Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 07:26 am GMT

PDB ID	:	5O82
Title	:	Crystal Structure of R67A/E173A Mutant of alpha-L-arabinofuranosidase Ara51 from Clostridium thermocellum in complex with arabinofuranose
Authors	:	Lafite, P.; Daniellou, R.
Deposited on	:	2017-06-12
Resolution	:	2.39 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

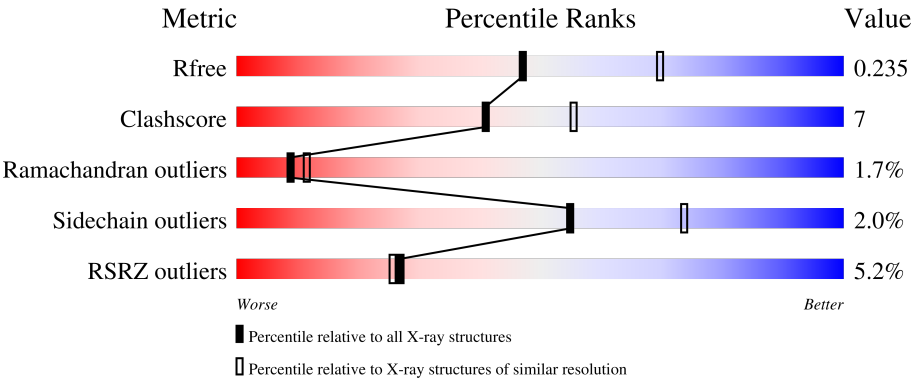
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.39 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.



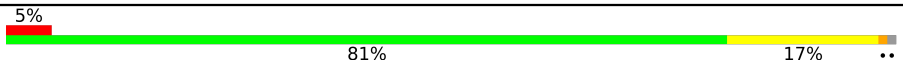
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	501	4% 84% 14%
1	B	501	3% 84% 14%
1	C	501	8% 79% 17%
1	D	501	5% 84% 14%
1	E	501	5% 83% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	501	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24076 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.

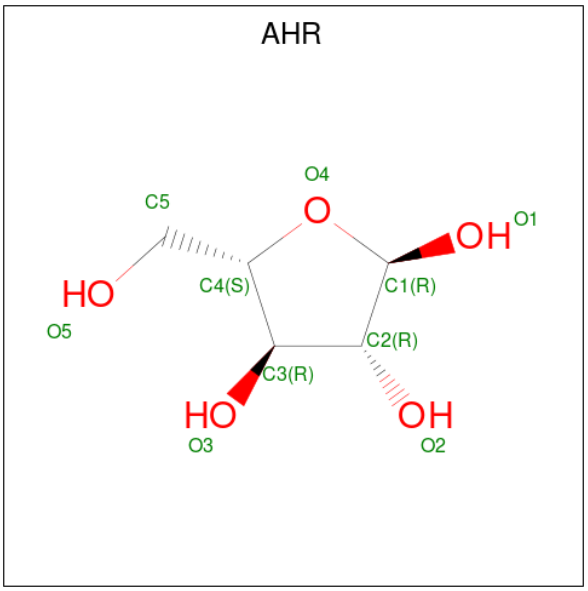
- Molecule 1 is a protein called Intracellular exo-alpha-(1->5)-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	1	0
			3954	2512	671	748	23			
1	B	496	Total	C	N	O	S	0	0	0
			3962	2519	673	748	22			
1	C	496	Total	C	N	O	S	0	0	0
			3965	2520	673	750	22			
1	D	496	Total	C	N	O	S	0	0	0
			3965	2520	673	750	22			
1	E	495	Total	C	N	O	S	0	0	0
			3956	2514	671	749	22			
1	F	495	Total	C	N	O	S	0	0	0
			3955	2514	671	748	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	ARG	engineered mutation	UNP A3DIH0
A	173	ALA	GLU	engineered mutation	UNP A3DIH0
B	67	ALA	ARG	engineered mutation	UNP A3DIH0
B	173	ALA	GLU	engineered mutation	UNP A3DIH0
C	67	ALA	ARG	engineered mutation	UNP A3DIH0
C	173	ALA	GLU	engineered mutation	UNP A3DIH0
D	67	ALA	ARG	engineered mutation	UNP A3DIH0
D	173	ALA	GLU	engineered mutation	UNP A3DIH0
E	67	ALA	ARG	engineered mutation	UNP A3DIH0
E	173	ALA	GLU	engineered mutation	UNP A3DIH0
F	67	ALA	ARG	engineered mutation	UNP A3DIH0
F	173	ALA	GLU	engineered mutation	UNP A3DIH0

- Molecule 2 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 10 5 5	0	0
2	E	1	Total C O 10 5 5	0	0
2	F	1	Total C O 10 5 5	0	0

- Molecule 3 is water.

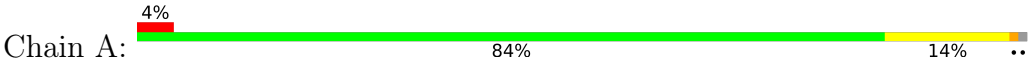
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	40	Total O 40 40	0	0
3	B	50	Total O 50 50	0	0
3	C	47	Total O 47 47	0	0
3	D	42	Total O 42 42	0	0
3	E	44	Total O 44 44	0	0
3	F	36	Total O 36 36	0	0

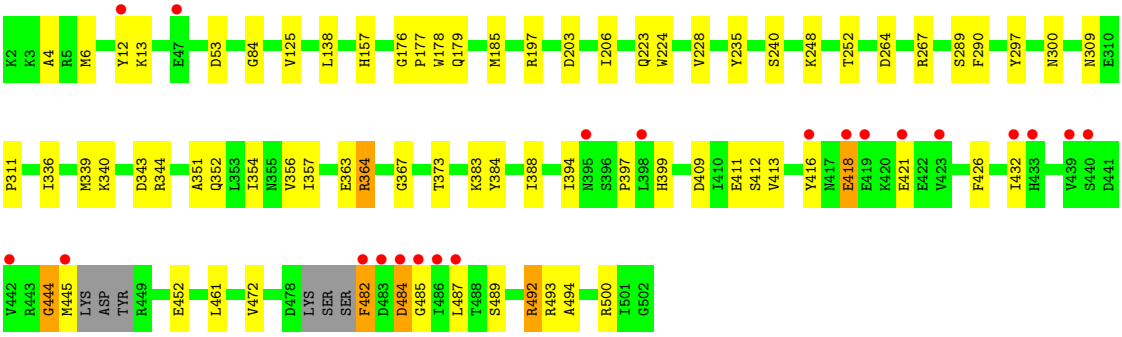
3 Residue-property plots (i)

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: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

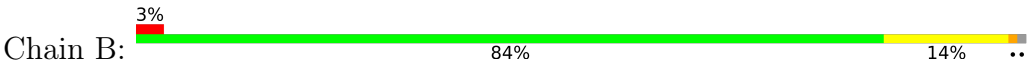
Chain A:

