



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:53 AM UTC

PDB ID : 3R6V / pdb_00003r6v
Title : Crystal structure of aspartase from Bacillus sp. YM55-1 with bound L-aspartate
Authors : Fibriansah, G.; Puthan Veetil, V.; Poelarends, G.J.; Thunnissen, A.-M.W.H.
Deposited on : 2011-03-22
Resolution : 2.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

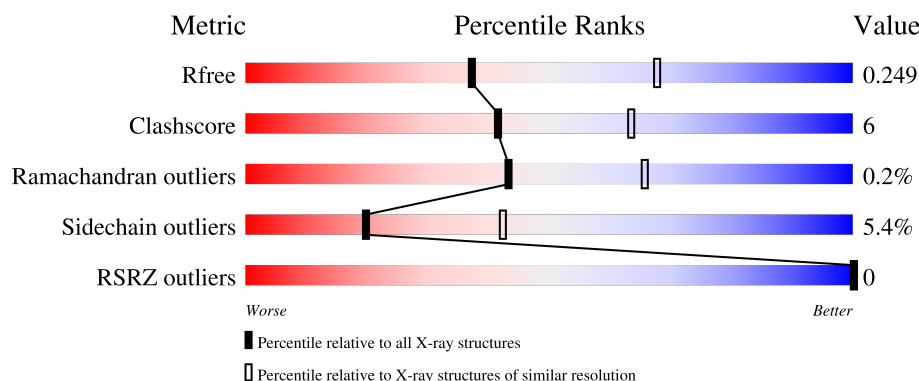
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	
1	B	468	
1	C	468	
1	D	468	
1	E	468	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	468	 81% 16% ..
1	G	468	 82% 16% ..
1	H	468	 80% 16% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28980 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
1	A	458	Total	C	N	O	S	0	0	0
			3547	2240	600	685	22			
1	B	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	C	462	Total	C	N	O	S	0	0	0
			3568	2253	604	689	22			
1	D	459	Total	C	N	O	S	0	0	0
			3551	2242	601	686	22			
1	E	459	Total	C	N	O	S	0	1	0
			3557	2246	601	688	22			
1	F	461	Total	C	N	O	S	0	0	0
			3564	2251	603	688	22			
1	G	463	Total	C	N	O	S	0	0	0
			3573	2256	605	690	22			
1	H	459	Total	C	N	O	S	0	0	0
			3551	2242	601	686	22			

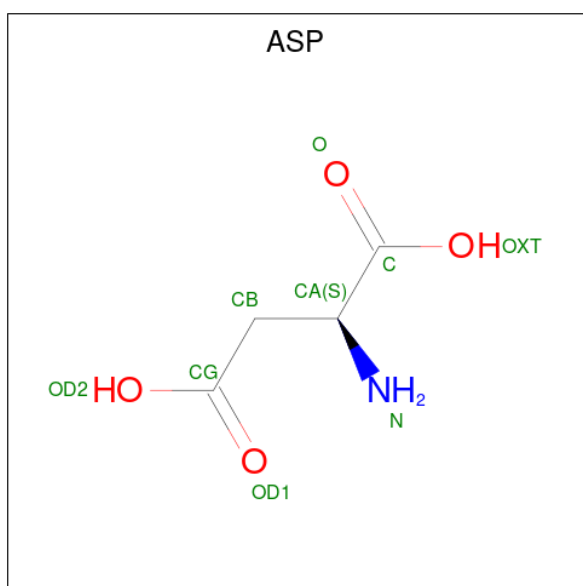
There are 8 discrepancies between the modelled and reference sequences:

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 (CCD ID: 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 ASPARTIC ACID (CCD ID: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 9 4 1 4	0	0
3	F	1	Total C N O 9 4 1 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	74	Total O 74 74	0	0
4	B	58	Total O 58 58	0	0
4	C	50	Total O 50 50	0	0
4	D	71	Total O 71 71	0	0

Continued on next page...

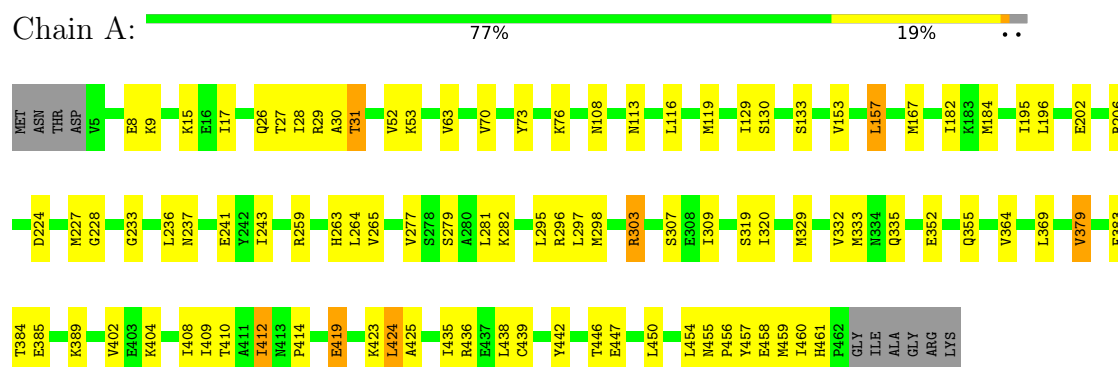
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	55	Total 55	O 55	0	0
4	F	66	Total 66	O 66	0	0
4	G	41	Total 41	O 41	0	0
4	H	64	Total 64	O 64	0	0

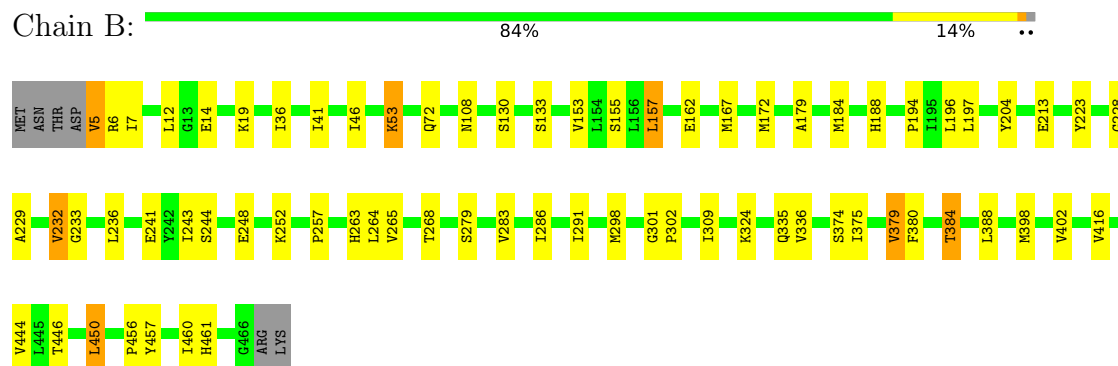
3 Residue-property plots [i](#)

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.

