



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:43 PM UTC

PDB ID : 2CGE / pdb_00002cge
Title : Crystal structure of an Hsp90-Sba1 closed chaperone complex
Authors : Ali, M.M.U.; Roe, S.M.; Prodromou, C.; Pearl, L.H.
Deposited on : 2006-03-01
Resolution : 3.00 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
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

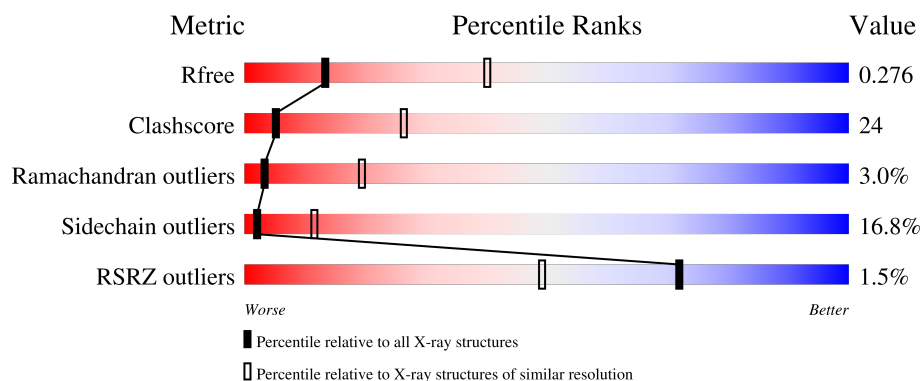
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	405	2% 57% 32% 8% .
1	B	405	% 54% 33% 10% .
1	D	405	% 50% 35% 13% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9882 atoms, of which 0 are hydrogens and 0 are deuteriums.

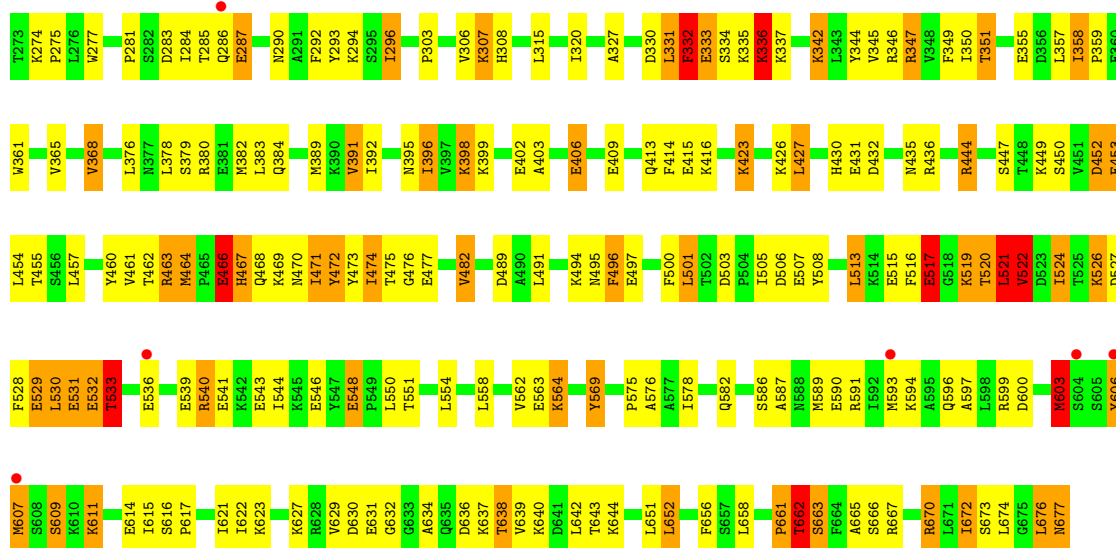
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP-DEPENDENT MOLECULAR CHAPERONE HSP82.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3294	2110	539	638	7			
1	B	405	Total	C	N	O	S	0	0	0
			3294	2110	539	638	7			
1	D	405	Total	C	N	O	S	0	0	0
			3294	2110	539	638	7			



• Molecule 1: ATP-DEPENDENT MOLECULAR CHAPERONE HSP82



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 105.56Å 289.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	288.67 – 3.00 99.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (288.67-3.00) 99.9 (99.16-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.257 , 0.288 0.245 , 0.276	Depositor DCC
R_{free} test set	2072 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 89.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9882	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% 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

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	1.07	4/3355 (0.1%)	1.19	18/4518 (0.4%)
1	B	1.01	5/3355 (0.1%)	1.20	18/4518 (0.4%)
1	D	1.26	20/3355 (0.6%)	1.31	23/4518 (0.5%)
All	All	1.12	29/10065 (0.3%)	1.24	59/13554 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	602	SER	CB-OG	17.67	1.77	1.42
1	D	463	ARG	C-O	13.12	1.41	1.24
1	D	473	TYR	C-N	9.25	1.44	1.33
1	D	471	ILE	C-O	8.72	1.33	1.24
1	B	522	VAL	CA-CB	8.72	1.64	1.54
1	D	462	THR	C-O	8.37	1.34	1.24
1	D	521	LEU	C-O	7.38	1.32	1.23
1	D	496	PHE	CA-C	7.01	1.61	1.52
1	D	464	MET	CA-C	6.63	1.60	1.52
1	D	464	MET	N-CA	6.48	1.56	1.46
1	D	467	HIS	CG-ND1	-6.34	1.31	1.38
1	D	472	TYR	C-O	6.26	1.31	1.24
1	D	522	VAL	CA-CB	6.21	1.60	1.54
1	D	475	THR	N-CA	-6.17	1.38	1.46
1	B	533	THR	CA-CB	6.09	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	467	HIS	CE1-NE2	-6.07	1.26	1.32
1	D	472	TYR	CA-C	5.91	1.60	1.52
1	B	522	VAL	CA-C	-5.91	1.46	1.52
1	B	384	GLN	CG-CD	5.74	1.66	1.52
1	D	365	VAL	CA-CB	-5.66	1.47	1.54
1	D	533	THR	CA-CB	5.57	1.62	1.53
1	A	520	THR	CA-CB	5.42	1.61	1.53
1	A	341	ILE	CA-CB	-5.28	1.47	1.54
1	D	468	GLN	CD-NE2	5.24	1.44	1.33
1	A	336	LYS	N-CA	5.18	1.52	1.46
1	D	494	LYS	C-O	5.16	1.30	1.24
1	B	384	GLN	CB-CG	5.14	1.67	1.52