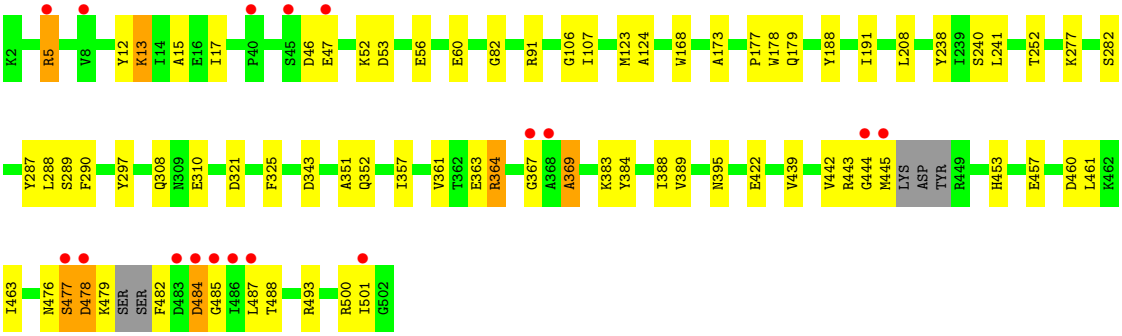




• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

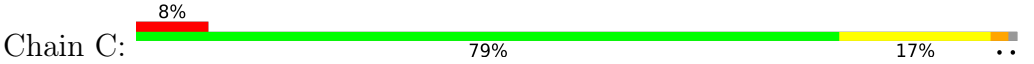
Chain B:

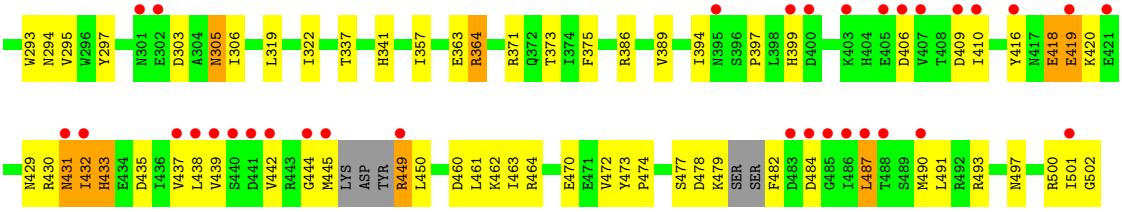




• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

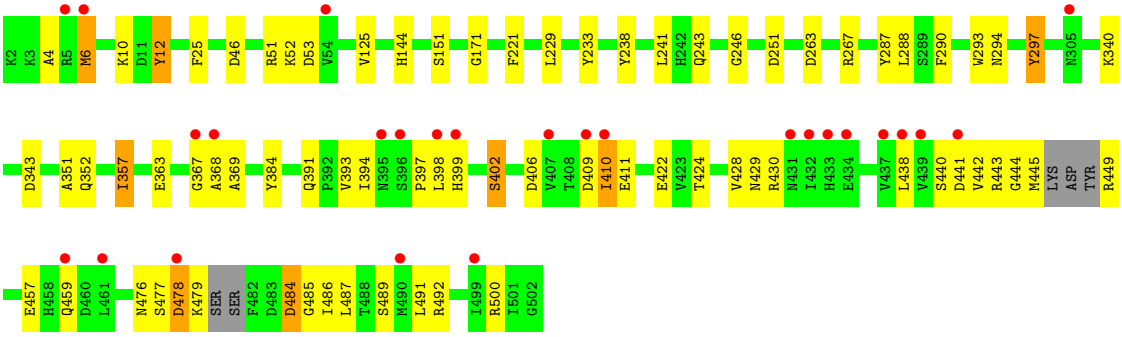
Chain C:





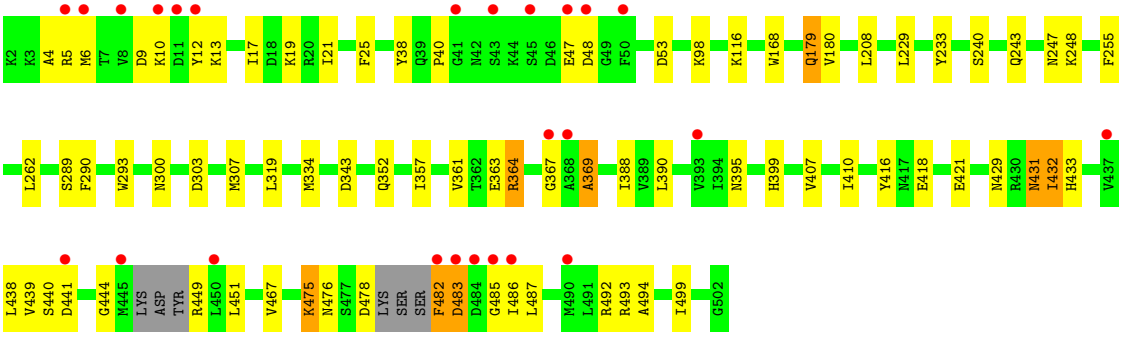
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain D:



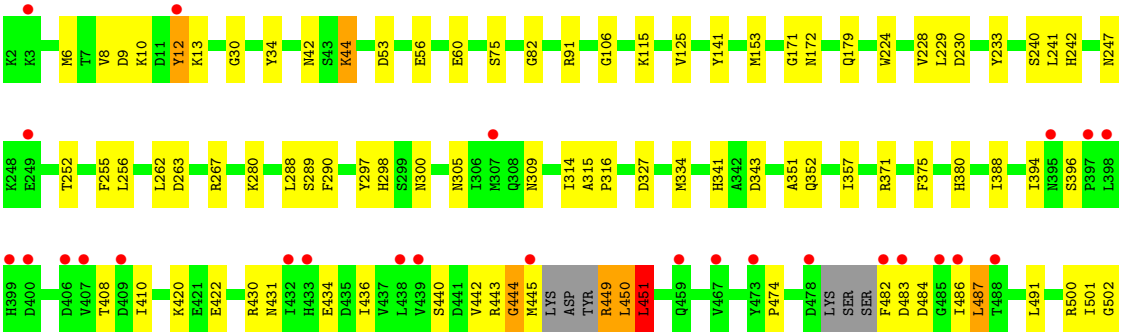
• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain E:



• Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	170.55Å 170.55Å 265.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.85 – 2.39 48.65 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.85-2.39) 99.8 (48.65-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.11.1	Depositor
R, R_{free}	0.187 , 0.237 0.187 , 0.235	Depositor DCC
R_{free} test set	7712 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24076	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.47	0/4044	0.61	0/5480
1	B	0.45	0/4052	0.65	0/5488
1	C	0.48	0/4055	0.64	0/5492
1	D	0.45	0/4055	0.61	0/5492
1	E	0.45	0/4046	0.60	0/5481
1	F	0.50	0/4045	0.61	0/5480
All	All	0.47	0/24297	0.62	0/32913

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	3954	0	3837	48	0
1	B	3962	0	3859	48	0
1	C	3965	0	3861	80	0
1	D	3965	0	3861	48	0
1	E	3956	0	3848	45	0
1	F	3955	0	3845	67	0
2	A	10	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	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	40	0	0	0	0
3	B	50	0	0	0	0
3	C	47	0	0	0	0
3	D	42	0	0	0	0
3	E	44	0	0	0	0
3	F	36	0	0	0	0
All	All	24076	0	23111	332	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 7.