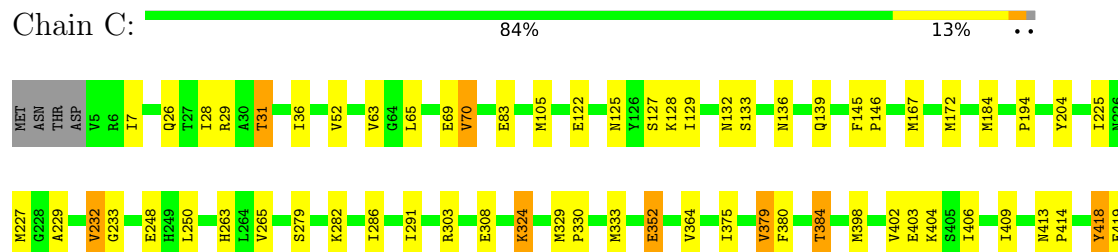
• Molecule 1: Aspartase



• Molecule 1: Aspartase



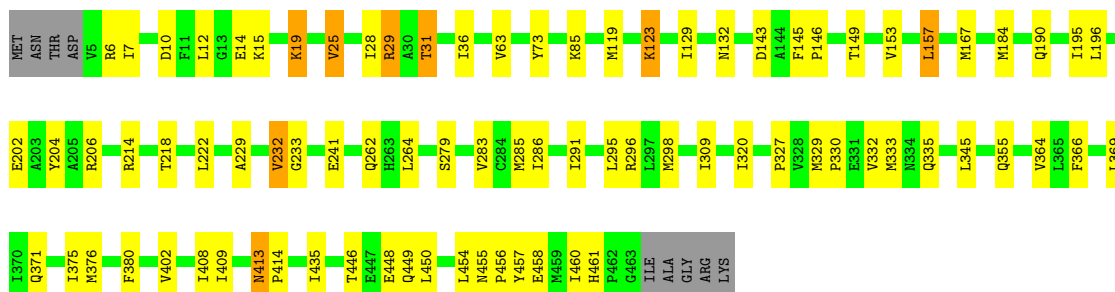
• Molecule 1: Aspartase





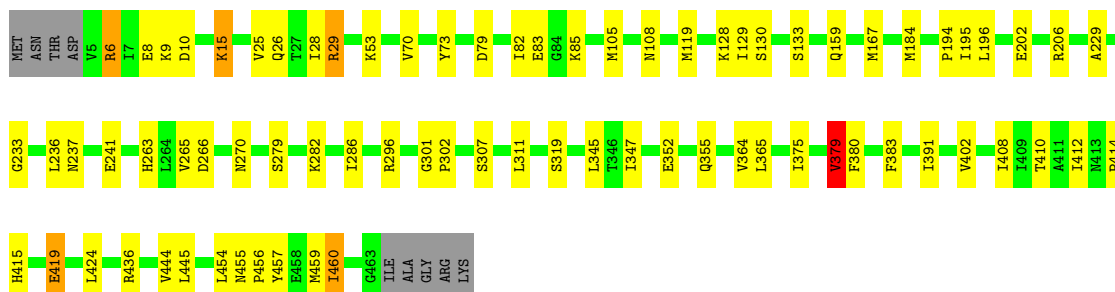
• Molecule 1: Aspartase

Chain D: 80% 16% ..



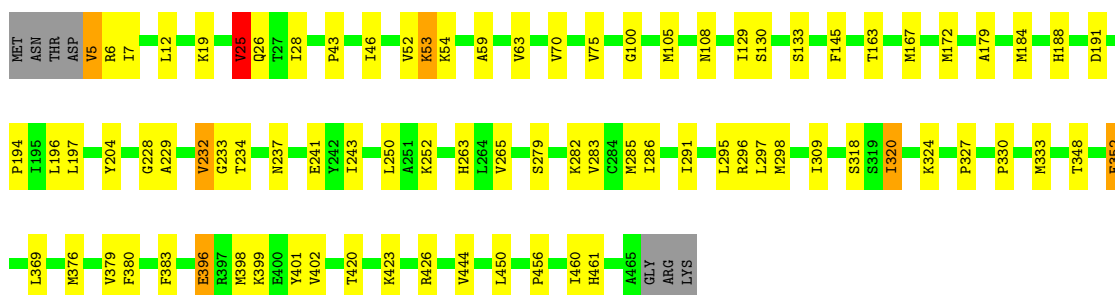
• Molecule 1: Aspartase

Chain E: 82% 15% ..



• Molecule 1: Aspartase

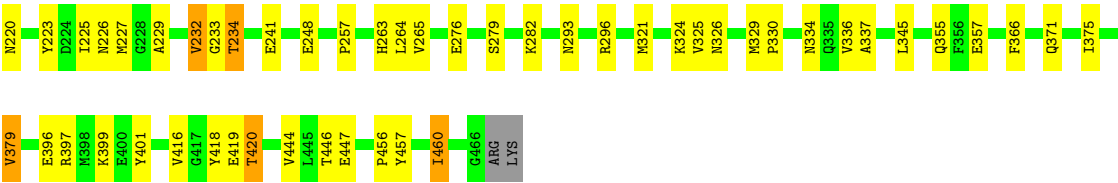
Chain F: 81% 16% ..



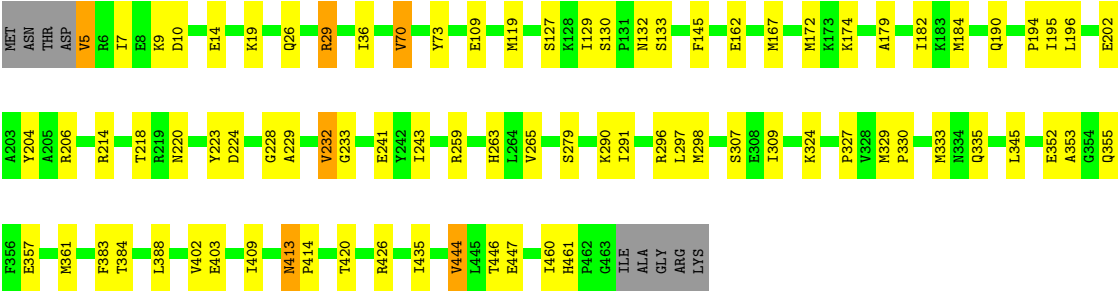
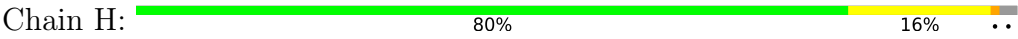
• Molecule 1: Aspartase

Chain G: 82% 16% ..