1	D	466	GLU	CD-OE2	5.03	1.34	1.25
1	D	520	THR	CA-CB	5.02	1.60	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	599	ARG	N-CA-C	-8.29	105.17	114.62
1	D	495	ASN	CA-C-N	-8.13	109.78	122.87
1	D	495	ASN	C-N-CA	-8.13	109.78	122.87
1	B	599	ARG	N-CA-C	-7.70	105.85	114.62
1	B	522	VAL	N-CA-C	-7.63	99.74	109.58
1	A	521	LEU	N-CA-C	7.21	121.31	109.06
1	D	463	ARG	CA-C-N	-7.21	111.01	120.67
1	D	463	ARG	C-N-CA	-7.21	111.01	120.67
1	B	302	ASP	CA-C-N	-7.02	113.43	120.31
1	B	302	ASP	C-N-CA	-7.02	113.43	120.31
1	A	505	ILE	CB-CA-C	-6.97	102.73	112.14
1	B	384	GLN	N-CA-C	-6.70	103.22	111.33
1	A	367	GLY	N-CA-C	6.67	118.83	110.29
1	D	469	LYS	N-CA-C	-6.64	105.80	114.04
1	D	468	GLN	OE1-CD-NE2	-6.48	116.12	122.60
1	D	495	ASN	N-CA-C	6.47	120.59	111.92
1	D	522	VAL	CB-CA-C	-6.39	100.90	111.32
1	D	472	TYR	CA-C-N	-6.23	111.92	123.01
1	D	472	TYR	C-N-CA	-6.23	111.92	123.01
1	D	327	ALA	CA-C-N	5.88	125.49	119.56
1	D	327	ALA	C-N-CA	5.88	125.49	119.56
1	B	521	LEU	N-CA-C	5.86	119.02	109.06
1	B	530	LEU	CB-CA-C	-5.85	109.85	116.63
1	B	292	PHE	N-CA-C	-5.75	104.92	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	PHE	N-CA-C	-5.71	104.97	111.14
1	B	672	ILE	N-CA-C	-5.65	106.30	111.67
1	B	607	MET	N-CA-C	-5.64	106.32	113.43
1	A	602	SER	CA-CB-OG	-5.63	99.83	111.10
1	D	550	LEU	N-CA-C	-5.53	104.11	111.24
1	B	349	PHE	CA-C-N	-5.44	116.15	122.63
1	B	349	PHE	C-N-CA	-5.44	116.15	122.63
1	D	522	VAL	N-CA-C	-5.44	101.80	109.63
1	B	286	GLN	N-CA-C	-5.37	101.38	109.60
1	D	521	LEU	N-CA-C	5.35	118.11	108.48
1	D	569	TYR	N-CA-C	-5.34	106.78	113.72
1	D	529	GLU	N-CA-C	5.33	118.09	109.40
1	A	423	LYS	N-CA-C	-5.31	105.53	112.23
1	B	300	TRP	N-CA-C	-5.31	106.30	112.89
1	A	356	ASP	N-CA-C	5.27	118.86	111.74
1	B	505	ILE	CB-CA-C	-5.27	103.99	112.16
1	A	314	GLN	N-CA-C	-5.26	104.60	111.02
1	B	330	ASP	N-CA-C	5.25	118.12	109.72
1	D	344	TYR	CA-C-N	-5.18	116.36	123.14
1	D	344	TYR	C-N-CA	-5.18	116.36	123.14
1	A	302	ASP	CA-C-N	-5.17	114.66	120.14
1	A	302	ASP	C-N-CA	-5.17	114.66	120.14
1	A	522	VAL	N-CA-C	-5.16	102.92	109.58
1	D	292	PHE	N-CA-C	-5.12	105.61	111.14
1	A	286	GLN	N-CA-C	-5.10	99.93	110.80
1	D	524	ILE	N-CA-C	-5.07	106.97	112.80
1	D	472	TYR	N-CA-C	5.06	117.86	109.46
1	B	327	ALA	CA-C-N	5.04	124.66	119.56
1	B	327	ALA	C-N-CA	5.04	124.66	119.56
1	A	333	GLU	CA-C-N	-5.03	115.29	122.68
1	A	333	GLU	C-N-CA	-5.03	115.29	122.68
1	A	522	VAL	CB-CA-C	-5.03	103.62	111.26
1	A	349	PHE	CA-C-N	-5.01	118.02	123.08
1	A	349	PHE	C-N-CA	-5.01	118.02	123.08
1	A	384	GLN	N-CA-C	-5.01	105.27	111.33

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	606	TYR	Peptide
1	D	517	GLU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	532	GLU	Peptide

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	3294	0	3323	145	0
1	B	3294	0	3323	173	0
1	D	3294	0	3323	181	0
All	All	9882	0	9969	486	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 24.