All (332) 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:B:444:GLY:HA3	1:B:445:MET:HG2	1.40	1.00
1:C:478:ASP:HA	1:C:479:LYS:HB3	1.45	0.96
1:C:10:LYS:NZ	1:C:445:MET:SD	2.39	0.96
1:A:176:GLY:H	1:A:179:GLN:HE21	1.14	0.90
1:D:478:ASP:HA	1:D:479:LYS:HB3	1.53	0.90
1:F:482:PHE:HB2	1:F:487:LEU:HD12	1.53	0.87
1:A:482:PHE:HB2	1:A:487:LEU:HA	1.55	0.87
1:C:418:GLU:O	1:C:420:LYS:N	2.08	0.87
1:F:6:MET:HB2	1:F:394:ILE:HD12	1.56	0.85
1:C:431:ASN:HA	1:C:432:ILE:HG22	1.58	0.85
1:C:435:ASP:HB3	1:C:490:MET:HE1	1.57	0.84
1:F:451:LEU:CD2	1:F:501:ILE:C	2.47	0.83
1:F:487:LEU:HD13	1:F:501:ILE:HD11	1.61	0.83
1:A:176:GLY:H	1:A:179:GLN:NE2	1.80	0.80
1:F:451:LEU:CD2	1:F:502:GLY:N	2.46	0.79
1:F:451:LEU:HD21	1:F:502:GLY:N	1.99	0.78
1:D:51:ARG:NH2	1:D:368:ALA:O	2.17	0.78
1:C:435:ASP:HB3	1:C:490:MET:CE	2.14	0.77
1:A:363:GLU:O	1:A:364:ARG:HB2	1.85	0.76
1:B:482:PHE:HB2	1:B:487:LEU:HD12	1.66	0.76
1:D:440:SER:HB2	1:D:487:LEU:HB3	1.67	0.75
1:C:12:TYR:HE2	1:F:12:TYR:HE2	1.33	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ILE:HD12	1:F:491:LEU:HD12	1.70	0.73
1:C:363:GLU:O	1:C:364:ARG:HB2	1.88	0.73
1:C:17:ILE:HD11	1:C:389:VAL:HG23	1.70	0.73
1:C:250:ASN:OD1	1:C:462:LYS:NZ	2.22	0.72
1:D:399:HIS:ND1	1:D:409:ASP:OD1	2.19	0.72
1:F:451:LEU:HD21	1:F:501:ILE:C	2.09	0.71
1:E:431:ASN:ND2	1:E:431:ASN:O	2.21	0.71
1:C:12:TYR:CE2	1:F:12:TYR:HE2	2.07	0.71
1:D:485:GLY:H	1:D:486:ILE:HD12	1.56	0.71
1:A:6:MET:HB2	1:A:394:ILE:HD12	1.71	0.70
1:E:363:GLU:HG2	1:E:467:VAL:HG11	1.74	0.69
1:C:4:ALA:HB2	1:C:397:PRO:HD2	1.76	0.68
1:F:75:SER:OG	1:F:179:GLN:NE2	2.26	0.68
1:C:257:ALA:HA	1:C:430:ARG:HH11	1.60	0.66
1:B:252:THR:HG21	1:B:461:LEU:HD13	1.77	0.66
1:F:13:LYS:HG2	1:F:388:ILE:HG21	1.76	0.66
1:B:487:LEU:HD13	1:B:501:ILE:HD11	1.75	0.66
1:A:444:GLY:HA2	1:A:445:MET:HB2	1.75	0.66
1:F:451:LEU:HD21	1:F:502:GLY:CA	2.25	0.66
1:D:410:ILE:HD12	1:D:491:LEU:HD12	1.76	0.66
1:C:6:MET:HB2	1:C:394:ILE:HD12	1.78	0.65
1:F:444:GLY:HA3	1:F:445:MET:HB3	1.79	0.65
1:D:424:THR:HG23	1:D:500:ARG:HG2	1.79	0.65
1:F:408:THR:HB	1:F:430:ARG:HH21	1.62	0.65
1:F:486:ILE:N	1:F:486:ILE:HD12	2.13	0.64
1:A:13:LYS:HG2	1:A:388:ILE:HG21	1.80	0.64
1:C:478:ASP:CA	1:C:479:LYS:HB3	2.23	0.64
1:C:10:LYS:HZ2	1:C:445:MET:CG	2.11	0.64
1:E:431:ASN:O	1:E:433:HIS:N	2.26	0.64
1:C:10:LYS:NZ	1:C:445:MET:CG	2.61	0.63
1:A:432:ILE:HG22	1:A:494:ALA:HB2	1.78	0.63
1:B:363:GLU:HB2	1:B:367:GLY:O	1.98	0.63
1:C:10:LYS:HZ2	1:C:445:MET:HG3	1.63	0.63
1:F:450:LEU:C	1:F:450:LEU:HD12	2.18	0.63
1:F:42:ASN:OD1	1:F:44:LYS:NZ	2.32	0.62
1:F:451:LEU:HD23	1:F:501:ILE:N	2.14	0.62
1:F:451:LEU:HD23	1:F:501:ILE:CA	2.29	0.62
1:B:439:VAL:HG22	1:B:488:THR:HG22	1.82	0.62
1:E:361:VAL:O	1:E:369:ALA:HA	2.00	0.62
1:A:492:ARG:HD3	1:A:493:ARG:O	2.00	0.61
1:D:410:ILE:HD13	1:D:429:ASN:HA	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:ASP:HB3	1:C:479:LYS:C	2.21	0.61
1:C:10:LYS:HE3	1:C:444:GLY:HA2	1.83	0.61
1:C:257:ALA:HA	1:C:430:ARG:NH1	2.15	0.60
1:B:107:ILE:HD13	1:B:123:MET:CE	2.32	0.59
1:E:482:PHE:HA	1:E:487:LEU:HD12	1.84	0.59
1:B:5:ARG:HG3	1:B:395:ASN:HB2	1.84	0.59
1:B:453:HIS:HB3	1:B:477:SER:HB2	1.85	0.59
1:B:477:SER:OG	1:B:479:LYS:HD3	2.02	0.59
1:B:107:ILE:HD13	1:B:123:MET:HE3	1.84	0.58
1:C:107:ILE:HD11	1:C:141:TYR:CE1	2.38	0.58
1:E:179:GLN:HE21	1:E:180:VAL:H	1.49	0.58
1:C:437:VAL:HA	1:C:490:MET:HA	1.85	0.58
1:C:460:ASP:HB3	1:C:463:ILE:HB	1.86	0.58
1:B:363:GLU:O	1:B:364:ARG:HB3	2.04	0.57
1:F:6:MET:HB2	1:F:394:ILE:CD1	2.32	0.57
1:D:363:GLU:HB2	1:D:367:GLY:O	2.04	0.57
1:A:252:THR:HG21	1:A:461:LEU:HD23	1.86	0.57
1:D:6:MET:SD	1:D:394:ILE:HD11	2.44	0.57
1:B:13:LYS:HD3	1:B:388:ILE:HG21	1.86	0.57
1:C:305:ASN:HB3	1:C:306:ILE:HD12	1.86	0.57
1:E:363:GLU:O	1:E:364:ARG:HB2	2.05	0.57
1:B:478:ASP:HA	1:B:479:LYS:HG2	1.86	0.56
1:F:487:LEU:CD1	1:F:501:ILE:HD11	2.33	0.56
1:A:452:GLU:OE2	1:A:500:ARG:NH1	2.39	0.56
1:B:361:VAL:O	1:B:369:ALA:HA	2.05	0.56
1:C:479:LYS:NZ	1:C:479:LYS:O	2.37	0.56
1:F:451:LEU:HD23	1:F:501:ILE:C	2.25	0.56
1:A:482:PHE:CB	1:A:487:LEU:HA	2.33	0.56
1:E:363:GLU:N	1:E:367:GLY:O	2.38	0.56
1:D:340:LYS:NZ	1:D:411:GLU:OE2	2.30	0.56
1:F:298:HIS:HE1	1:F:327:ASP:OD2	1.89	0.56
1:C:399:HIS:HD2	1:C:409:ASP:OD1	1.89	0.56
1:E:13:LYS:HD3	1:E:388:ILE:HG21	1.86	0.56
1:A:343:ASP:OD1	1:A:343:ASP:N	2.40	0.55
1:D:384:TYR:HB3	1:D:424:THR:HG21	1.88	0.55
1:A:185:MET:SD	1:A:223:GLN:HG2	2.46	0.55
1:A:264:ASP:OD1	1:A:267:ARG:NH2	2.39	0.55
1:A:363:GLU:O	1:A:364:ARG:CB	2.55	0.55
1:E:363:GLU:HG2	1:E:467:VAL:CG1	2.35	0.55
1:A:340:LYS:HG3	1:A:413:VAL:HG11	1.88	0.54
1:E:483:ASP:HB3	1:E:486:ILE:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:HD11	1:C:141:TYR:HE1	1.73	0.54
1:A:309:ASN:OD1	1:A:309:ASN:N	2.40	0.54
1:A:416:TYR:CZ	1:A:418:GLU:HB3	2.43	0.54
1:F:141:TYR:HE2	1:F:153:MET:HG2	1.72	0.53
1:C:9:ASP:C	1:C:11:ASP:H	2.11	0.53
1:F:91:ARG:NH2	1:F:314:ILE:HD11	2.23	0.53
1:C:435:ASP:CB	1:C:490:MET:HE1	2.34	0.53
1:E:47:GLU:CD	1:E:47:GLU:H	2.11	0.53
1:B:107:ILE:CD1	1:B:123:MET:HE3	2.37	0.52
1:C:432:ILE:HG23	1:C:432:ILE:O	2.08	0.52
1:C:500:ARG:HG2	1:C:500:ARG:HH11	1.74	0.52
1:F:267:ARG:HE	1:F:341:HIS:HE1	1.58	0.52
1:E:9:ASP:HB3	1:E:12:TYR:CD1	2.44	0.52
1:E:487:LEU:HD21	1:E:499:ILE:HG21	1.90	0.52
1:D:241:LEU:HD11	1:D:288:LEU:HG	1.91	0.52
1:D:251:ASP:OD2	1:D:402:SER:HB2	2.08	0.52
1:E:303:ASP:OD2	1:E:319:LEU:HD12	2.10	0.51
1:F:486:ILE:N	1:F:486:ILE:CD1	2.73	0.51
1:B:478:ASP:HA	1:B:479:LYS:NZ	2.26	0.51
1:C:479:LYS:HE3	1:C:490:MET:HG2	1.91	0.51
1:E:390:LEU:HD11	1:E:416:TYR:HB2	1.92	0.51
1:F:125:VAL:O	1:F:171:GLY:HA2	2.10	0.51
1:C:487:LEU:HD13	1:C:501:ILE:HD11	1.92	0.51
1:F:410:ILE:HD11	1:F:436:ILE:HB	1.92	0.51
1:F:6:MET:O	1:F:440:SER:HA	2.11	0.51
1:B:478:ASP:HA	1:B:479:LYS:HZ2	1.76	0.50
1:E:248:LYS:NZ	1:E:300:ASN:OD1	2.42	0.50
1:E:439:VAL:HG23	1:E:486:ILE:HG23	1.92	0.50
1:F:371:ARG:HD3	1:F:375:PHE:CE1	2.47	0.50
1:B:460:ASP:HB3	1:B:463:ILE:HB	1.93	0.50
1:D:484:ASP:HB3	1:D:486:ILE:HD12	1.94	0.50
1:C:209:VAL:HG22	1:C:238:TYR:HB2	1.93	0.50
1:D:444:GLY:HA2	1:D:445:MET:HE2	1.93	0.50
1:E:416:TYR:CZ	1:E:418:GLU:HG2	2.47	0.50
1:A:363:GLU:HB2	1:A:367:GLY:HA3	1.93	0.49
1:C:65:ILE:HD11	1:C:122:MET:HB2	1.93	0.49
1:F:450:LEU:O	1:F:450:LEU:HG	2.12	0.49
1:B:277:LYS:NZ	1:B:282:SER:O	2.46	0.49
1:C:240:SER:HA	1:C:289:SER:O	2.12	0.49
1:A:336:ILE:HA	1:A:339:MET:CE	2.42	0.49
1:A:340:LYS:NZ	1:A:411:GLU:OE2	2.37	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:OE1	1:B:500:ARG:NH1	2.46	0.49
1:F:343:ASP:N	1:F:343:ASP:OD1	2.45	0.49
1:C:229:LEU:O	1:C:233:TYR:HB2	2.13	0.49
1:D:343:ASP:OD1	1:D:343:ASP:N	2.46	0.49
1:F:482:PHE:CD1	1:F:487:LEU:HB2	2.48	0.49
1:F:451:LEU:HD23	1:F:500:ARG:C	2.33	0.49
1:E:9:ASP:HB3	1:E:12:TYR:HD1	1.78	0.49
1:E:179:GLN:HE21	1:E:180:VAL:N	2.10	0.49
1:C:439:VAL:HA	1:C:487:LEU:O	2.13	0.48
1:F:34:TYR:HB2	1:F:315:ALA:HB2	1.95	0.48
1:C:477:SER:HB3	1:C:478:ASP:OD1	2.12	0.48
1:D:478:ASP:HA	1:D:479:LYS:CB	2.35	0.48
1:D:442:VAL:O	1:D:444:GLY:N	2.44	0.48
1:E:53:ASP:N	1:E:53:ASP:OD1	2.47	0.48
1:E:432:ILE:HA	1:E:494:ALA:HB2	1.95	0.48
1:F:172:ASN:HB3	1:F:179:GLN:HE22	1.78	0.48
1:C:8:VAL:CG1	1:C:442:VAL:HG12	2.44	0.48
1:C:478:ASP:HA	1:C:479:LYS:CB	2.32	0.48
1:F:240:SER:HA	1:F:289:SER:O	2.14	0.48
1:B:107:ILE:CD1	1:B:123:MET:CE	2.92	0.48
1:A:176:GLY:N	1:A:179:GLN:HE21	1.96	0.47
1:C:294:ASN:OD1	1:C:295:VAL:N	2.47	0.47
1:F:451:LEU:CD2	1:F:501:ILE:CA	2.90	0.47
1:C:12:TYR:CE2	1:F:12:TYR:CE2	2.96	0.47
1:E:431:ASN:C	1:E:433:HIS:H	2.14	0.47