• Molecule 1: Aspartase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.85Å 118.96Å 141.41Å 89.93° 89.93° 76.42°	Depositor
Resolution (Å)	39.73 – 2.60 39.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.73-2.60) 97.5 (39.73-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.193 , 0.250 0.194 , 0.249	Depositor DCC
R_{free} test set	7250 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 5.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.457 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	28980	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.60	0/3606	0.88	0/4880
1	B	0.60	0/3627	0.88	0/4908
1	C	0.60	0/3627	0.88	2/4908 (0.0%)
1	D	0.60	0/3610	0.88	0/4885
1	E	0.59	0/3619	0.85	1/4897 (0.0%)
1	F	0.59	0/3623	0.88	1/4903 (0.0%)
1	G	0.58	0/3632	0.92	3/4915 (0.1%)
1	H	0.60	0/3610	0.88	4/4885 (0.1%)
All	All	0.60	0/28954	0.88	11/39181 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	325	VAL	N-CA-C	5.98	115.34	106.85
1	G	321	MET	CA-C-N	5.90	127.22	119.84
1	G	321	MET	C-N-CA	5.90	127.22	119.84
1	H	145	PHE	CA-C-N	-5.89	112.95	119.19
1	H	145	PHE	C-N-CA	-5.89	112.95	119.19
1	C	324	LYS	N-CA-C	5.48	118.18	110.23
1	C	418	TYR	N-CA-C	5.42	116.87	111.07
1	E	379	VAL	CB-CA-C	-5.33	104.86	112.22
1	F	25	VAL	CB-CA-C	-5.25	105.25	111.97
1	H	413	ASN	CA-C-N	-5.19	115.53	120.83
1	H	413	ASN	C-N-CA	-5.19	115.53	120.83

