:71:GLY:HA3	2.50	0.51
1:A:336:VAL:HG21	1:A:379:VAL:CG1	2.40	0.51
1:G:455:ASN:HD22	1:G:458:GLU:HG3	1.74	0.51
1:A:456:PRO:O	1:A:460:ILE:HG13	2.10	0.51
1:H:63:VAL:HG12	1:H:63:VAL:O	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:CYS:O	1:A:277:VAL:HG23	2.10	0.50
1:E:228:GLY:HA3	1:E:243:ILE:HG12	1.93	0.50
1:A:70:VAL:HG12	1:A:119:MET:HE1	1.94	0.50
1:D:318:SER:HB3	1:D:321:MET:HB2	1.92	0.50
1:D:460:ILE:CD1	1:D:461:HIS:ND1	2.72	0.50
1:H:167:MET:CE	1:H:383:PHE:HD1	2.25	0.50
1:A:10:ASP:HB2	1:A:25:VAL:HG21	1.93	0.50
1:A:460:ILE:HD12	1:A:461:HIS:ND1	2.26	0.50
1:C:37:THR:HB	1:C:39:TYR:CD1	2.47	0.50
1:G:235:GLY:O	1:H:462:PRO:HA	2.12	0.50
1:A:184:MET:HE3	1:A:402:VAL:HA	1.94	0.50
1:C:416:VAL:HG13	1:C:420:THR:HB	1.93	0.49
1:H:54:LYS:HD2	1:H:79:ASP:OD2	2.12	0.49
1:A:232:VAL:HG22	1:A:357:GLU:HG3	1.94	0.49
1:H:319:SER:O	1:H:320:ILE:HG23	2.12	0.49
1:F:460:ILE:HD11	1:F:461:HIS:CE1	2.46	0.49
1:H:450:LEU:O	1:H:454:LEU:HB2	2.12	0.49
1:A:6:ARG:HG2	1:A:7:ILE:N	2.28	0.49
1:G:206:ARG:NH2	1:H:262:GLN:OE1	2.46	0.49
1:F:70:VAL:HG13	1:F:129:ILE:HG12	1.94	0.49
1:H:167:MET:HE2	1:H:383:PHE:HD1	1.78	0.49
1:D:136:ASN:O	1:D:139:GLN:HG2	2.13	0.49
1:E:184:MET:CE	1:E:402:VAL:HG22	2.43	0.48
1:C:196:LEU:CD1	1:C:460:ILE:HD13	2.43	0.48
1:A:321:MET:O	1:A:321:MET:HG3	2.13	0.48
1:B:202:GLU:O	1:B:206:ARG:HG3	2.14	0.48
1:C:196:LEU:CD1	1:C:460:ILE:CD1	2.91	0.48
1:A:379:VAL:HG13	1:D:36:ILE:HD12	1.96	0.48
1:G:70:VAL:HG13	1:G:129:ILE:HG12	1.96	0.48
1:F:297:LEU:HD23	1:H:189:LEU:HD13	1.96	0.48
1:C:292:ALA:O	1:C:296:ARG:HG3	2.13	0.48
1:E:196:LEU:CD2	1:E:460:ILE:HD13	2.43	0.48
1:E:459:MET:O	1:F:236:LEU:HD13	2.13	0.48
1:C:71:GLY:O	1:C:75:VAL:HG23	2.13	0.48
1:B:222:LEU:HD11	1:B:277:VAL:HG21	1.94	0.48
1:H:167:MET:HE1	1:H:383:PHE:CD1	2.49	0.48
1:F:282:LYS:HB3	1:F:282:LYS:HE3	1.61	0.47
1:C:229:ALA:HB1	1:C:233:GLY:HA2	1.95	0.47
1:F:19:LYS:HE3	1:F:19:LYS:O	2.14	0.47
1:D:395:GLU:CD	1:D:395:GLU:H	2.17	0.47
1:B:227:MET:HG3	1:B:250:LEU:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ALA:O	1:C:196:LEU:HD13	2.15	0.47
1:H:44:GLU:HG2	1:H:156:LEU:HG	1.96	0.47
1:A:179:ALA:O	1:A:196:LEU:HD13	2.15	0.47
1:B:282:LYS:HE3	1:B:282:LYS:HB3	1.43	0.47