All (486) 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:602:SER:CB	1:A:602:SER:OG	1.77	1.31
1:D:593:MET:SD	1:D:607:MET:HE2	1.94	1.07
1:D:597:ALA:HB3	1:D:606:TYR:HE2	1.19	1.06
1:A:332:PHE:O	1:A:333:GLU:HB2	1.56	1.05
1:B:526:LYS:HB3	1:B:582:GLN:HG2	1.36	1.05
1:B:332:PHE:O	1:B:333:GLU:HB2	1.52	1.02
1:D:524:ILE:HD11	1:D:586:SER:HB2	1.41	1.01
1:D:597:ALA:HB3	1:D:606:TYR:CE2	1.95	1.00
1:B:636:ASP:HB2	1:B:639:VAL:HG23	1.44	0.99
1:D:530:LEU:O	1:D:532:GLU:N	1.97	0.97
1:D:335:LYS:HG3	1:D:336:LYS:H	1.29	0.96
1:A:636:ASP:HB2	1:A:639:VAL:HG23	1.47	0.95
1:D:449:LYS:HD2	1:D:497:GLU:HB2	1.48	0.95
1:D:636:ASP:HB2	1:D:639:VAL:HG23	1.47	0.95
1:A:335:LYS:HG3	1:A:336:LYS:H	1.28	0.95
1:D:332:PHE:O	1:D:333:GLU:HB2	1.63	0.93
1:A:540:ARG:HG3	1:A:540:ARG:HH11	1.38	0.88
1:B:494:LYS:NZ	1:B:530:LEU:HD12	1.88	0.88
1:A:531:GLU:HB3	1:A:534:ASP:OD1	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:ALA:CB	1:D:606:TYR:HE2	1.87	0.85
1:B:517:GLU:OE2	1:B:517:GLU:HA	1.76	0.84
1:D:426:LYS:HE2	1:D:506:ASP:OD1	1.78	0.84
1:B:494:LYS:HZ3	1:B:530:LEU:HD12	1.41	0.83
1:A:526:LYS:HB3	1:A:582:GLN:HG2	1.58	0.83
1:A:426:LYS:HD3	1:A:505:ILE:HD12	1.57	0.83
1:B:335:LYS:HG3	1:B:336:LYS:H	1.44	0.82
1:B:526:LYS:CB	1:B:582:GLN:HG2	2.09	0.82
1:B:670:ARG:HA	1:B:673:SER:HB2	1.60	0.81
1:D:389:MET:HE3	1:D:389:MET:HA	1.63	0.81
1:B:540:ARG:HG3	1:B:540:ARG:HH11	1.45	0.81
1:A:470:ASN:HB3	1:A:521:LEU:HD21	1.61	0.81
1:D:426:LYS:HD3	1:D:505:ILE:HD12	1.62	0.80
1:A:529:GLU:CD	1:A:530:LEU:HD12	2.06	0.80
1:D:636:ASP:HB3	1:D:638:THR:HG23	1.62	0.79
1:D:461:VAL:HA	1:D:464:MET:HE2	1.63	0.79
1:D:470:ASN:HB3	1:D:521:LEU:HD21	1.62	0.79
1:D:593:MET:SD	1:D:607:MET:CE	2.70	0.79
1:D:358:ILE:HG12	1:D:359:PRO:HD2	1.64	0.78
1:B:470:ASN:HB3	1:B:521:LEU:HD21	1.63	0.78
1:D:526:LYS:HB3	1:D:582:GLN:HG2	1.65	0.78
1:A:361:TRP:HB3	1:A:427:LEU:CD1	2.13	0.78
1:D:501:LEU:HB3	1:D:506:ASP:HB3	1.66	0.77
1:A:333:GLU:HG3	1:B:376:LEU:HD13	1.66	0.77
1:D:673:SER:O	1:D:677:ASN:N	2.17	0.77
1:A:521:LEU:HD23	1:A:521:LEU:N	2.00	0.76
1:B:426:LYS:HE2	1:B:506:ASP:OD1	1.85	0.76
1:D:330:ASP:O	1:D:334:SER:HB3	1.86	0.76
1:A:636:ASP:HB3	1:A:638:THR:HG23	1.69	0.75
1:A:531:GLU:CB	1:A:534:ASP:OD1	2.35	0.75
1:B:361:TRP:HB3	1:B:427:LEU:HD12	1.69	0.75
1:D:554:LEU:HD22	1:D:643:THR:HG23	1.69	0.74
1:D:461:VAL:HG22	1:D:464:MET:HE2	1.69	0.74
1:A:540:ARG:O	1:A:544:ILE:HG13	1.87	0.74
1:D:540:ARG:HG3	1:D:540:ARG:HH11	1.50	0.74
1:A:540:ARG:HH11	1:A:540:ARG:CG	2.01	0.73
1:B:526:LYS:HB3	1:B:582:GLN:CG	2.17	0.73
1:A:449:LYS:HD2	1:A:497:GLU:HB2	1.70	0.73
1:B:540:ARG:HH11	1:B:540:ARG:CG	2.02	0.73
1:B:503:ASP:O	1:B:506:ASP:HB2	1.88	0.72
1:B:540:ARG:O	1:B:544:ILE:HG13	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:PRO:HG3	1:B:621:ILE:HD13	1.70	0.72
1:D:575:PRO:HG3	1:D:621:ILE:HD13	1.71	0.72
1:B:670:ARG:CB	1:B:670:ARG:HH11	2.03	0.72
1:A:503:ASP:O	1:A:506:ASP:HB2	1.90	0.72