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	3547	0	3563	59	0
1	B	3568	0	3585	45	0
1	C	3568	0	3585	36	0
1	D	3551	0	3566	57	0
1	E	3557	0	3572	51	0
1	F	3564	0	3582	57	0
1	G	3573	0	3587	49	0
1	H	3551	0	3566	53	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	B	9	0	3	0	0
3	F	9	0	3	0	0
4	A	74	0	0	0	0
4	B	58	0	0	0	0
4	C	50	0	0	1	0
4	D	71	0	0	0	0
4	E	55	0	0	0	0
4	F	66	0	0	0	0
4	G	41	0	0	2	0
4	H	64	0	0	1	0
All	All	28980	0	28612	367	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 (367) 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:A:53:LYS:HE2	1:A:108:ASN:OD1	1.75	0.87
1:D:285:MET:HE3	1:D:376:MET:HE3	1.53	0.87
1:D:119:MET:HE3	1:D:129:ILE:HD11	1.56	0.86
1:F:285:MET:HE3	1:F:376:MET:HE3	1.57	0.85
1:F:460:ILE:HD12	1:F:461:HIS:ND1	1.92	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:ALA:HB1	1:D:233:GLY:HA2	1.61	0.82
1:A:184:MET:CE	1:A:402:VAL:HA	2.13	0.77
1:G:279:SER:HB3	1:H:279:SER:HB3	1.67	0.77
1:B:460:ILE:HD12	1:B:461:HIS:ND1	1.99	0.77
1:A:184:MET:HE3	1:A:402:VAL:HA	1.68	0.76
1:E:184:MET:HE3	1:E:402:VAL:HA	1.68	0.75
1:H:229:ALA:HB1	1:H:233:GLY:HA2	1.69	0.75
1:B:380:PHE:O	1:B:384:THR:HG23	1.89	0.73
1:A:457:TYR:HA	1:A:460:ILE:HD11	1.72	0.72
1:D:460:ILE:HD12	1:D:461:HIS:ND1	2.05	0.72
1:C:279:SER:HB3	1:D:279:SER:HB3	1.70	0.71
1:H:202:GLU:O	1:H:206:ARG:HG3	1.91	0.71
1:H:184:MET:HE3	1:H:402:VAL:HA	1.73	0.70
1:H:7:ILE:HD11	1:H:14:GLU:HB3	1.73	0.70
1:H:460:ILE:HD12	1:H:461:HIS:CE1	2.26	0.70
1:D:285:MET:HE1	1:D:380:PHE:CZ	2.27	0.70
1:A:73:TYR:CD1	1:A:119:MET:HE2	2.27	0.69
1:E:457:TYR:HA	1:E:460:ILE:CD1	2.20	0.69
1:F:5:VAL:N	1:F:19:LYS:HE2	2.07	0.69
1:C:380:PHE:O	1:C:384:THR:HG23	1.91	0.69
1:F:285:MET:HA	1:F:285:MET:HE2	1.73	0.69
1:D:298:MET:HB3	1:D:309:ILE:HG12	1.74	0.69
1:C:145:PHE:HB3	1:C:146:PRO:HD3	1.76	0.68
1:D:10:ASP:OD1	1:D:29:ARG:HD3	1.93	0.68
1:C:26:GLN:OE1	1:C:105:MET:HE2	1.94	0.68
1:E:236:LEU:O	1:E:237:ASN:HB2	1.94	0.68
1:B:229:ALA:HB1	1:B:233:GLY:HA2	1.76	0.67
1:E:15:LYS:HG2	1:E:28:ILE:HG21	1.75	0.67
1:A:279:SER:HB3	1:B:279:SER:HB3	1.76	0.67
1:G:229:ALA:HB1	1:G:233:GLY:HA2	1.76	0.67
1:B:179:ALA:O	1:B:196:LEU:HD13	1.95	0.67
1:H:460:ILE:HD12	1:H:461:HIS:ND1	2.09	0.67
1:H:460:ILE:CD1	1:H:461:HIS:CE1	2.78	0.67
1:D:202:GLU:O	1:D:206:ARG:HG3	1.94	0.67
1:E:73:TYR:CD1	1:E:119:MET:HE2	2.30	0.66
1:H:119:MET:HE3	1:H:129:ILE:HD11	1.78	0.65
1:F:179:ALA:O	1:F:196:LEU:HD13	1.96	0.65
1:B:36:ILE:HD12	1:C:379:VAL:HG13	1.77	0.65
1:F:460:ILE:HD12	1:F:461:HIS:HD1	1.60	0.65
1:E:229:ALA:HB1	1:E:233:GLY:HA2	1.80	0.64
1:B:184:MET:HE3	1:B:402:VAL:HA	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ARG:NH1	1:G:8:GLU:OE2	2.31	0.63
1:A:195:ILE:HD12	1:B:232:VAL:CG1	2.28	0.63
1:E:379:VAL:HG13	1:H:36:ILE:HD12	1.79	0.63
1:B:6:ARG:HG2	1:B:7:ILE:H	1.64	0.62
1:F:229:ALA:HB1	1:F:233:GLY:HA2	1.81	0.62
1:A:296:ARG:NH2	1:D:355:GLN:NE2	2.47	0.62
1:B:6:ARG:HG2	1:B:7:ILE:N	2.14	0.62
1:D:285:MET:HE1	1:D:380:PHE:CE1	2.34	0.62
1:A:167:MET:HE2	1:A:383:PHE:CD1	2.33	0.62
1:C:460:ILE:HD12	1:C:461:HIS:ND1	2.15	0.62
1:B:184:MET:HE1	1:B:194:PRO:HG3	1.83	0.61
1:H:259:ARG:HD3	4:H:508:HOH:O	1.98	0.61
1:H:167:MET:HE2	1:H:383:PHE:CD1	2.35	0.61
1:A:119:MET:HE3	1:A:129:ILE:HD11	1.83	0.61
1:E:355:GLN:OE1	1:H:296:ARG:NH2	2.34	0.61
1:A:303:ARG:HD2	1:C:404:LYS:O	2.01	0.60
1:H:10:ASP:OD1	1:H:29:ARG:HD3	2.00	0.60
1:E:457:TYR:HA	1:E:460:ILE:HD11	1.82	0.60
1:H:184:MET:HE1	1:H:194:PRO:HG3	1.83	0.60
1:H:167:MET:HE1	1:H:333:MET:HE1	1.84	0.59
1:B:446:THR:O	1:B:450:LEU:HD12	2.03	0.59
1:A:113:ASN:HA	1:A:116:LEU:HD12	1.85	0.59
1:A:63:VAL:O	1:A:63:VAL:HG12	2.03	0.58
1:G:263:HIS:CE1	1:G:265:VAL:HB	2.39	0.58
1:G:196:LEU:CD1	1:G:460:ILE:HD13	2.34	0.58
1:D:184:MET:HE3	1:D:402:VAL:HA	1.85	0.57
1:F:184:MET:HE1	1:F:194:PRO:HG3	1.85	0.57
1:B:379:VAL:HG13	1:C:36:ILE:HD12	1.85	0.57
1:E:202:GLU:O	1:E:206:ARG:HG3	2.04	0.57
1:C:28:ILE:O	1:C:31:THR:HB	2.05	0.57
1:D:19:LYS:O	1:D:123:LYS:NZ	2.38	0.57
1:A:167:MET:HE1	1:A:333:MET:HE1	1.87	0.56
1:G:196:LEU:CD1	1:G:460:ILE:CD1	2.83	0.56
1:H:420:THR:HG21	1:H:444:VAL:HG21	1.87	0.56
1:A:233:GLY:HA3	1:A:265:VAL:HA	1.87	0.56
1:F:460:ILE:CD1	1:F:461:HIS:ND1	2.67	0.56
1:A:355:GLN:OE1	1:D:296:ARG:NH2	2.38	0.56
1:A:404:LYS:O	1:C:303:ARG:HD3	2.05	0.56
1:B:456:PRO:O	1:B:460:ILE:HG13	2.06	0.56
1:F:460:ILE:CD1	1:F:461:HIS:CE1	2.88	0.56
1:G:416:VAL:HG12	1:G:420:THR:HB	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ILE:CD1	1:B:461:HIS:ND1	2.68	0.56
1:G:226:ASN:HA	1:G:264:LEU:HD22	1.87	0.56
1:C:184:MET:HE1	1:C:194:PRO:HG3	1.88	0.56
1:G:196:LEU:HG	1:G:460:ILE:HD13	1.87	0.56
1:A:296:ARG:NH2	1:D:355:GLN:HE22	2.04	0.55
1:E:455:ASN:C	1:E:457:TYR:H	2.13	0.55
1:A:409:ILE:HD13	1:A:425:ALA:HB2	1.89	0.55
1:G:456:PRO:O	1:G:460:ILE:HG12	2.07	0.55
1:E:130:SER:HB3	1:E:133:SER:HB2	1.89	0.55
1:F:456:PRO:O	1:F:460:ILE:HG13	2.07	0.55
1:C:136:ASN:O	1:C:139:GLN:HG2	2.07	0.54
1:E:263:HIS:CE1	1:E:265:VAL:HB	2.42	0.54
1:F:43:PRO:HA	1:F:46:ILE:HD12	1.89	0.54
1:C:229:ALA:HB1	1:C:233:GLY:HA2	1.89	0.54
1:F:130:SER:HB3	1:F:133:SER:HB2	1.90	0.54
1:E:184:MET:CE	1:E:402:VAL:HG22	2.37	0.54
1:E:167:MET:HE2	1:E:383:PHE:HD1	1.71	0.54
1:E:70:VAL:HG22	1:E:119:MET:HE1	1.88	0.54
1:E:10:ASP:OD1	1:E:29:ARG:HD3	2.08	0.54
1:E:184:MET:CE	1:E:402:VAL:HA	2.37	0.54
1:F:296:ARG:NH2	1:G:355:GLN:OE1	2.41	0.53
1:A:236:LEU:O	1:A:237:ASN:HB2	2.06	0.53
1:B:384:THR:HA	1:B:388:LEU:HB3	1.90	0.53
1:G:234:THR:OG1	1:H:460:ILE:HA	2.08	0.53
1:C:352:GLU:HG3	4:C:498:HOH:O	2.09	0.53
1:A:335:GLN:HB3	1:D:364:VAL:HB	1.90	0.53
1:B:283:VAL:HA	1:B:286:ILE:HD12	1.91	0.53
1:B:324:LYS:HG3	1:D:190:GLN:HG2	1.91	0.53
1:F:167:MET:HE2	1:F:383:PHE:CD1	2.43	0.53
1:E:196:LEU:HG	1:E:460:ILE:HG13	1.90	0.53
1:B:375:ILE:O	1:B:379:VAL:HG22	2.09	0.52
1:C:413:ASN:C	1:C:413:ASN:OD1	2.52	0.52
1:E:184:MET:HE2	1:E:184:MET:HA	1.90	0.52
1:F:184:MET:HA	1:F:184:MET:HE2	1.91	0.52
1:C:70:VAL:CG2	1:C:129:ILE:HG12	2.39	0.52