1:A:224:TRP:O	1:A:228:VAL:HG23	2.14	0.47
1:B:383:LYS:HD3	1:B:384:TYR:CZ	2.50	0.47
1:B:444:GLY:HA3	1:B:445:MET:CG	2.30	0.47
1:D:4:ALA:HB2	1:D:397:PRO:HD2	1.96	0.47
1:B:188:TYR:HA	1:B:191:ILE:HG22	1.97	0.47
1:C:252:THR:HG21	1:C:461:LEU:HD13	1.97	0.47
1:C:373:THR:HG22	1:C:472:VAL:HB	1.96	0.47
1:E:431:ASN:O	1:E:432:ILE:HG22	2.14	0.47
1:F:247:ASN:HB2	1:F:255:PHE:CD1	2.49	0.47
1:B:476:ASN:HB3	1:B:477:SER:HB3	1.96	0.47
1:C:38:TYR:CZ	1:C:40:PRO:HG3	2.50	0.47
1:C:482:PHE:HB2	1:C:487:LEU:HD12	1.98	0.46
1:E:343:ASP:OD1	1:E:343:ASP:N	2.46	0.46
1:B:173:ALA:O	1:B:179:GLN:NE2	2.49	0.46
1:E:243:GLN:O	1:E:293:TRP:HA	2.16	0.46
1:D:238:TYR:HA	1:D:287:TYR:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:449:ARG:HG3	1:C:450:LEU:H	1.80	0.46
1:D:477:SER:O	1:D:478:ASP:HB2	2.15	0.46
1:A:484:ASP:OD1	1:A:485:GLY:N	2.48	0.46
1:D:125:VAL:O	1:D:171:GLY:HA2	2.16	0.46
1:E:492:ARG:HG2	1:E:493:ARG:N	2.31	0.46
1:C:437:VAL:HG22	1:C:490:MET:HB3	1.98	0.45
1:F:263:ASP:O	1:F:267:ARG:HG3	2.16	0.45
1:C:252:THR:HG22	1:C:432:ILE:HD12	1.97	0.45
1:A:12:TYR:CE1	1:D:393:VAL:HG21	2.51	0.45
1:A:309:ASN:C	1:A:311:PRO:HD3	2.37	0.45
1:B:17:ILE:HG12	1:B:389:VAL:HG23	1.98	0.45
1:D:4:ALA:O	1:D:438:LEU:HA	2.16	0.45
1:D:6:MET:O	1:D:441:ASP:N	2.49	0.45
1:D:53:ASP:OD1	1:D:53:ASP:N	2.49	0.45
1:A:354:ILE:O	1:A:356:VAL:N	2.43	0.45
1:D:457:GLU:CD	1:D:492:ARG:HD2	2.38	0.45
1:B:53:ASP:N	1:B:53:ASP:OD1	2.45	0.45
1:E:38:TYR:CZ	1:E:40:PRO:HG3	2.52	0.45
1:F:449:ARG:O	1:F:502:GLY:N	2.40	0.45
1:D:351:ALA:O	1:D:357:ILE:HD12	2.16	0.45
1:F:224:TRP:O	1:F:228:VAL:HG23	2.16	0.45
1:C:482:PHE:HA	1:C:487:LEU:HA	1.98	0.44
1:D:484:ASP:HB3	1:D:486:ILE:CD1	2.47	0.44
1:B:241:LEU:HD11	1:B:288:LEU:HG	1.98	0.44
1:B:484:ASP:HB3	1:B:485:GLY:H	1.54	0.44
1:D:293:TRP:O	1:D:294:ASN:HB2	2.16	0.44
1:C:303:ASP:OD2	1:C:319:LEU:HD12	2.18	0.44
1:A:197:ARG:NH1	1:A:235:TYR:OH	2.51	0.44
1:B:238:TYR:HA	1:B:287:TYR:O	2.17	0.44
1:B:442:VAL:O	1:B:444:GLY:N	2.50	0.44
1:E:410:ILE:HD13	1:E:429:ASN:HA	2.00	0.44
1:F:431:ASN:ND2	1:F:434:GLU:HB3	2.32	0.44
1:D:246:GLY:HA2	1:D:297:TYR:CD1	2.53	0.44
1:E:4:ALA:O	1:E:438:LEU:HD12	2.18	0.44
1:F:8:VAL:HG23	1:F:442:VAL:HA	2.00	0.44
1:F:30:GLY:HA2	1:F:316:PRO:O	2.18	0.44
1:A:399:HIS:ND1	1:A:409:ASP:OD1	2.39	0.44
1:A:177:PRO:HD2	1:A:178:TRP:CZ3	2.53	0.44
1:A:336:ILE:HG23	1:A:413:VAL:HG22	2.00	0.44
1:C:419:GLU:HG3	1:C:420:LYS:HG3	1.99	0.44
1:E:17:ILE:HD12	1:E:21:ILE:HD11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:SER:HA	1:B:289:SER:O	2.18	0.43
1:F:351:ALA:HA	1:F:352:GLN:HA	1.66	0.43
1:F:451:LEU:HD22	1:F:502:GLY:N	2.31	0.43
1:D:229:LEU:O	1:D:233:TYR:HB2	2.18	0.43
1:E:240:SER:HA	1:E:289:SER:O	2.19	0.43
1:B:363:GLU:O	1:B:364:ARG:CB	2.65	0.43
1:E:262:LEU:HD22	1:E:334:MET:HG2	2.01	0.43
1:F:241:LEU:HD11	1:F:288:LEU:HG	2.01	0.43
1:F:420:LYS:HB3	1:F:422:GLU:HG3	2.00	0.43
1:A:178:TRP:CD1	1:A:179:GLN:HG2	2.53	0.43
1:A:240:SER:HA	1:A:289:SER:O	2.19	0.43
1:C:140:GLU:HG2	1:C:150:TYR:HB2	2.00	0.43
1:C:430:ARG:O	1:C:431:ASN:HB3	2.18	0.43
1:F:305:ASN:O	1:F:309:ASN:HB2	2.19	0.43
1:A:53:ASP:OD1	1:A:53:ASP:N	2.52	0.43
1:A:84:GLY:HA2	1:A:157:HIS:CD2	2.53	0.43
1:B:478:ASP:H	1:B:479:LYS:HA	1.83	0.43
1:F:262:LEU:HD22	1:F:334:MET:HG2	2.00	0.43
1:C:144:HIS:HB3	1:C:151:SER:HB3	2.00	0.43
1:C:432:ILE:O	1:C:433:HIS:CG	2.72	0.43
1:C:449:ARG:HB3	1:C:502:GLY:H	1.83	0.43
1:D:351:ALA:HA	1:D:352:GLN:HA	1.76	0.43
1:D:398:LEU:HD13	1:D:406:ASP:HB3	1.99	0.43
1:A:248:LYS:NZ	1:A:300:ASN:HD22	2.16	0.43
1:B:308:GLN:O	1:B:310:GLU:N	2.46	0.43
1:D:428:VAL:HG12	1:D:430:ARG:HB2	2.00	0.43
1:E:168:TRP:HB2	1:E:208:LEU:HD23	2.01	0.43
1:B:343:ASP:OD1	1:B:343:ASP:N	2.48	0.42
1:B:351:ALA:HA	1:B:352:GLN:HA	1.76	0.42
1:C:435:ASP:HB3	1:C:490:MET:HE3	1.98	0.42
1:E:399:HIS:O	1:E:407:VAL:HG22	2.20	0.42
1:A:125:VAL:HG12	1:A:138:LEU:HD23	2.01	0.42
1:A:383:LYS:HG2	1:A:384:TYR:CD1	2.53	0.42
1:C:416:TYR:CE1	1:C:418:GLU:OE2	2.72	0.42
1:C:293:TRP:O	1:C:294:ASN:HB2	2.19	0.42
1:C:416:TYR:CZ	1:C:418:GLU:OE2	2.72	0.42
1:A:373:THR:HG22	1:A:472:VAL:HB	2.01	0.42
1:E:48:ASP:OD2	1:E:116:LYS:NZ	2.52	0.42
1:A:344:ARG:HA	1:A:344:ARG:HD2	1.87	0.42
1:C:17:ILE:HD11	1:C:389:VAL:CG2	2.45	0.42
1:C:432:ILE:H	1:C:493:ARG:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:PHE:O	1:E:352:GLN:HB3	2.20	0.42
1:F:380:HIS:CE1	1:F:474:PRO:HB3	2.55	0.42
1:F:422:GLU:OE1	1:F:500:ARG:NH1	2.52	0.42
1:B:325:PHE:CZ	1:B:457:GLU:HA	2.54	0.42
1:F:451:LEU:HD22	1:F:451:LEU:H	1.84	0.42
1:D:478:ASP:HB3	1:D:479:LYS:C	2.39	0.42
1:B:168:TRP:HB2	1:B:208:LEU:HD23	2.01	0.42
1:C:337:THR:O	1:C:341:HIS:HD2	2.03	0.42
1:E:363:GLU:CG	1:E:467:VAL:HG11	2.47	0.42
1:F:229:LEU:O	1:F:233:TYR:HB2	2.20	0.42
1:D:12:TYR:CE1	1:D:391:GLN:HG2	2.54	0.42
1:D:410:ILE:HA	1:D:428:VAL:O	2.20	0.42
1:B:46:ASP:HB3	1:B:52:LYS:HD2	2.02	0.41
1:F:56:GLU:O	1:F:60:GLU:HG3	2.20	0.41
1:C:461:LEU:HD23	1:C:461:LEU:HA	1.88	0.41
1:D:263:ASP:CG	1:D:267:ARG:HH11	2.22	0.41
1:E:475:LYS:HB2	1:E:475:LYS:HE2	1.76	0.41
1:A:203:ASP:O	1:A:206:ILE:HG12	2.21	0.41
1:B:47:GLU:CD	1:B:47:GLU:H	2.23	0.41
1:C:473:TYR:HB2	1:C:474:PRO:HD2	2.02	0.41
1:F:44:LYS:HZ2	1:F:44:LYS:HG3	1.72	0.41
1:C:449:ARG:HG3	1:C:450:LEU:N	2.35	0.41
1:D:422:GLU:OE1	1:D:500:ARG:NH2	2.51	0.41
1:E:449:ARG:HD3	1:E:449:ARG:N	2.35	0.41
1:B:82:GLY:O	1:B:106:GLY:HA3	2.20	0.41
1:C:10:LYS:HB3	1:C:416:TYR:CZ	2.56	0.41
1:C:491:LEU:HD22	1:C:497:ASN:CG	2.41	0.41
1:D:46:ASP:HB3	1:D:52:LYS:HD2	2.01	0.41
1:E:6:MET:O	1:E:440:SER:HA	2.20	0.41
1:E:229:LEU:O	1:E:233:TYR:HB2	2.21	0.41
1:C:438:LEU:HD12	1:C:438:LEU:HA	1.96	0.41
1:E:229:LEU:HD23	1:E:229:LEU:HA	1.84	0.41
1:A:13:LYS:HG2	1:A:388:ILE:CG2	2.49	0.41
1:A:412:SER:HA	1:A:426:PHE:O	2.21	0.41
1:B:56:GLU:O	1:B:60:GLU:HG3	2.20	0.41
1:B:177:PRO:HD2	1:B:178:TRP:CZ3	2.56	0.41
1:C:53:ASP:N	1:C:53:ASP:OD1	2.54	0.41
1:C:256:LEU:HD23	1:C:256:LEU:HA	1.86	0.41
1:D:25:PHE:O	1:D:352:GLN:HB3	2.21	0.41
1:D:394:ILE:HD13	1:D:394:ILE:HA	1.85	0.41
1:F:82:GLY:O	1:F:106:GLY:HA3	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HA	1:A:339:MET:HE2	2.03	0.41
1:A:351:ALA:HA	1:A:352:GLN:HA	1.77	0.41
1:E:247:ASN:HB2	1:E:255:PHE:CD1	2.56	0.41
1:F:9:ASP:OD1	1:F:443:ARG:HB2	2.21	0.41
1:F:115:LYS:HD3	1:F:115:LYS:HA	1.93	0.41
1:F:230:ASP:O	1:F:280:LYS:NZ	2.42	0.41
1:C:10:LYS:HZ1	1:C:445:MET:CG	2.33	0.40
1:C:17:ILE:CD1	1:C:389:VAL:HG23	2.44	0.40
1:C:322:ILE:HG21	1:C:464:ARG:CZ	2.51	0.40
1:D:144:HIS:HB3	1:D:151:SER:HB3	2.03	0.40
1:A:4:ALA:HB2	1:A:397:PRO:HD3	2.02	0.40
1:F:371:ARG:HD3	1:F:375:PHE:CD1	2.56	0.40
1:C:62:ASN:HB3	1:C:386:ARG:NH2	2.36	0.40
1:C:410:ILE:HD13	1:C:429:ASN:HA	2.03	0.40
1:F:53:ASP:OD1	1:F:53:ASP:N	2.54	0.40
1:B:15:ALA:HB2	1:B:343:ASP:HB3	2.04	0.40
1:B:123:MET:HG3	1:B:124:ALA:N	2.36	0.40
1:F:252:THR:O	1:F:256:LEU:HG	2.21	0.40
1:A:340:LYS:HG3	1:A:413:VAL:CG1	2.52	0.40
1:C:371:ARG:HD3	1:C:375:PHE:CD1	2.56	0.40
1:D:221:PHE:CD1	1:D:221:PHE:C	2.95	0.40
1:D:243:GLN:O	1:D:293:TRP:HA	2.21	0.40
1:D:478:ASP:CA	1:D:479:LYS:HB3	2.35	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	490/501 (98%)	465 (95%)	19 (4%)	6 (1%)	13 19
1	B	490/501 (98%)	461 (94%)	21 (4%)	8 (2%)	9 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	490/501 (98%)	448 (91%)	29 (6%)	13 (3%)	5 5
1	D	490/501 (98%)	450 (92%)	33 (7%)	7 (1%)	11 15
1	E	489/501 (98%)	454 (93%)	25 (5%)	10 (2%)	7 9
1	F	489/501 (98%)	463 (95%)	21 (4%)	5 (1%)	15 23
All	All	2938/3006 (98%)	2741 (93%)	148 (5%)	49 (2%)	9 11