1:D:461:VAL:HG22	1:D:464:MET:CE	2.19	0.72
1:B:636:ASP:HB3	1:B:638:THR:HG23	1.70	0.71
1:D:335:LYS:HG3	1:D:336:LYS:N	2.03	0.71
1:D:597:ALA:CB	1:D:606:TYR:CE2	2.66	0.71
1:B:334:SER:HB2	1:D:349:PHE:O	1.89	0.71
1:A:357:LEU:HD12	1:A:389:MET:HE2	1.71	0.71
1:A:357:LEU:HD13	1:A:389:MET:HE1	1.73	0.70
1:B:441:LYS:O	1:B:444:ARG:NH2	2.24	0.70
1:B:554:LEU:HD22	1:B:643:THR:HG23	1.72	0.70
1:D:470:ASN:CB	1:D:521:LEU:HD21	2.20	0.70
1:A:361:TRP:HB3	1:A:427:LEU:HD12	1.73	0.70
1:D:361:TRP:HB3	1:D:427:LEU:CD1	2.22	0.70
1:D:516:PHE:O	1:D:517:GLU:CD	2.35	0.70
1:A:335:LYS:HG3	1:A:336:LYS:N	2.05	0.70
1:A:357:LEU:HD12	1:A:389:MET:CE	2.21	0.70
1:D:449:LYS:HD2	1:D:497:GLU:CB	2.22	0.69
1:A:530:LEU:C	1:A:532:GLU:H	2.00	0.69
1:A:532:GLU:HG2	1:A:540:ARG:HE	1.55	0.69
1:D:361:TRP:HB3	1:D:427:LEU:HD12	1.75	0.69
1:A:357:LEU:CD1	1:A:389:MET:HE1	2.22	0.69
1:D:517:GLU:OE2	1:D:517:GLU:HA	1.92	0.68
1:D:529:GLU:OE2	1:D:530:LEU:HG	1.93	0.68
1:D:530:LEU:C	1:D:532:GLU:H	1.98	0.68
1:B:274:LYS:HG2	1:B:275:PRO:HD2	1.76	0.68
1:B:636:ASP:HB2	1:B:639:VAL:CG2	2.20	0.68
1:B:516:PHE:O	1:B:517:GLU:CD	2.37	0.67
1:B:389:MET:HE3	1:B:389:MET:HA	1.77	0.67
1:D:293:TYR:CG	1:D:303:PRO:HG3	2.29	0.67
1:D:670:ARG:CB	1:D:670:ARG:HH11	2.07	0.67
1:B:361:TRP:HB3	1:B:427:LEU:CD1	2.25	0.67
1:A:334:SER:HB2	1:B:349:PHE:O	1.95	0.67
1:D:378:LEU:HD22	1:D:382:MET:HG3	1.77	0.67
1:B:461:VAL:HG22	1:B:464:MET:HE2	1.77	0.66
1:D:455:THR:OG1	1:D:463:ARG:NH2	2.28	0.66
1:D:667:ARG:HG2	1:D:667:ARG:HH11	1.60	0.66
1:A:357:LEU:CD1	1:A:389:MET:CE	2.74	0.66
1:D:392:ILE:O	1:D:396:ILE:HG12	1.94	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ILE:HG12	1:B:359:PRO:HD2	1.78	0.65
1:A:554:LEU:HD22	1:A:643:THR:HG23	1.78	0.65
1:A:607:MET:SD	1:A:607:MET:C	2.79	0.65
1:B:426:LYS:HD3	1:B:505:ILE:HD12	1.77	0.65
1:B:449:LYS:HD2	1:B:497:GLU:HB2	1.78	0.65
1:B:378:LEU:HD22	1:B:382:MET:HG3	1.79	0.65
1:B:392:ILE:O	1:B:396:ILE:HG12	1.96	0.65
1:D:501:LEU:HB3	1:D:506:ASP:CB	2.26	0.65
1:A:636:ASP:HB2	1:A:639:VAL:CG2	2.24	0.65
1:D:540:ARG:O	1:D:544:ILE:HG13	1.96	0.65
1:A:575:PRO:HG3	1:A:621:ILE:HD13	1.79	0.64
1:A:361:TRP:HB3	1:A:427:LEU:HD13	1.78	0.64
1:B:594:LYS:HB2	1:B:606:TYR:OH	1.97	0.64
1:A:536:GLU:HB3	1:A:540:ARG:NH1	2.12	0.64
1:D:426:LYS:HD3	1:D:505:ILE:CD1	2.26	0.64
1:A:532:GLU:O	1:A:536:GLU:HB2	1.96	0.64
1:A:358:ILE:HG12	1:A:359:PRO:HD2	1.80	0.64
1:B:536:GLU:HB3	1:B:540:ARG:NH1	2.13	0.63
1:A:652:LEU:HD21	1:A:658:LEU:HD22	1.80	0.63
1:D:460:TYR:C	1:D:460:TYR:CD2	2.77	0.63
1:B:652:LEU:HD21	1:B:658:LEU:HD22	1.81	0.63
1:D:477:GLU:CD	1:D:591:ARG:HD3	2.24	0.63
1:A:350:ILE:HG22	1:A:351:THR:HG22	1.80	0.62
1:D:636:ASP:HB2	1:D:639:VAL:CG2	2.26	0.62
1:B:461:VAL:HA	1:B:464:MET:HE2	1.81	0.62
1:A:517:GLU:HA	1:A:517:GLU:OE2	2.00	0.62
1:B:455:THR:OG1	1:B:463:ARG:NH2	2.25	0.62
1:B:452:ASP:OD1	1:B:452:ASP:C	2.43	0.62
1:A:333:GLU:O	1:A:334:SER:C	2.42	0.62
1:D:516:PHE:O	1:D:517:GLU:OE2	2.18	0.62