1:E:167:MET:CE	1:E:380:PHE:HA	2.39	0.52
1:G:70:VAL:HG13	1:G:129:ILE:HG12	1.91	0.52
1:G:447:GLU:HB2	4:G:494:HOH:O	2.08	0.52
1:H:174:LYS:HE3	1:H:388:LEU:O	2.09	0.52
1:B:197:LEU:HD22	1:B:398:MET:HE1	1.92	0.52
1:E:26:GLN:NE2	1:E:105:MET:HG3	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:MET:HG3	1:H:384:THR:OG1	2.10	0.52
1:C:413:ASN:HB3	1:C:414:PRO:HD3	1.92	0.51
1:E:286:ILE:HD11	1:F:348:THR:HG23	1.91	0.51
1:E:53:LYS:HE2	1:E:108:ASN:OD1	2.10	0.51
1:H:409:ILE:HD13	1:H:435:ILE:HD12	1.92	0.51
1:C:375:ILE:O	1:C:379:VAL:HG22	2.10	0.51
1:E:311:LEU:HD23	1:E:391:ILE:HG12	1.92	0.51
1:A:28:ILE:O	1:A:31:THR:HB	2.10	0.51
1:D:7:ILE:HD11	1:D:14:GLU:HB3	1.92	0.51
1:D:409:ILE:HB	1:D:435:ILE:HD13	1.93	0.51
1:G:225:ILE:HD12	1:G:227:MET:HB2	1.93	0.51
1:A:460:ILE:HD12	1:A:461:HIS:ND1	2.26	0.51
1:F:53:LYS:HE3	1:F:108:ASN:OD1	2.11	0.51
1:F:59:ALA:O	1:F:63:VAL:HG23	2.10	0.51
1:C:184:MET:HE3	1:C:402:VAL:HA	1.91	0.51
1:A:184:MET:HE2	1:A:402:VAL:HG22	1.94	0.50
1:A:379:VAL:HG13	1:D:36:ILE:HD12	1.93	0.50
1:A:409:ILE:HD12	1:A:435:ILE:HD13	1.94	0.50
1:H:298:MET:HB3	1:H:309:ILE:HG12	1.94	0.50
1:D:285:MET:HE1	1:D:380:PHE:HZ	1.75	0.50
1:A:182:ILE:HD13	1:A:456:PRO:HA	1.92	0.50
1:C:204:TYR:CD1	1:C:291:ILE:HG12	2.47	0.50
1:E:167:MET:HE1	1:E:380:PHE:HA	1.93	0.50
1:B:457:TYR:HA	1:B:460:ILE:HD11	1.93	0.50
1:H:228:GLY:HA3	1:H:243:ILE:HG12	1.93	0.50
1:A:195:ILE:HD12	1:B:232:VAL:HG13	1.94	0.50
1:C:167:MET:HE1	1:C:333:MET:HE1	1.94	0.50
1:G:37:THR:HG21	1:G:95:ILE:HD12	1.93	0.50
1:D:73:TYR:CD1	1:D:119:MET:HE2	2.47	0.49
1:H:73:TYR:CD1	1:H:119:MET:HE2	2.47	0.49
1:D:456:PRO:O	1:D:460:ILE:HG13	2.12	0.49
1:E:408:ILE:HG13	1:E:459:MET:HE1	1.94	0.49
1:A:319:SER:HB2	1:C:418:TYR:OH	2.13	0.49
1:E:375:ILE:O	1:E:379:VAL:HG22	2.11	0.49
1:G:196:LEU:CG	1:G:460:ILE:HD13	2.43	0.49
1:A:224:ASP:CG	1:A:259:ARG:HH21	2.20	0.49
1:A:408:ILE:HD11	1:A:454:LEU:HD13	1.94	0.49
1:A:424:LEU:HD13	1:A:438:LEU:HB3	1.95	0.49
1:G:179:ALA:O	1:G:196:LEU:HD13	2.12	0.49
1:B:336:VAL:HG21	1:B:379:VAL:HG11	1.94	0.49
1:G:145:PHE:HB3	1:G:146:PRO:HD3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:324:LYS:NZ	1:G:326:ASN:HD21	2.11	0.49
1:A:196:LEU:HD21	1:A:456:PRO:O	2.13	0.49
1:A:263:HIS:CE1	1:A:265:VAL:HB	2.48	0.48
1:F:25:VAL:O	1:F:28:ILE:HG22	2.13	0.48
1:F:420:THR:HG21	1:F:444:VAL:HG21	1.95	0.48
1:F:396:GLU:H	1:F:396:GLU:CD	2.21	0.48
1:F:460:ILE:HD12	1:F:461:HIS:CE1	2.47	0.48
1:F:6:ARG:HG2	1:F:7:ILE:N	2.29	0.48
1:D:285:MET:CE	1:D:376:MET:HE3	2.35	0.48
1:G:336:VAL:HG13	1:G:375:ILE:HD12	1.96	0.48
1:C:263:HIS:CE1	1:C:265:VAL:HB	2.48	0.48
1:D:283:VAL:HA	1:D:286:ILE:HD12	1.96	0.48
1:E:412:ILE:HD11	1:E:454:LEU:HD21	1.94	0.48
1:G:126:TYR:HA	1:G:129:ILE:O	2.14	0.48
1:H:413:ASN:HB3	1:H:414:PRO:HD3	1.96	0.48
1:B:130:SER:HB3	1:B:133:SER:HB2	1.95	0.48
1:B:184:MET:HE3	1:B:402:VAL:HG22	1.96	0.48
1:E:319:SER:HB3	1:G:418:TYR:OH	2.14	0.48
1:E:415:HIS:HB3	1:E:445:LEU:HD21	1.96	0.48
1:F:204:TYR:CD1	1:F:291:ILE:HG12	2.49	0.48
1:G:329:MET:HB2	1:G:330:PRO:HD3	1.96	0.48
1:D:153:VAL:O	1:D:157:LEU:HB2	2.14	0.47
1:A:298:MET:HB3	1:A:309:ILE:HG12	1.95	0.47
1:E:279:SER:HB3	1:F:279:SER:HB3	1.96	0.47
1:G:196:LEU:HD11	1:G:460:ILE:HD11	1.95	0.47
1:A:153:VAL:HG12	1:A:157:LEU:HD22	1.97	0.47
1:C:70:VAL:HG23	1:C:129:ILE:HG12	1.96	0.47
1:G:61:MET:SD	1:G:71:GLY:HA3	2.54	0.47
1:A:455:ASN:HB3	1:A:458:GLU:HB2	1.97	0.47
1:B:153:VAL:O	1:B:157:LEU:HB2	2.15	0.47
1:D:10:ASP:C	1:D:12:LEU:H	2.22	0.47
1:D:455:ASN:HB3	1:D:458:GLU:HB2	1.96	0.47
1:G:145:PHE:HB3	1:G:146:PRO:CD	2.45	0.47
1:D:204:TYR:CD1	1:D:291:ILE:HG12	2.50	0.46
1:E:119:MET:HE3	1:E:129:ILE:HD11	1.97	0.46
1:G:375:ILE:O	1:G:379:VAL:HG22	2.15	0.46
1:H:214:ARG:O	1:H:218:THR:HG23	2.16	0.46
1:E:167:MET:HE2	1:E:383:PHE:CD1	2.50	0.46
1:C:167:MET:HB2	1:C:384:THR:HG21	1.98	0.46
1:E:296:ARG:NH2	1:H:355:GLN:OE1	2.49	0.46
1:F:184:MET:HE3	1:F:402:VAL:HG13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:SER:HB3	1:H:133:SER:HB2	1.98	0.46
1:E:26:GLN:HE22	1:E:105:MET:HG3	1.80	0.46
1:F:283:VAL:HA	1:F:286:ILE:HD12	1.98	0.46
1:B:336:VAL:HG21	1:B:379:VAL:CG1	2.46	0.46
1:A:277:VAL:O	1:A:281:LEU:HG	2.15	0.46
1:B:184:MET:HE2	1:B:184:MET:HA	1.97	0.46
1:H:5:VAL:N	1:H:19:LYS:HG3	2.31	0.46
1:A:329:MET:O	1:A:332:VAL:HG12	2.16	0.46
1:H:290:LYS:HD3	1:H:290:LYS:C	2.40	0.46
1:H:26:GLN:HB2	1:H:109:GLU:OE2	2.16	0.45
1:C:232:VAL:HG13	1:D:195:ILE:HD12	1.98	0.45
1:D:460:ILE:CD1	1:D:461:HIS:CE1	2.99	0.45
1:G:293:ASN:HA	1:G:296:ARG:HH11	1.81	0.45
1:H:232:VAL:HG13	1:H:357:GLU:HG2	1.98	0.45
1:D:28:ILE:O	1:D:31:THR:HB	2.16	0.45
1:G:15:LYS:HG2	1:G:28:ILE:HG21	1.98	0.45
1:B:263:HIS:CE1	1:B:265:VAL:HB	2.52	0.45
1:B:204:TYR:CD1	1:B:291:ILE:HG12	2.51	0.45
1:E:263:HIS:HE1	1:E:265:VAL:HB	1.81	0.45
1:F:263:HIS:CE1	1:F:265:VAL:HB	2.52	0.45
1:G:73:TYR:CD1	1:G:119:MET:HE2	2.52	0.45
1:H:329:MET:HB2	1:H:330:PRO:HD3	1.97	0.45
1:F:228:GLY:HA3	1:F:243:ILE:HG12	1.99	0.45
1:H:460:ILE:CD1	1:H:461:HIS:ND1	2.79	0.45
1:A:296:ARG:HH22	1:D:355:GLN:NE2	2.13	0.45
1:F:191:ASP:O	1:H:324:LYS:HE2	2.17	0.45
1:G:457:TYR:O	1:G:460:ILE:HG13	2.17	0.45
1:E:364:VAL:HB	1:H:335:GLN:HB3	1.98	0.45
1:D:145:PHE:HB3	1:D:146:PRO:HD3	2.00	0.44
1:F:26:GLN:NE2	1:F:105:MET:HG3	2.32	0.44
1:D:10:ASP:C	1:D:12:LEU:N	2.74	0.44
1:B:335:GLN:HB3	1:C:364:VAL:HB	1.99	0.44
1:D:460:ILE:CD1	1:D:461:HIS:ND1	2.79	0.44
1:F:324:LYS:HG3	1:H:190:GLN:HG2	1.99	0.44
1:A:130:SER:HB3	1:A:133:SER:HB2	2.00	0.44
1:D:329:MET:O	1:D:332:VAL:HG12	2.18	0.44
1:E:347:ILE:HG23	1:E:365:LEU:HD21	1.99	0.44
1:G:196:LEU:HD12	1:G:460:ILE:HD13	1.98	0.44
1:H:204:TYR:CD1	1:H:291:ILE:HG12	2.53	0.44
1:B:298:MET:HB3	1:B:309:ILE:HG12	2.00	0.43
1:B:456:PRO:O	1:B:460:ILE:CG1	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:MET:HB2	1:C:330:PRO:HD3	1.99	0.43
1:E:460:ILE:HA	1:F:234:THR:HB	2.00	0.43
1:G:232:VAL:HG13	1:H:195:ILE:HD12	2.00	0.43
1:G:106:ASN:C	1:G:106:ASN:HD22	2.26	0.43