1:D:145:PHE:HB3	1:D:146:PRO:CD	2.44	0.47
1:F:448:GLU:CD	1:F:448:GLU:H	2.18	0.47
1:H:52:VAL:HA	1:H:250:LEU:HD21	1.97	0.47
1:H:54:LYS:HG3	1:H:75:VAL:HG13	1.96	0.47
1:E:279:SER:HB3	1:F:279:SER:HB3	1.97	0.47
1:G:298:MET:HB3	1:G:309:ILE:HG12	1.96	0.47
1:E:345:LEU:HD12	1:H:345:LEU:HD12	1.97	0.46
1:F:192:ALA:O	1:F:407:GLY:HA3	2.15	0.46
1:G:357:GLU:OE1	1:H:200:GLU:OE2	2.33	0.46
1:H:29:ARG:HD3	1:H:29:ARG:HA	1.76	0.46
1:A:436:ARG:C	1:A:438:LEU:H	2.19	0.46
1:C:11:PHE:HB3	3:C:515:HOH:O	2.14	0.46
1:C:436:ARG:HG3	1:C:450:LEU:HD13	1.96	0.46
1:D:464:ILE:CG1	1:D:465:ALA:H	2.23	0.46
1:H:186:ARG:NH1	1:H:308:GLU:OE1	2.44	0.46
1:A:194:PRO:HG2	1:A:459:MET:HG2	1.96	0.46
1:D:413:ASN:HB3	1:D:414:PRO:CD	2.46	0.46
1:E:335:GLN:HB3	1:H:364:VAL:HB	1.96	0.46
1:H:70:VAL:HG13	1:H:129:ILE:HG12	1.98	0.46
1:B:52:VAL:HA	1:B:250:LEU:HD21	1.98	0.46
1:B:413:ASN:HD22	1:D:320:ILE:HD13	1.81	0.46
1:E:413:ASN:HB3	1:E:414:PRO:HD3	1.97	0.46
1:H:179:ALA:O	1:H:196:LEU:HD13	2.14	0.46
1:A:296:ARG:NH2	1:D:355:GLN:OE1	2.48	0.46
1:A:8:GLU:HB2	1:A:17:ILE:HD12	1.97	0.46
1:B:6:ARG:NH1	1:B:8:GLU:OE2	2.49	0.46
1:C:456:PRO:O	1:C:460:ILE:HG12	2.15	0.46
1:F:196:LEU:HD12	1:F:460:ILE:HD13	1.98	0.46
1:D:75:VAL:HG11	1:F:431:THR:HG22	1.97	0.46
1:G:424:LEU:HD22	1:G:438:LEU:HB3	1.98	0.46
1:H:228:GLY:HA3	1:H:243:ILE:HG12	1.97	0.46
1:C:398:MET:O	1:C:402:VAL:HG23	2.15	0.45
1:F:422:ALA:HB1	1:H:320:ILE:CG2	2.46	0.45
1:C:408:ILE:CG2	1:C:435:ILE:HD12	2.46	0.45
1:C:419:GLU:HG3	1:C:420:THR:H	1.80	0.45
1:B:209:ALA:HA	1:B:212:ILE:HD12	1.97	0.45
1:H:167:MET:CE	1:H:383:PHE:CD1	2.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:HB3	1:A:70:VAL:HG22	1.98	0.45
1:A:335:GLN:HB3	1:D:364:VAL:HB	1.97	0.45
1:F:420:THR:HG21	1:F:444:VAL:HG21	1.98	0.45
1:E:184:MET:HE1	1:E:402:VAL:HG22	1.98	0.45
1:G:6:ARG:NH1	1:G:8:GLU:OE2	2.50	0.45
1:A:228:GLY:HA3	1:A:243:ILE:HG12	1.99	0.45
1:E:460:ILE:CD1	1:E:461:HIS:CE1	2.99	0.45
1:H:5:VAL:HG12	1:H:18:PRO:HA	1.99	0.45
1:H:196:LEU:HD11	1:H:460:ILE:HD11	1.99	0.45
1:A:420:THR:HG21	1:A:444:VAL:HG11	1.99	0.45
1:F:136:ASN:O	1:F:139:GLN:HG2	2.17	0.45
1:A:375:ILE:O	1:A:379:VAL:HG22	2.17	0.44
1:C:396:GLU:CD	1:C:396:GLU:H	2.21	0.44
1:D:6:ARG:HG2	1:D:7:ILE:N	2.33	0.44