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	A	484	ASP
1	B	364	ARG
1	B	478	ASP
1	C	10	LYS
1	C	305	ASN
1	C	364	ARG
1	E	364	ARG
1	E	483	ASP
1	F	483	ASP
1	B	443	ARG
1	B	477	SER
1	C	406	ASP
1	C	418	GLU
1	E	369	ALA
1	E	432	ILE
1	E	444	GLY
1	F	297	TYR
1	F	444	GLY
1	A	297	TYR
1	B	297	TYR
1	C	297	TYR
1	C	470	GLU
1	D	369	ALA
1	D	484	ASP
1	E	10	LYS
1	A	421	GLU
1	A	444	GLY
1	B	493	ARG
1	C	419	GLU
1	C	484	ASP
1	D	297	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	443	ARG
1	D	478	ASP
1	E	441	ASP
1	E	451	LEU
1	A	357	ILE
1	B	369	ALA
1	C	431	ASN
1	D	410	ILE
1	F	451	LEU
1	B	357	ILE
1	C	432	ILE
1	C	433	HIS
1	C	357	ILE
1	E	357	ILE
1	E	485	GLY
1	F	357	ILE
1	D	357	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	425/438 (97%)	420 (99%)	5 (1%)	71	85
1	B	426/438 (97%)	419 (98%)	7 (2%)	62	79
1	C	427/438 (98%)	421 (99%)	6 (1%)	67	82
1	D	427/438 (98%)	418 (98%)	9 (2%)	53	72
1	E	426/438 (97%)	413 (97%)	13 (3%)	40	60
1	F	425/438 (97%)	413 (97%)	12 (3%)	43	63
All	All	2556/2628 (97%)	2504 (98%)	52 (2%)	55	74