1:G:200:GLU:OE2	1:H:357:GLU:OE1	2.35	0.43
1:D:446:THR:HG23	1:D:449:GLN:H	1.82	0.43
1:F:456:PRO:O	1:F:460:ILE:CG1	2.66	0.43
1:D:413:ASN:HB3	1:D:414:PRO:HD3	2.00	0.43
1:F:54:LYS:HG3	1:F:75:VAL:HG13	2.01	0.43
1:G:334:ASN:O	1:G:337:ALA:HB3	2.18	0.43
1:H:224:ASP:CG	1:H:259:ARG:HH21	2.26	0.43
1:F:167:MET:HE1	1:F:333:MET:HE1	2.00	0.43
1:F:188:HIS:HB3	1:H:327:PRO:HD2	2.00	0.43
1:C:184:MET:HE2	1:C:184:MET:HA	2.00	0.43
1:H:184:MET:CE	1:H:402:VAL:HG22	2.48	0.43
1:A:436:ARG:NH2	1:A:450:LEU:HB3	2.34	0.43
1:B:252:LYS:HA	1:B:252:LYS:HD2	1.90	0.43
1:A:167:MET:HE2	1:A:383:PHE:HD1	1.82	0.43
1:F:52:VAL:HA	1:F:250:LEU:HD21	2.01	0.43
1:F:285:MET:HE1	1:F:380:PHE:CZ	2.54	0.43
1:H:263:HIS:CE1	1:H:265:VAL:HB	2.54	0.43
1:H:353:ALA:CB	1:H:361:MET:HG3	2.49	0.43
1:A:408:ILE:HG22	1:A:435:ILE:HD12	2.01	0.42
1:A:439:CYS:HB2	1:A:450:LEU:HD21	2.00	0.42
1:B:301:GLY:HA3	1:B:302:PRO:HA	1.90	0.42
1:D:460:ILE:HD12	1:D:461:HIS:HD1	1.83	0.42
1:D:149:THR:HG21	1:D:366:PHE:CD2	2.54	0.42
1:D:460:ILE:HD12	1:D:461:HIS:CE1	2.53	0.42
1:D:143:ASP:C	1:D:146:PRO:HD2	2.44	0.42
1:A:167:MET:CE	1:A:383:PHE:CD1	3.00	0.42
1:D:371:GLN:O	1:D:375:ILE:HG12	2.18	0.42
1:H:179:ALA:O	1:H:196:LEU:HD13	2.20	0.42
1:H:196:LEU:CD1	1:H:460:ILE:HD13	2.49	0.42
1:D:327:PRO:HB2	1:D:330:PRO:HG2	2.00	0.42
1:F:327:PRO:O	1:F:330:PRO:HD2	2.20	0.42
1:F:423:LYS:HA	1:F:426:ARG:HH11	1.84	0.42
1:A:167:MET:HG3	1:A:384:THR:OG1	2.20	0.42
1:B:184:MET:CE	1:B:402:VAL:HG22	2.49	0.42
1:G:196:LEU:HD12	1:G:460:ILE:CD1	2.50	0.42
1:G:220:ASN:ND2	4:G:491:HOH:O	2.36	0.42
1:D:456:PRO:O	1:D:460:ILE:CG1	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LYS:HA	1:E:15:LYS:HD3	1.82	0.42
1:F:167:MET:HE2	1:F:383:PHE:HD1	1.81	0.42
1:F:232:VAL:O	1:F:232:VAL:CG1	2.67	0.42
1:G:133:SER:O	1:G:137:MET:HB2	2.19	0.42
1:E:53:LYS:CE	1:E:108:ASN:OD1	2.68	0.42
1:E:410:THR:O	1:F:237:ASN:ND2	2.53	0.42
1:G:218:THR:HG22	1:G:276:GLU:HG2	2.01	0.42
1:A:364:VAL:HB	1:D:335:GLN:HB3	2.02	0.41
1:A:423:LYS:HE3	1:A:442:TYR:OH	2.20	0.41
1:D:196:LEU:CD1	1:D:460:ILE:HD13	2.50	0.41
1:H:182:ILE:HG13	1:H:402:VAL:HG21	2.02	0.41
1:A:202:GLU:O	1:A:206:ARG:HG3	2.21	0.41
1:B:167:MET:HG3	1:B:384:THR:HG22	2.03	0.41
1:C:406:ILE:O	1:C:409:ILE:HG22	2.21	0.41
1:E:6:ARG:NH1	1:E:8:GLU:OE2	2.53	0.41
1:F:70:VAL:HG13	1:F:129:ILE:HG12	2.02	0.41
1:H:224:ASP:OD2	1:H:259:ARG:NH2	2.49	0.41
1:A:8:GLU:HB2	1:A:17:ILE:CD1	2.50	0.41
1:A:412:ILE:HD11	1:A:454:LEU:HD21	2.02	0.41
1:C:52:VAL:HA	1:C:250:LEU:HD21	2.02	0.41
1:C:409:ILE:HB	1:C:435:ILE:CD1	2.49	0.41
1:D:457:TYR:HA	1:D:460:ILE:HD11	2.02	0.41
1:E:286:ILE:HG23	1:F:352:GLU:HB3	2.02	0.41
1:D:214:ARG:O	1:D:218:THR:HG23	2.20	0.41
1:D:408:ILE:HG12	1:D:454:LEU:HD22	2.02	0.41
1:F:297:LEU:CD2	1:H:297:LEU:HD21	2.50	0.41
1:A:459:MET:O	1:B:236:LEU:HD13	2.21	0.41
1:B:223:TYR:CE2	1:B:257:PRO:HD2	2.56	0.41
1:F:100:GLY:HA3	1:F:145:PHE:CE2	2.56	0.41
1:F:285:MET:HA	1:F:285:MET:CE	2.47	0.41
1:F:295:LEU:HA	1:F:298:MET:HE3	2.03	0.41
1:B:228:GLY:HA3	1:B:243:ILE:HG12	2.02	0.41
1:C:308:GLU:O	1:C:398:MET:HE2	2.21	0.41
1:D:6:ARG:HG2	1:D:7:ILE:N	2.35	0.41
1:E:79:ASP:HA	1:E:82:ILE:HD12	2.02	0.41
1:E:194:PRO:HG2	1:E:459:MET:HE2	2.02	0.41
1:F:285:MET:HE1	1:F:380:PHE:CE1	2.56	0.41
1:B:53:LYS:HE3	1:B:108:ASN:OD1	2.21	0.41
1:G:263:HIS:HE1	1:G:265:VAL:HB	1.85	0.41
1:G:371:GLN:O	1:G:375:ILE:HG12	2.21	0.41
1:A:52:VAL:HG13	1:A:227:MET:HE1	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE1	1:A:402:VAL:HA	1.98	0.41
1:D:330:PRO:O	1:D:333:MET:HB3	2.20	0.41
1:F:63:VAL:O	1:F:63:VAL:HG12	2.20	0.41
1:G:149:THR:HG21	1:G:366:PHE:CG	2.56	0.41
1:G:184:MET:HE2	1:G:184:MET:HA	2.03	0.41
1:G:397:ARG:NH2	1:G:401:TYR:OH	2.52	0.41
1:H:184:MET:HE3	1:H:402:VAL:HG22	2.03	0.41
1:C:122:GLU:O	1:C:125:ASN:HB2	2.20	0.41
1:C:282:LYS:O	1:C:286:ILE:HG13	2.21	0.41
1:E:455:ASN:C	1:E:457:TYR:N	2.79	0.41
1:H:70:VAL:HG22	1:H:119:MET:HE1	2.02	0.41
1:D:232:VAL:O	1:D:232:VAL:CG1	2.68	0.40
1:E:301:GLY:HA3	1:E:302:PRO:HA	1.82	0.40
1:F:318:SER:HB2	1:F:320:ILE:HG22	2.02	0.40
1:B:5:VAL:N	1:B:19:LYS:HG3	2.35	0.40
1:C:225:ILE:HD12	1:C:227:MET:HB2	2.04	0.40
1:D:167:MET:HE1	1:D:333:MET:HE1	2.03	0.40
1:E:266:ASP:OD1	1:E:270:ASN:ND2	2.40	0.40
1:B:41:ILE:HD11	1:B:46:ILE:HG13	2.03	0.40
1:B:264:LEU:O	1:B:268:THR:OG1	2.39	0.40
1:D:15:LYS:HB2	1:D:25:VAL:HG12	2.03	0.40
1:G:196:LEU:CD1	1:G:460:ILE:HD11	2.52	0.40
1:H:220:ASN:HA	1:H:223:TYR:CD1	2.57	0.40
1:A:27:THR:O	1:A:30:ALA:HB3	2.20	0.40
1:B:188:HIS:HB3	1:D:327:PRO:HD2	2.03	0.40
1:E:10:ASP:HB2	1:E:25:VAL:HG21	2.03	0.40
1:F:197:LEU:HD22	1:F:398:MET:HE1	2.04	0.40
1:G:223:TYR:CE2	1:G:257:PRO:HD2	2.57	0.40
1:A:70:VAL:HA	1:A:119:MET:HE1	2.03	0.40
1:A:228:GLY:HA3	1:A:243:ILE:HG12	2.03	0.40
1:A:385:GLU:CD	1:A:389:LYS:HZ2	2.30	0.40
1:F:184:MET:HE3	1:F:402:VAL:HA	2.04	0.40
1:F:298:MET:HB3	1:F:309:ILE:HG12	2.04	0.40
1:G:232:VAL:HG22	1:G:357:GLU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/468 (97%)	440 (96%)	13 (3%)	3 (1%)	18	38
1	B	460/468 (98%)	444 (96%)	16 (4%)	0	100	100
1	C	460/468 (98%)	449 (98%)	11 (2%)	0	100	100
1	D	457/468 (98%)	442 (97%)	14 (3%)	1 (0%)	43	66
1	E	458/468 (98%)	439 (96%)	16 (4%)	3 (1%)	18	38
1	F	459/468 (98%)	440 (96%)	19 (4%)	0	100	100
1	G	461/468 (98%)	450 (98%)	11 (2%)	0	100	100
1	H	457/468 (98%)	442 (97%)	15 (3%)	0	100	100
All	All	3668/3744 (98%)	3546 (97%)	115 (3%)	7 (0%)	43	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	419	GLU
1	E	419	GLU
1	A	414	PRO
1	E	456	PRO
1	A	447	GLU
1	E	414	PRO
1	D	413	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	387/394 (98%)	364 (94%)	23 (6%)	18	38
1	B	388/394 (98%)	368 (95%)	20 (5%)	21	44
1	C	388/394 (98%)	364 (94%)	24 (6%)	16	36
1	D	387/394 (98%)	367 (95%)	20 (5%)	21	44
1	E	388/394 (98%)	368 (95%)	20 (5%)	21	44
1	F	388/394 (98%)	370 (95%)	18 (5%)	24	49
1	G	388/394 (98%)	365 (94%)	23 (6%)	18	38
1	H	387/394 (98%)	369 (95%)	18 (5%)	23	48
All	All	3101/3152 (98%)	2935 (95%)	166 (5%)	20	42