1:E:36:ILE:CD1	1:H:379:VAL:HG12	2.41	0.44
1:D:29:ARG:HA	1:D:29:ARG:HD2	1.66	0.44
1:A:277:VAL:O	1:A:281:LEU:HG	2.17	0.44
1:C:192:ALA:O	1:C:407:GLY:HA3	2.17	0.44
1:A:63:VAL:CG1	1:A:239:ASP:OD1	2.55	0.44
1:G:460:ILE:HD12	1:G:461:HIS:CE1	2.53	0.44
1:H:40:ARG:HD2	1:H:91:ILE:HA	2.00	0.44
1:E:196:LEU:HD23	1:E:460:ILE:CD1	2.45	0.44
1:F:5:VAL:HG21	1:F:16:GLU:HB3	1.98	0.44
1:D:408:ILE:HG12	1:D:454:LEU:HD22	2.00	0.43
1:E:79:ASP:HA	1:E:82:ILE:HD12	2.00	0.43
1:A:223:TYR:CE2	1:A:257:PRO:HD2	2.53	0.43
1:B:15:LYS:HG2	1:B:28:ILE:HD11	1.99	0.43
1:C:460:ILE:CD1	1:C:461:HIS:CE1	3.00	0.43
1:E:10:ASP:HB2	1:E:25:VAL:HG21	2.00	0.43
1:E:201:PHE:HA	1:E:204:TYR:CD2	2.53	0.43
1:D:151:ILE:HG23	1:D:254:SER:HB2	1.99	0.43
1:E:26:GLN:HG2	1:H:316:PRO:HG3	2.00	0.43
1:E:282:LYS:HE2	3:F:795:HOH:O	2.18	0.43
1:F:441:LYS:HD3	1:F:442:TYR:CZ	2.53	0.43
1:B:15:LYS:HG2	1:B:28:ILE:CD1	2.48	0.43
1:D:52:VAL:HA	1:D:250:LEU:HD21	2.01	0.43
1:H:329:MET:HB2	1:H:330:PRO:HD3	1.99	0.43
1:E:404:LYS:O	1:G:303:ARG:NH1	2.51	0.43
1:F:204:TYR:CD1	1:F:291:ILE:HG12	2.52	0.43
1:B:400:GLU:HG3	1:B:404:LYS:HE2	2.01	0.43
1:E:169:GLN:HA	1:E:169:GLN:OE1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:460:ILE:CD1	1:H:461:HIS:ND1	2.82	0.43
1:B:379:VAL:CG1	1:C:36:ILE:HD12	2.48	0.43
1:C:261:ALA:HB3	1:C:264:LEU:HD23	2.01	0.43
1:E:8:GLU:HB2	1:E:17:ILE:CD1	2.49	0.43
1:C:282:LYS:HE2	1:C:344:ASP:OD1	2.19	0.42
1:H:301:GLY:HA3	1:H:302:PRO:HA	1.82	0.42
1:H:460:ILE:HD11	1:H:461:HIS:CE1	2.54	0.42
1:F:214:ARG:O	1:F:218:THR:HG23	2.19	0.42
1:G:10:ASP:HB2	1:G:25:VAL:HG21	2.01	0.42
1:B:227:MET:HG3	1:B:250:LEU:CD1	2.50	0.42
1:F:402:VAL:HG13	1:F:408:ILE:CD1	2.49	0.42
1:D:7:ILE:HD11	1:D:14:GLU:HB3	2.02	0.42
1:F:142:ASN:ND2	1:F:231:ALA:O	2.49	0.42
1:H:8:GLU:HB2	1:H:25:VAL:HG13	2.01	0.42
1:H:345:LEU:C	1:H:345:LEU:CD2	2.87	0.42
1:C:443:GLY:HA2	3:C:651:HOH:O	2.19	0.42
1:E:214:ARG:O	1:E:218:THR:HG23	2.19	0.42
1:F:441:LYS:HD3	1:F:442:TYR:CE2	2.54	0.42
1:B:379:VAL:HG12	1:C:36:ILE:HD12	2.02	0.42
1:F:319:SER:HG	1:H:418:TYR:HH	1.65	0.42
1:D:347:ILE:HG23	1:D:365:LEU:HD21	2.02	0.42
1:A:341:PHE:HB3	1:D:345:LEU:HD21	2.02	0.42
1:A:401:TYR:O	1:A:405:SER:HB3	2.20	0.42