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	418	GLU
1	A	482	PHE
1	A	489	SER
1	A	492	ARG
1	B	5	ARG
1	B	12	TYR
1	B	13	LYS
1	B	91	ARG
1	B	290	PHE
1	B	321	ASP
1	B	484	ASP
1	C	5	ARG
1	C	11	ASP
1	C	216	LYS
1	C	290	PHE
1	C	449	ARG
1	C	487	LEU
1	D	6	MET
1	D	10	LYS
1	D	12	TYR
1	D	290	PHE
1	D	402	SER
1	D	449	ARG
1	D	459	GLN
1	D	476	ASN
1	D	489	SER
1	E	5	ARG
1	E	19	LYS
1	E	98	LYS
1	E	179	GLN
1	E	290	PHE
1	E	307	MET
1	E	395	ASN
1	E	421	GLU
1	E	431	ASN
1	E	475	LYS
1	E	476	ASN
1	E	478	ASP
1	E	482	PHE
1	F	10	LYS
1	F	12	TYR
1	F	44	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	242	HIS
1	F	290	PHE
1	F	300	ASN
1	F	396	SER
1	F	449	ARG
1	F	450	LEU
1	F	451	LEU
1	F	484	ASP
1	F	487	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	GLN
1	A	300	ASN
1	B	395	ASN
1	E	179	GLN
1	E	395	ASN
1	F	172	ASN
1	F	179	GLN
1	F	497	ASN