All (166) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	15	LYS
1	A	26	GLN
1	A	29	ARG
1	A	31	THR
1	A	76	LYS
1	A	157	LEU
1	A	241	GLU
1	A	264	LEU
1	A	282	LYS
1	A	295	LEU
1	A	297	LEU
1	A	303	ARG
1	A	307	SER
1	A	320	ILE
1	A	352	GLU
1	A	369	LEU
1	A	379	VAL
1	A	410	THR
1	A	412	ILE
1	A	419	GLU
1	A	424	LEU
1	A	446	THR
1	B	5	VAL
1	B	12	LEU
1	B	14	GLU
1	B	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	72	GLN
1	B	155	SER
1	B	157	LEU
1	B	162	GLU
1	B	172	MET
1	B	213	GLU
1	B	232	VAL
1	B	241	GLU
1	B	244	SER
1	B	248	GLU
1	B	374	SER
1	B	379	VAL
1	B	384	THR
1	B	416	VAL
1	B	444	VAL
1	B	450	LEU
1	C	7	ILE
1	C	29	ARG
1	C	31	THR
1	C	63	VAL
1	C	65	LEU
1	C	69	GLU
1	C	70	VAL
1	C	83	GLU
1	C	127	SER
1	C	128	LYS
1	C	132	ASN
1	C	133	SER
1	C	172	MET
1	C	232	VAL
1	C	248	GLU
1	C	324	LYS
1	C	352	GLU
1	C	379	VAL
1	C	384	THR
1	C	403	GLU
1	C	419	GLU
1	C	420	THR
1	C	436	ARG
1	C	444	VAL
1	D	19	LYS
1	D	25	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	29	ARG
1	D	31	THR
1	D	63	VAL
1	D	85	LYS
1	D	123	LYS
1	D	132	ASN
1	D	157	LEU
1	D	222	LEU
1	D	232	VAL
1	D	241	GLU
1	D	262	GLN
1	D	264	LEU
1	D	295	LEU
1	D	320	ILE
1	D	345	LEU
1	D	369	LEU
1	D	448	GLU
1	D	450	LEU
1	E	6	ARG
1	E	9	LYS
1	E	15	LYS
1	E	29	ARG
1	E	83	GLU
1	E	85	LYS
1	E	128	LYS
1	E	159	GLN
1	E	195	ILE
1	E	241	GLU
1	E	282	LYS
1	E	307	SER
1	E	345	LEU
1	E	352	GLU
1	E	379	VAL
1	E	419	GLU
1	E	424	LEU
1	E	436	ARG
1	E	444	VAL
1	E	460	ILE
1	F	5	VAL
1	F	12	LEU
1	F	25	VAL
1	F	53	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	163	THR
1	F	172	MET
1	F	232	VAL
1	F	241	GLU
1	F	252	LYS
1	F	282	LYS
1	F	320	ILE
1	F	352	GLU
1	F	369	LEU
1	F	379	VAL
1	F	396	GLU
1	F	399	LYS
1	F	401	TYR
1	F	450	LEU
1	G	5	VAL
1	G	15	LYS
1	G	25	VAL
1	G	29	ARG
1	G	63	VAL
1	G	69	GLU
1	G	132	ASN
1	G	133	SER
1	G	172	MET
1	G	232	VAL
1	G	234	THR
1	G	241	GLU
1	G	248	GLU
1	G	282	LYS
1	G	345	LEU
1	G	379	VAL
1	G	396	GLU
1	G	399	LYS
1	G	419	GLU
1	G	420	THR
1	G	444	VAL
1	G	446	THR
1	G	460	ILE
1	H	5	VAL
1	H	9	LYS
1	H	29	ARG
1	H	70	VAL
1	H	127	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	132	ASN
1	H	162	GLU
1	H	172	MET
1	H	232	VAL
1	H	241	GLU
1	H	307	SER
1	H	345	LEU
1	H	352	GLU
1	H	403	GLU
1	H	426	ARG
1	H	444	VAL
1	H	446	THR
1	H	447	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	96	GLN
1	A	169	GLN
1	A	190	GLN
1	A	334	ASN
1	A	368	ASN
1	A	413	ASN
1	B	132	ASN
1	B	256	HIS
1	B	449	GLN
1	B	451	ASN
1	C	96	GLN
1	C	104	ASN
1	C	132	ASN
1	C	142	ASN
1	C	190	GLN
1	C	220	ASN
1	C	334	ASN
1	D	26	GLN
1	D	220	ASN
1	D	249	HIS
1	D	339	GLN
1	D	355	GLN
1	D	386	ASN
1	E	26	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	96	GLN
1	E	249	HIS
1	E	451	ASN
1	F	26	GLN
1	F	72	GLN
1	F	169	GLN
1	F	220	ASN
1	F	249	HIS
1	F	315	GLN
1	F	334	ASN
1	F	368	ASN
1	G	142	ASN
1	G	269	GLN
1	G	326	ASN
1	G	343	ASN
1	G	371	GLN
1	G	413	ASN
1	G	461	HIS
1	H	132	ASN
1	H	142	ASN
1	H	262	GLN
1	H	269	GLN
1	H	334	ASN
1	H	386	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ASP	B	469	-	7,8,8	1.07	1 (14%)	6,10,10	1.28	1 (16%)
3	ASP	F	469	-	7,8,8	1.10	1 (14%)	6,10,10	1.19	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	B	469	-	-	4/8/8/8	-
3	ASP	F	469	-	-	3/8/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	469	ASP	OXT-C	-2.09	1.24	1.30
3	B	469	ASP	OXT-C	-2.07	1.24	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	469	ASP	OXT-C-O	-2.02	119.50	124.08