1:B:670:ARG:HH11	1:B:670:ARG:CG	2.14	0.61
1:D:540:ARG:HH11	1:D:540:ARG:CG	2.14	0.61
1:D:452:ASP:OD1	1:D:452:ASP:C	2.44	0.61
1:A:455:THR:OG1	1:A:463:ARG:NH2	2.26	0.61
1:B:335:LYS:HG3	1:B:336:LYS:N	2.13	0.61
1:D:477:GLU:OE1	1:D:591:ARG:HD3	2.01	0.61
1:A:376:LEU:HD13	1:D:333:GLU:HG3	1.82	0.60
1:A:330:ASP:O	1:A:334:SER:HB3	2.02	0.60
1:B:516:PHE:O	1:B:517:GLU:OE2	2.19	0.60
1:B:382:MET:O	1:B:385:GLN:HG2	2.01	0.60
1:B:529:GLU:HG3	1:B:530:LEU:HG	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:331:LEU:O	1:B:332:PHE:O	2.20	0.60
1:B:517:GLU:OE2	1:B:517:GLU:CA	2.49	0.60
1:A:274:LYS:HG2	1:A:275:PRO:HD2	1.82	0.60
1:A:307:LYS:HG3	1:A:403:ALA:HB2	1.84	0.60
1:A:392:ILE:O	1:A:396:ILE:HG12	2.02	0.60
1:B:667:ARG:HG2	1:B:667:ARG:HH11	1.66	0.59
1:A:426:LYS:HE2	1:A:506:ASP:OD1	2.01	0.59
1:D:662:THR:O	1:D:663:SER:C	2.44	0.59
1:A:342:LYS:HB2	1:A:368:VAL:HG12	1.84	0.59
1:B:531:GLU:HB2	1:B:534:ASP:OD1	2.02	0.59
1:B:636:ASP:CB	1:B:639:VAL:HG23	2.25	0.59
1:B:307:LYS:HG3	1:B:403:ALA:HB2	1.85	0.59
1:B:531:GLU:O	1:B:534:ASP:N	2.31	0.59
1:D:672:ILE:HG22	1:D:673:SER:N	2.18	0.59
1:B:333:GLU:HG3	1:D:376:LEU:HD13	1.85	0.58
1:D:331:LEU:O	1:D:332:PHE:O	2.21	0.58
1:B:670:ARG:HH11	1:B:670:ARG:HB2	1.67	0.58
1:B:438:ALA:O	1:B:441:LYS:HB2	2.04	0.58
1:A:461:VAL:HG22	1:A:464:MET:HE2	1.86	0.58
1:D:342:LYS:HB2	1:D:368:VAL:HG12	1.85	0.57
1:A:531:GLU:HA	1:A:537:LYS:HD3	1.86	0.57
1:A:670:ARG:CB	1:A:670:ARG:HH11	2.17	0.57
1:B:286:GLN:O	1:B:288:GLU:N	2.36	0.57
1:D:597:ALA:HA	1:D:603:MET:HG3	1.86	0.57
1:B:521:LEU:N	1:B:521:LEU:HD23	2.20	0.57
1:A:378:LEU:HD22	1:A:382:MET:HG3	1.87	0.57
1:A:501:LEU:HB3	1:A:506:ASP:HB3	1.87	0.57
1:A:516:PHE:O	1:A:517:GLU:OE2	2.22	0.57
1:A:532:GLU:CG	1:A:540:ARG:HE	2.16	0.57
1:D:521:LEU:HD23	1:D:521:LEU:N	2.19	0.57
1:D:644:LYS:HG3	1:D:667:ARG:NH2	2.20	0.57
1:D:670:ARG:HH11	1:D:670:ARG:HB2	1.69	0.57
1:B:629:VAL:C	1:B:631:GLU:H	2.11	0.56
1:D:636:ASP:CB	1:D:639:VAL:HG23	2.30	0.56
1:D:670:ARG:HH11	1:D:670:ARG:CG	2.18	0.56
1:B:524:ILE:HD11	1:B:586:SER:HB2	1.86	0.56
1:D:600:ASP:O	1:D:603:MET:HB2	2.05	0.56
1:D:350:ILE:HG22	1:D:351:THR:HG22	1.86	0.56
1:B:426:LYS:CB	1:B:505:ILE:HD12	2.36	0.56
1:B:470:ASN:CB	1:B:521:LEU:HD21	2.33	0.56
1:D:296:ILE:HD11	1:D:342:LYS:HE2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ARG:HD3	1:B:513:LEU:HA	1.88	0.56
1:B:315:LEU:HD22	1:B:391:VAL:CG2	2.36	0.56
1:B:332:PHE:O	1:B:333:GLU:CB	2.33	0.56
1:A:330:ASP:OD2	1:A:334:SER:HB3	2.06	0.55
1:A:461:VAL:HG22	1:A:464:MET:CE	2.36	0.55
1:B:606:TYR:HD1	1:B:608:SER:H	1.53	0.55
1:D:476:GLY:HA3	1:D:482:VAL:HG23	1.87	0.55
1:A:452:ASP:C	1:A:452:ASP:OD1	2.48	0.55
1:A:629:VAL:C	1:A:631:GLU:H	2.13	0.55
1:A:411:SER:OG	1:A:412:GLU:N	2.39	0.55
1:B:461:VAL:HG22	1:B:464:MET:CE	2.37	0.55
1:D:526:LYS:CB	1:D:582:GLN:HG2	2.35	0.55
1:B:430:HIS:HD2	1:B:431:GLU:OE1	1.90	0.55
1:D:286:GLN:O	1:D:287:GLU:HB2	2.07	0.55
1:D:432:ASP:O	1:D:436:ARG:HB2	2.07	0.55