1:C:436:ARG:O	1:C:440:ILE:HG12	2.18	0.42
1:D:455:ASN:HD22	1:D:458:GLU:HG2	1.85	0.42
1:C:419:GLU:HG3	1:C:420:THR:N	2.35	0.42
1:F:455:ASN:HD22	1:F:458:GLU:HB2	1.84	0.42
1:B:60:ASN:HB3	1:B:66:LEU:HB2	2.02	0.41
1:C:223:TYR:CE2	1:C:257:PRO:HD2	2.55	0.41
1:G:301:GLY:HA3	1:G:302:PRO:HA	1.93	0.41
1:H:130:SER:HB3	1:H:133:SER:HB2	2.02	0.41
1:A:329:MET:HB2	1:A:330:PRO:HD3	2.02	0.41
1:F:222:LEU:HD11	1:F:277:VAL:HG21	2.02	0.41
1:A:184:MET:HE1	1:A:194:PRO:HG3	2.01	0.41
1:D:6:ARG:HG2	1:D:7:ILE:H	1.85	0.41
1:G:232:VAL:HG23	1:G:234:THR:HG23	2.01	0.41
1:B:315:GLN:HB2	1:B:316:PRO:HD2	2.02	0.41
1:C:440:ILE:HG22	1:C:441:LYS:HE3	2.02	0.41
1:G:63:VAL:HG12	1:G:65:LEU:HG	2.02	0.41
1:G:242:TYR:O	1:G:246:VAL:HG12	2.20	0.41
1:G:263:HIS:HB3	1:G:266:ASP:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ASN:HA	1:C:381:LYS:HE2	2.03	0.41
1:G:196:LEU:CD1	1:G:460:ILE:CD1	2.98	0.41
1:G:224:ASP:CG	1:G:259:ARG:HH21	2.24	0.41
1:F:422:ALA:CB	1:H:320:ILE:CG2	2.98	0.41
1:A:196:LEU:HG	1:A:460:ILE:HG12	2.03	0.41
1:A:200:GLU:O	1:A:203:ALA:HB3	2.21	0.41
1:B:196:LEU:CD2	1:B:460:ILE:HD13	2.50	0.41
1:C:206:ARG:NH1	1:D:266:ASP:OD2	2.53	0.41
1:G:196:LEU:HD11	1:G:460:ILE:HD11	2.03	0.41
1:B:400:GLU:O	1:B:404:LYS:HG2	2.21	0.41
1:B:145:PHE:HB3	1:B:146:PRO:CD	2.51	0.40
1:C:53:LYS:HA	1:C:53:LYS:HD3	1.98	0.40
1:A:229:ALA:HB1	1:A:233:GLY:HA2	2.03	0.40
1:A:404:LYS:O	1:C:303:ARG:NH1	2.52	0.40
1:G:61:MET:SD	1:G:71:GLY:HA3	2.60	0.40
1:A:52:VAL:HA	1:A:250:LEU:HD21	2.03	0.40
1:B:291:ILE:O	1:B:294:ASP:HB2	2.22	0.40
1:E:15:LYS:HG2	1:E:28:ILE:HG21	2.04	0.40
1:E:96:GLN:OE1	1:E:102:SER:HB2	2.21	0.40
1:E:375:ILE:O	1:E:379:VAL:HG22	2.21	0.40
1:F:422:ALA:HB1	1:H:320:ILE:HG22	2.04	0.40
1:F:460:ILE:CD1	1:F:461:HIS:ND1	2.81	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	462/468 (99%)	439 (95%)	21 (4%)	2 (0%)	34 48
1	B	460/468 (98%)	446 (97%)	12 (3%)	2 (0%)	34 48
1	C	460/468 (98%)	444 (96%)	13 (3%)	3 (1%)	22 32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	460/468 (98%)	447 (97%)	12 (3%)	1 (0%)	47 62
1	E	460/468 (98%)	446 (97%)	13 (3%)	1 (0%)	47 62
1	F	461/468 (98%)	446 (97%)	14 (3%)	1 (0%)	47 62
1	G	460/468 (98%)	450 (98%)	10 (2%)	0	100 100