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)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AHR	E	600	-	10,10,10	1.49	2 (20%)	13,14,14	1.52	3 (23%)
2	AHR	C	600	-	10,10,10	1.80	3 (30%)	13,14,14	1.38	3 (23%)
2	AHR	B	600	-	10,10,10	1.75	3 (30%)	13,14,14	1.32	2 (15%)
2	AHR	F	600	-	10,10,10	1.82	2 (20%)	13,14,14	1.39	1 (7%)
2	AHR	A	600	-	10,10,10	1.71	2 (20%)	13,14,14	1.44	2 (15%)
2	AHR	D	600	-	10,10,10	1.77	2 (20%)	13,14,14	1.31	2 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AHR	E	600	-	-	0/2/18/18	0/1/1/1
2	AHR	C	600	-	-	2/2/18/18	0/1/1/1
2	AHR	B	600	-	-	2/2/18/18	0/1/1/1
2	AHR	F	600	-	-	1/2/18/18	0/1/1/1
2	AHR	A	600	-	-	2/2/18/18	0/1/1/1
2	AHR	D	600	-	-	2/2/18/18	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	AHR	C2-C3	-3.52	1.43	1.53
2	A	600	AHR	C2-C3	-3.44	1.43	1.53
2	F	600	AHR	C2-C3	-3.40	1.44	1.53
2	F	600	AHR	C1-C2	-3.28	1.48	1.52
2	C	600	AHR	C2-C3	-3.16	1.44	1.53
2	C	600	AHR	C1-C2	-3.13	1.49	1.52
2	B	600	AHR	C2-C3	-3.12	1.44	1.53
2	B	600	AHR	C1-C2	-3.01	1.49	1.52
2	E	600	AHR	C2-C3	-2.95	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	AHR	C1-C2	-2.72	1.49	1.52
2	A	600	AHR	C1-C2	-2.71	1.49	1.52
2	D	600	AHR	C1-C2	-2.59	1.49	1.52
2	C	600	AHR	O4-C1	2.02	1.45	1.43
2	B	600	AHR	C3-C4	-2.02	1.47	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	AHR	O1-C1-O4	-3.55	106.59	111.13
2	F	600	AHR	C1-C2-C3	3.15	106.24	102.30
2	C	600	AHR	O4-C4-C5	2.86	115.39	109.21
2	E	600	AHR	C1-C2-C3	2.61	105.57	102.30
2	C	600	AHR	C1-C2-C3	2.57	105.52	102.30
2	A	600	AHR	O4-C4-C3	-2.55	100.07	105.11
2	B	600	AHR	C1-C2-C3	2.51	105.45	102.30
2	E	600	AHR	O1-C1-O4	-2.48	107.96	111.13
2	D	600	AHR	O4-C1-C2	2.40	107.41	104.46
2	D	600	AHR	O1-C1-O4	-2.31	108.17	111.13
2	E	600	AHR	O5-C5-C4	2.18	118.78	111.29
2	B	600	AHR	O1-C1-O4	-2.05	108.50	111.13
2	C	600	AHR	O4-C1-C2	2.03	106.96	104.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	AHR	O4-C4-C5-O5
2	B	600	AHR	O4-C4-C5-O5
2	C	600	AHR	O4-C4-C5-O5
2	C	600	AHR	C3-C4-C5-O5
2	D	600	AHR	O4-C4-C5-O5
2	F	600	AHR	O4-C4-C5-O5
2	A	600	AHR	C3-C4-C5-O5
2	B	600	AHR	C3-C4-C5-O5
2	D	600	AHR	C3-C4-C5-O5