1:D:513:LEU:HD22	1:D:515:GLU:O	2.07	0.55
1:D:529:GLU:HG3	1:D:530:LEU:HB2	1.88	0.55
1:D:652:LEU:HD21	1:D:658:LEU:HD22	1.89	0.55
1:D:293:TYR:CD2	1:D:303:PRO:HG3	2.41	0.55
1:A:516:PHE:O	1:A:517:GLU:CD	2.50	0.55
1:D:308:HIS:CD2	1:D:320:ILE:HG12	2.42	0.55
1:D:307:LYS:HG3	1:D:403:ALA:HB2	1.89	0.55
1:D:395:ASN:O	1:D:396:ILE:C	2.45	0.55
1:D:472:TYR:HH	1:D:529:GLU:CD	2.13	0.55
1:D:491:LEU:HD12	1:D:496:PHE:HB2	1.89	0.55
1:B:399:LYS:O	1:B:402:GLU:HB3	2.06	0.54
1:D:507:GLU:CD	1:D:589:MET:HE2	2.32	0.54
1:B:350:ILE:HG22	1:B:351:THR:HG22	1.87	0.54
1:A:285:THR:C	1:A:286:GLN:O	2.48	0.54
1:A:667:ARG:HH11	1:A:667:ARG:HG2	1.72	0.54
1:A:636:ASP:CB	1:A:639:VAL:HG23	2.29	0.54
1:D:524:ILE:HD11	1:D:586:SER:CB	2.26	0.54
1:D:406:GLU:O	1:D:409:GLU:HB2	2.07	0.54
1:D:471:ILE:HB	1:D:520:THR:HG22	1.90	0.54
1:D:296:ILE:O	1:D:296:ILE:CG2	2.56	0.53
1:B:661:PRO:HG2	1:B:662:THR:H	1.73	0.53
1:B:408:ALA:HA	1:B:414:PHE:CD2	2.44	0.53
1:A:602:SER:OG	1:A:602:SER:CA	2.54	0.53
1:B:285:THR:OG1	1:B:286:GLN:O	2.19	0.53
1:D:629:VAL:C	1:D:631:GLU:H	2.15	0.53
1:B:532:GLU:CB	1:B:536:GLU:HB2	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:THR:O	1:A:663:SER:C	2.52	0.53
1:B:501:LEU:HB3	1:B:506:ASP:HB3	1.90	0.53
1:B:522:VAL:CG1	1:B:524:ILE:HG12	2.38	0.53
1:B:334:SER:H	1:D:350:ILE:HD12	1.73	0.52
1:B:532:GLU:HB2	1:B:536:GLU:HB2	1.91	0.52
1:B:530:LEU:C	1:B:531:GLU:HG3	2.35	0.52
1:A:349:PHE:O	1:D:334:SER:HB2	2.08	0.52
1:B:522:VAL:HG11	1:B:524:ILE:HG12	1.90	0.52
1:A:651:LEU:O	1:A:656:PHE:HB2	2.10	0.52
1:A:426:LYS:HD3	1:A:505:ILE:CD1	2.34	0.52
1:A:603:MET:HE3	1:A:605:SER:O	2.10	0.52
1:A:533:THR:O	1:A:535:GLU:N	2.42	0.52
1:A:661:PRO:HG2	1:A:662:THR:H	1.74	0.52
1:D:590:GLU:OE2	1:D:609:SER:OG	2.26	0.52
1:D:673:SER:O	1:D:676:LEU:N	2.41	0.52
1:D:562:VAL:HG12	1:D:563:GLU:N	2.24	0.52
1:A:670:ARG:HH11	1:A:670:ARG:HB2	1.74	0.52
1:B:651:LEU:O	1:B:656:PHE:HB2	2.10	0.52
1:D:414:PHE:O	1:D:415:GLU:C	2.52	0.52
1:D:452:ASP:OD1	1:D:453:GLU:N	2.43	0.51
1:A:408:ALA:HA	1:A:414:PHE:CD2	2.44	0.51
1:A:522:VAL:CG1	1:A:524:ILE:HG12	2.40	0.51
1:B:452:ASP:OD1	1:B:453:GLU:N	2.44	0.51
1:D:315:LEU:HD22	1:D:391:VAL:CG2	2.40	0.51
1:A:623:LYS:O	1:A:627:LYS:HG2	2.11	0.51
1:A:334:SER:HA	1:B:350:ILE:HA	1.93	0.51
1:B:383:LEU:HA	1:B:386:ASN:HD22	1.76	0.51
1:B:590:GLU:OE2	1:B:609:SER:HB3	2.10	0.51
1:B:440:ALA:HA	1:B:443:LEU:HD12	1.93	0.51
1:D:274:LYS:HG2	1:D:275:PRO:HD2	1.93	0.51
1:B:576:ALA:HA	1:B:614:GLU:O	2.10	0.51
1:D:536:GLU:HB3	1:D:540:ARG:NH1	2.25	0.51
1:A:383:LEU:HA	1:A:386:ASN:HD22	1.76	0.51
1:A:529:GLU:OE2	1:A:530:LEU:HD12	2.11	0.51
1:D:470:ASN:HB3	1:D:521:LEU:CD2	2.37	0.51
1:B:378:LEU:HD22	1:B:382:MET:CG	2.40	0.50
1:D:661:PRO:HG2	1:D:662:THR:H	1.76	0.50
1:D:308:HIS:CG	1:D:320:ILE:HG12	2.45	0.50
1:A:350:ILE:HA	1:D:334:SER:HA	1.94	0.50
1:D:435:ASN:O	1:D:436:ARG:C	2.52	0.50
1:D:515:GLU:HB3	1:D:519:LYS:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ILE:HD11	1:A:586:SER:HB2	1.93	0.50