1	H	460/468 (98%)	445 (97%)	13 (3%)	2 (0%)	34 48
All	All	3683/3744 (98%)	3563 (97%)	108 (3%)	12 (0%)	41 55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	408	ILE
1	C	465	ALA
1	B	408	ILE
1	H	464	ILE
1	B	230	THR
1	A	320	ILE
1	A	437	GLU
1	C	230	THR
1	D	413	ASN
1	E	465	ALA
1	F	230	THR
1	H	320	ILE

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	390/394 (99%)	376 (96%)	14 (4%)	35 54
1	B	388/394 (98%)	378 (97%)	10 (3%)	46 66
1	C	388/394 (98%)	374 (96%)	14 (4%)	35 54
1	D	388/394 (98%)	376 (97%)	12 (3%)	40 60
1	E	388/394 (98%)	372 (96%)	16 (4%)	30 48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	389/394 (99%)	374 (96%)	15 (4%)	32	50
1	G	388/394 (98%)	373 (96%)	15 (4%)	32	50
1	H	388/394 (98%)	370 (95%)	18 (5%)	27	43
All	All	3107/3152 (99%)	2993 (96%)	114 (4%)	34	53

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	79	ASP
1	A	106	ASN
1	A	128	LYS
1	A	159	GLN
1	A	232	VAL
1	A	306	LEU
1	A	320	ILE
1	A	352	GLU
1	A	357	GLU
1	A	379	VAL
1	A	400	GLU
1	A	435	ILE
1	A	459	MET
1	B	19	LYS
1	B	106	ASN
1	B	176	ASP
1	B	260	SER
1	B	307	SER
1	B	385	GLU
1	B	404	LYS
1	B	423	LYS
1	B	435	ILE
1	B	452	GLU
1	C	5	VAL
1	C	9	LYS
1	C	19	LYS
1	C	20	ASP
1	C	29	ARG
1	C	106	ASN
1	C	232	VAL
1	C	352	GLU
1	C	418	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	420	THR
1	C	423	LYS
1	C	441	LYS
1	C	444	VAL
1	C	460	ILE
1	D	9	LYS
1	D	29	ARG
1	D	106	ASN
1	D	127	SER
1	D	218	THR
1	D	282	LYS
1	D	315	GLN
1	D	320	ILE
1	D	379	VAL
1	D	400	GLU
1	D	434	SER
1	D	441	LYS
1	E	6	ARG
1	E	9	LYS
1	E	83	GLU
1	E	106	ASN
1	E	123	LYS
1	E	128	LYS
1	E	190	GLN
1	E	222	LEU
1	E	282	LYS
1	E	289	SER
1	E	352	GLU
1	E	357	GLU
1	E	385	GLU
1	E	403	GLU
1	E	452	GLU
1	E	459	MET
1	F	6	ARG
1	F	19	LYS
1	F	29	ARG
1	F	106	ASN
1	F	140	SER
1	F	232	VAL
1	F	252	LYS
1	F	303	ARG
1	F	307	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	399	LYS
1	F	404	LYS
1	F	416	VAL
1	F	419	GLU
1	F	423	LYS
1	F	444	VAL
1	G	20	ASP
1	G	29	ARG
1	G	40	ARG
1	G	76	LYS
1	G	106	ASN
1	G	172	MET
1	G	248	GLU
1	G	264	LEU
1	G	307	SER
1	G	352	GLU
1	G	379	VAL
1	G	385	GLU
1	G	419	GLU
1	G	438	LEU
1	G	444	VAL
1	H	15	LYS
1	H	58	LEU
1	H	76	LYS
1	H	102	SER
1	H	106	ASN
1	H	140	SER
1	H	172	MET
1	H	248	GLU