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, 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	495/501 (98%)	0.19	21 (4%)	36	35	32, 44, 75, 99	0
1	B	496/501 (99%)	0.20	17 (3%)	45	44	31, 43, 77, 100	0
1	C	496/501 (99%)	0.36	40 (8%)	12	11	32, 46, 89, 115	0
1	D	496/501 (99%)	0.26	26 (5%)	27	26	30, 48, 82, 100	0
1	E	495/501 (98%)	0.29	25 (5%)	28	26	30, 45, 84, 116	0
1	F	495/501 (98%)	0.31	26 (5%)	26	25	32, 49, 87, 113	0
All	All	2973/3006 (98%)	0.27	155 (5%)	27	26	30, 45, 83, 116	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	445	MET	7.8
1	C	416	TYR	6.5
1	C	486	ILE	6.1
1	C	432	ILE	5.1
1	B	483	ASP	4.8
1	F	432	ILE	4.6
1	F	398	LEU	4.4
1	C	485	GLY	4.3
1	A	418	GLU	4.3
1	B	485	GLY	4.3
1	C	483	ASP	4.1
1	F	486	ILE	4.1
1	C	12	TYR	4.0
1	D	368	ALA	3.9
1	D	432	ILE	3.9
1	A	483	ASP	3.9
1	D	478	ASP	3.9
1	C	438	LEU	3.9
1	F	483	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	416	TYR	3.8
1	B	8	VAL	3.7
1	A	485	GLY	3.7
1	D	6	MET	3.7
1	A	432	ILE	3.6
1	C	484	ASP	3.6
1	E	368	ALA	3.5
1	C	405	GLU	3.4
1	D	433	HIS	3.4
1	B	486	ILE	3.4
1	A	12	TYR	3.3
1	B	478	ASP	3.3
1	C	421	GLU	3.3
1	C	419	GLU	3.2
1	A	486	ILE	3.2
1	F	395	ASN	3.2
1	C	441	ASP	3.2
1	F	439	VAL	3.2
1	D	441	ASP	3.1
1	F	478	ASP	3.1
1	F	307	MET	3.1
1	F	473	TYR	3.1
1	F	12	TYR	3.1
1	D	367	GLY	3.1
1	E	45	SER	3.0
1	D	398	LEU	3.0
1	E	43	SER	3.0
1	B	487	LEU	2.9
1	A	445	MET	2.9
1	B	40	PRO	2.9
1	E	485	GLY	2.9
1	D	434	GLU	2.8
1	E	10	LYS	2.8
1	D	439	VAL	2.8
1	C	444	GLY	2.8
1	E	47	GLU	2.8
1	E	486	ILE	2.8
1	C	439	VAL	2.8
1	A	47	GLU	2.8
1	A	423	VAL	2.8
1	C	9	ASP	2.8
1	C	406	ASP	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	3	LYS	2.8
1	A	398	LEU	2.7
1	E	483	ASP	2.7
1	E	484	ASP	2.7
1	C	11	ASP	2.7
1	E	5	ARG	2.7
1	B	484	ASP	2.7
1	F	438	LEU	2.7
1	E	41	GLY	2.7
1	C	501	ILE	2.7
1	F	488	THR	2.7
1	C	253	ALA	2.6
1	C	437	VAL	2.6
1	E	6	MET	2.6
1	E	8	VAL	2.6
1	C	449	ARG	2.6
1	E	441	ASP	2.6
1	D	5	ARG	2.6
1	E	450	LEU	2.6
1	D	409	ASP	2.6
1	C	431	ASN	2.6
1	C	440	SER	2.5
1	A	439	VAL	2.5
1	C	442	VAL	2.5
1	A	433	HIS	2.5
1	B	47	GLU	2.5
1	B	367	GLY	2.5
1	B	477	SER	2.5
1	D	437	VAL	2.5
1	D	410	ILE	2.5
1	E	11	ASP	2.5
1	D	431	ASN	2.5
1	B	45	SER	2.4
1	F	249	GLU	2.4
1	F	445	MET	2.4
1	F	406	ASP	2.4
1	B	444	GLY	2.4
1	F	433	HIS	2.4
1	F	400	ASP	2.4
1	C	410	ILE	2.4
1	E	482	PHE	2.4
1	C	445	MET	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	484	ASP	2.3
1	E	12	TYR	2.3
1	C	409	ASP	2.3
1	A	487	LEU	2.3
1	D	490	MET	2.3
1	F	409	ASP	2.3
1	F	467	VAL	2.3
1	A	419	GLU	2.3
1	E	48	ASP	2.3
1	D	459	GLN	2.3
1	A	395	ASN	2.3
1	D	499	ILE	2.3
1	F	459	GLN	2.3
1	F	399	HIS	2.3
1	D	407	VAL	2.3
1	A	482	PHE	2.2
1	C	399	HIS	2.2
1	A	440	SER	2.2
1	D	396	SER	2.2
1	A	442	VAL	2.2
1	D	438	LEU	2.2
1	C	490	MET	2.2
1	C	395	ASN	2.2
1	F	407	VAL	2.2
1	C	302	GLU	2.2
1	C	400	ASP	2.2
1	C	403	LYS	2.1
1	D	54	VAL	2.1
1	E	393	VAL	2.1
1	C	8	VAL	2.1
1	C	407	VAL	2.1
1	E	50	PHE	2.1
1	C	301	ASN	2.1
1	F	485	GLY	2.1
1	D	399	HIS	2.1
1	D	395	ASN	2.1
1	F	482	PHE	2.1
1	A	421	GLU	2.1
1	C	488	THR	2.1
1	C	487	LEU	2.0
1	E	367	GLY	2.0
1	F	397	PRO	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	461	LEU	2.0
1	B	445	MET	2.0
1	C	7	THR	2.0
1	B	5	ARG	2.0
1	E	437	VAL	2.0
1	D	305	ASN	2.0
1	B	501	ILE	2.0
1	C	47	GLU	2.0
1	E	490	MET	2.0
1	B	368	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 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	B-factors(Å^2)	Q<0.9
2	AHR	C	600	10/10	0.67	0.36	34,44,50,53	10
2	AHR	E	600	10/10	0.73	0.32	36,43,48,50	10
2	AHR	F	600	10/10	0.73	0.32	41,47,51,54	10
2	AHR	A	600	10/10	0.76	0.35	35,42,47,49	10
2	AHR	D	600	10/10	0.79	0.23	38,48,56,59	10
2	AHR	B	600	10/10	0.81	0.27	38,40,48,49	10

6.5 Other polymers (i)

There are no such residues in this entry.