1:D:426:LYS:CB	1:D:505:ILE:HD12	2.41	0.50
1:B:455:THR:HG1	1:B:463:ARG:HH22	1.54	0.50
1:A:293:TYR:CG	1:A:303:PRO:HG3	2.46	0.50
1:B:459:ASP:HB3	1:B:463:ARG:NH2	2.27	0.50
1:B:608:SER:O	1:B:609:SER:CB	2.59	0.50
1:D:357:LEU:HD12	1:D:389:MET:HE2	1.94	0.50
1:D:281:PRO:C	1:D:283:ASP:H	2.20	0.50
1:D:505:ILE:HG13	1:D:506:ASP:N	2.27	0.49
1:A:520:THR:C	1:A:521:LEU:HD23	2.38	0.49
1:A:522:VAL:HG11	1:A:524:ILE:HG12	1.93	0.49
1:B:334:SER:CB	1:D:349:PHE:O	2.60	0.49
1:B:474:ILE:HG12	1:B:482:VAL:HG22	1.92	0.49
1:D:665:ALA:O	1:D:666:SER:C	2.56	0.49
1:A:621:ILE:HD12	1:A:621:ILE:H	1.77	0.49
1:B:608:SER:O	1:B:609:SER:HB3	2.11	0.49
1:D:460:TYR:CE1	1:D:497:GLU:HB3	2.46	0.49
1:A:648:GLU:HA	1:A:651:LEU:HD12	1.95	0.49
1:B:644:LYS:HG3	1:B:667:ARG:NH2	2.28	0.49
1:D:333:GLU:O	1:D:334:SER:C	2.55	0.49
1:B:422:SER:O	1:B:425:ILE:HB	2.12	0.49
1:B:662:THR:O	1:B:663:SER:C	2.56	0.49
1:D:284:ILE:HG22	1:D:285:THR:O	2.12	0.49
1:B:284:ILE:HG22	1:B:285:THR:O	2.13	0.48
1:B:426:LYS:HD3	1:B:505:ILE:CD1	2.43	0.48
1:B:281:PRO:C	1:B:283:ASP:H	2.21	0.48
1:B:648:GLU:HA	1:B:651:LEU:HD12	1.95	0.48
1:D:516:PHE:O	1:D:517:GLU:OE1	2.31	0.48
1:D:651:LEU:O	1:D:656:PHE:N	2.46	0.48
1:B:477:GLU:OE2	1:B:591:ARG:HD3	2.12	0.48
1:D:522:VAL:HG11	1:D:524:ILE:HG12	1.95	0.48
1:D:474:ILE:HG12	1:D:482:VAL:HG22	1.95	0.48
1:D:533:THR:HB	1:D:536:GLU:HG2	1.93	0.48
1:A:562:VAL:HG12	1:A:563:GLU:N	2.28	0.48
1:D:461:VAL:CG2	1:D:464:MET:HE2	2.43	0.48
1:D:623:LYS:O	1:D:627:LYS:HG2	2.13	0.48
1:D:361:TRP:HB3	1:D:427:LEU:HD13	1.94	0.48
1:B:523:ASP:O	1:B:579:ARG:NH1	2.47	0.48
1:D:358:ILE:HG12	1:D:359:PRO:CD	2.39	0.48
1:B:644:LYS:HZ2	1:B:667:ARG:NH1	2.12	0.47
1:A:562:VAL:HG12	1:A:564:LYS:N	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLU:O	1:B:334:SER:C	2.57	0.47
1:B:426:LYS:HB2	1:B:505:ILE:HD12	1.96	0.47
1:D:315:LEU:HD22	1:D:391:VAL:HG21	1.96	0.47
1:D:378:LEU:O	1:D:379:SER:C	2.57	0.47
1:B:426:LYS:CD	1:B:505:ILE:HD12	2.44	0.47
1:A:530:LEU:C	1:A:532:GLU:N	2.68	0.47
1:D:505:ILE:HG13	1:D:506:ASP:H	1.79	0.47
1:A:423:LYS:H	1:A:423:LYS:HG3	1.37	0.47
1:D:423:LYS:H	1:D:423:LYS:HG3	1.41	0.47
1:B:406:GLU:O	1:B:406:GLU:HG3	2.13	0.47
1:B:494:LYS:NZ	1:B:530:LEU:CD1	2.69	0.47
1:A:452:ASP:OD1	1:A:453:GLU:N	2.48	0.47
1:A:558:LEU:HD13	1:A:562:VAL:HG21	1.95	0.47
1:D:576:ALA:HA	1:D:614:GLU:O	2.15	0.47
1:A:432:ASP:O	1:A:436:ARG:HB2	2.15	0.47
1:D:524:ILE:HD12	1:D:587:ALA:HB3	1.96	0.47
1:B:536:GLU:HB3	1:B:540:ARG:CZ	2.44	0.46
1:D:277:TRP:HA	1:D:320:ILE:HD11	1.96	0.46
1:A:470:ASN:CB	1:A:521:LEU:HD21	2.37	0.46
1:D:505:ILE:O	1:D:506:ASP:C	2.55	0.46
1:A:286:GLN:O	1:A:287:GLU:HB2	2.14	0.46
1:B:315:LEU:HD22	1:B:391:VAL:HG21	1.97	0.46
1:A:670:ARG:HH11	1:A:670:ARG:CG	2.28	0.46
1:A:460:TYR:CD2	1:A:460:TYR:C	2.93	0.46
1:B:275:PRO:HG2	1:B:278:THR:HG23	1.97	0.46
1:B:334:SER:HA	1:D:350:ILE:HA	1.98	0.46
1:B:411:SER:OG	1:B:412:GLU:N	2.49	0.46