1	H	282	LYS
1	H	320	ILE
1	H	349	SER
1	H	352	GLU
1	H	381	LYS
1	H	400	GLU
1	H	406	ILE
1	H	430	LEU
1	H	444	VAL
1	H	454	LEU

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

Mol	Chain	Res	Type
1	A	96	GLN
1	A	449	GLN
1	A	451	ASN
1	A	455	ASN
1	C	96	GLN
1	C	413	ASN
1	C	451	ASN
1	C	461	HIS
1	D	96	GLN
1	D	451	ASN
1	D	455	ASN
1	E	190	GLN
1	E	386	ASN
1	E	451	ASN
1	F	26	GLN
1	G	26	GLN
1	G	455	ASN
1	G	461	HIS
1	H	96	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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, 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	462/468 (98%)	-0.35	12 (2%) 56 54	7, 21, 71, 79	0
1	B	462/468 (98%)	-0.37	2 (0%) 92 91	10, 26, 49, 69	0
1	C	462/468 (98%)	-0.34	7 (1%) 73 72	8, 28, 55, 70	0
1	D	462/468 (98%)	-0.49	4 (0%) 84 82	7, 21, 47, 60	0
1	E	462/468 (98%)	-0.41	8 (1%) 70 68	8, 20, 70, 76	0
1	F	463/468 (98%)	-0.36	2 (0%) 92 91	8, 26, 47, 66	0
1	G	462/468 (98%)	-0.41	4 (0%) 84 82	8, 27, 53, 66	0
1	H	462/468 (98%)	-0.48	7 (1%) 73 72	6, 22, 47, 60	0
All	All	3697/3744 (98%)	-0.40	46 (1%) 79 77	6, 23, 56, 79	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	464	ILE	6.6
1	H	466	GLY	6.5
1	A	464	ILE	6.5
1	D	465	ALA	5.5
1	A	466	GLY	5.2
1	A	463	GLY	4.5
1	H	465	ALA	4.5
1	A	465	ALA	4.4
1	E	465	ALA	4.4
1	E	418	TYR	3.9
1	E	466	GLY	3.8
1	A	448	GLU	3.8
1	A	319	SER	3.8
1	C	465	ALA	3.6
1	A	419	GLU	3.4
1	D	466	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	444	VAL	3.3
1	H	418	TYR	3.2
1	D	464	ILE	3.2
1	C	466	GLY	3.1
1	E	419	GLU	3.0
1	B	320	ILE	3.0
1	H	320	ILE	3.0
1	B	418	TYR	2.7
1	H	319	SER	2.7
1	A	418	TYR	2.6
1	C	7	ILE	2.6
1	C	320	ILE	2.5
1	G	466	GLY	2.5
1	E	317	GLY	2.5
1	G	317	GLY	2.5
1	H	464	ILE	2.4
1	F	418	TYR	2.4
1	A	446	THR	2.3
1	E	463	GLY	2.2
1	C	319	SER	2.2
1	A	440	ILE	2.2
1	E	320	ILE	2.2
1	F	317	GLY	2.2
1	A	429	TYR	2.2
1	D	418	TYR	2.1
1	C	464	ILE	2.1
1	G	5	VAL	2.1
1	G	418	TYR	2.1
1	H	444	VAL	2.0
1	C	65	LEU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	469	1/1	0.90	0.09	42,42,42,42	0
2	CA	E	469	1/1	0.92	0.12	38,38,38,38	0
2	CA	H	469	1/1	0.95	0.10	34,34,34,34	0
2	CA	D	469	1/1	0.97	0.10	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.