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	469	ASP	C-CA-CB-CG
3	F	469	ASP	N-CA-CB-CG
3	B	469	ASP	OXT-C-CA-N
3	F	469	ASP	OXT-C-CA-N
3	B	469	ASP	O-C-CA-N
3	B	469	ASP	CA-CB-CG-OD2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	469	ASP	CA-CB-CG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	458/468 (97%)	-1.74	0 100 100	16, 27, 120, 131	0
1	B	462/468 (98%)	-1.86	0 100 100	16, 31, 53, 63	0
1	C	462/468 (98%)	-1.84	0 100 100	18, 33, 60, 78	0
1	D	459/468 (98%)	-1.88	0 100 100	16, 27, 50, 58	0
1	E	459/468 (98%)	-1.73	0 100 100	13, 27, 120, 131	1 (0%)
1	F	461/468 (98%)	-1.85	0 100 100	18, 31, 52, 65	0
1	G	463/468 (98%)	-1.83	0 100 100	18, 34, 60, 81	0
1	H	459/468 (98%)	-1.87	0 100 100	16, 27, 51, 59	0
All	All	3683/3744 (98%)	-1.82	0 100 100	13, 29, 61, 131	1 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

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($\text{\AA}^2$)	Q<0.9
2	CA	D	469	1/1	0.99	0.01	43,43,43,43	0
3	ASP	F	469	9/9	0.99	0.05	42,42,43,43	0
2	CA	E	469	1/1	1.00	0.01	67,67,67,67	0
2	CA	H	469	1/1	1.00	0.02	49,49,49,49	0
3	ASP	B	469	9/9	1.00	0.04	42,43,44,44	0
2	CA	A	469	1/1	1.00	0.02	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.