1:B:532:GLU:HG2	1:B:540:ARG:HH21	1.80	0.46
1:B:661:PRO:O	1:B:662:THR:C	2.58	0.46
1:D:670:ARG:O	1:D:674:LEU:HD12	2.14	0.46
1:B:296:ILE:HA	1:B:296:ILE:HD13	1.56	0.45
1:D:651:LEU:O	1:D:656:PHE:HB2	2.16	0.45
1:B:357:LEU:HD12	1:B:389:MET:CE	2.46	0.45
1:D:496:PHE:CZ	1:D:530:LEU:HD12	2.52	0.45
1:B:285:THR:C	1:B:286:GLN:O	2.57	0.45
1:B:501:LEU:HD13	1:B:506:ASP:HB3	1.97	0.45
1:A:531:GLU:O	1:A:537:LYS:HB2	2.17	0.45
1:B:658:LEU:H	1:B:658:LEU:HD23	1.82	0.45
1:B:516:PHE:O	1:B:517:GLU:OE1	2.34	0.45
1:A:541:GLU:CD	1:A:541:GLU:H	2.23	0.45
1:A:284:ILE:HG22	1:A:285:THR:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ILE:HG12	1:A:482:VAL:HG22	1.99	0.45
1:A:507:GLU:O	1:A:511:THR:HG23	2.17	0.45
1:A:562:VAL:HG12	1:A:564:LYS:H	1.81	0.45
1:D:541:GLU:CD	1:D:541:GLU:H	2.24	0.45
1:D:578:ILE:CG2	1:D:611:LYS:HG3	2.47	0.45
1:A:644:LYS:HG3	1:A:667:ARG:NH2	2.31	0.45
1:B:670:ARG:CG	1:B:670:ARG:NH1	2.79	0.45
1:A:315:LEU:HD22	1:A:391:VAL:CG2	2.47	0.45
1:A:426:LYS:CD	1:A:505:ILE:HD12	2.38	0.45
1:A:276:LEU:HD12	1:A:279:ARG:NH1	2.31	0.44
1:B:651:LEU:O	1:B:656:PHE:N	2.50	0.44
1:D:472:TYR:OH	1:D:529:GLU:OE1	2.31	0.44
1:A:531:GLU:HB2	1:A:534:ASP:OD1	2.15	0.44
1:B:383:LEU:O	1:B:387:LYS:HG2	2.17	0.44
1:B:447:SER:OG	1:B:450:SER:N	2.49	0.44
1:B:471:ILE:HB	1:B:520:THR:HG22	1.98	0.44
1:D:399:LYS:O	1:D:402:GLU:HB3	2.17	0.44
1:D:543:GLU:O	1:D:546:GLU:N	2.50	0.44
1:B:396:ILE:HG22	1:B:400:LEU:HD12	1.99	0.44
1:D:383:LEU:O	1:D:384:GLN:C	2.59	0.44
1:D:426:LYS:CE	1:D:506:ASP:OD1	2.59	0.44
1:A:357:LEU:HD13	1:A:389:MET:CE	2.43	0.44
1:B:530:LEU:HB3	1:B:531:GLU:H	1.48	0.44
1:D:285:THR:C	1:D:286:GLN:O	2.57	0.44
1:D:463:ARG:HD2	1:D:497:GLU:OE2	2.18	0.44
1:D:661:PRO:O	1:D:662:THR:C	2.60	0.44
1:D:667:ARG:HG2	1:D:667:ARG:NH1	2.30	0.44
1:A:315:LEU:HD22	1:A:391:VAL:HG22	2.00	0.44
1:D:472:TYR:OH	1:D:529:GLU:CD	2.61	0.44
1:D:658:LEU:HD23	1:D:658:LEU:H	1.83	0.43
1:B:532:GLU:HG2	1:B:540:ARG:NH2	2.33	0.43
1:B:621:ILE:HD12	1:B:621:ILE:H	1.83	0.43
1:B:665:ALA:O	1:B:666:SER:C	2.61	0.43
1:B:459:ASP:O	1:B:460:TYR:C	2.61	0.43
1:A:339:ASN:HD21	1:A:341:ILE:HB	1.83	0.43
1:A:466:GLU:OE2	1:A:466:GLU:HA	2.19	0.43
1:A:532:GLU:OE2	1:A:537:LYS:HD2	2.18	0.43
1:D:461:VAL:HA	1:D:464:MET:CE	2.43	0.43
1:B:342:LYS:HB2	1:B:368:VAL:HG12	2.01	0.43
1:A:280:ASN:O	1:A:283:ASP:HB3	2.18	0.43
1:A:661:PRO:O	1:A:662:THR:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:398:LYS:O	1:D:399:LYS:C	2.60	0.43
1:D:540:ARG:HG2	1:D:569:TYR:CE1	2.53	0.43
1:A:432:ASP:OD1	1:A:432:ASP:C	2.62	0.43
1:B:460:TYR:CE1	1:B:497:GLU:HB3	2.52	0.43
1:A:396:ILE:HG12	1:A:396:ILE:H	1.68	0.43
1:D:296:ILE:HA	1:D:296:ILE:HD13	1.74	0.43
1:B:357:LEU:CD1	1:B:389:MET:HE1	2.49	0.43
1:D:500:PHE:C	1:D:501:LEU:HD23	2.44	0.43
1:D:501:LEU:CB	1:D:506:ASP:HB3	2.45	0.43
1:A:331:LEU:O	1:A:332:PHE:O	2.37	0.42
1:B:531:GLU:O	1:B:534:ASP:HA	2.19	0.42
1:D:346:ARG:O	1:D:347:ARG:HB2	2.19	0.42
1:B:330:ASP:OD2	1:B:334:SER:HB3	2.19	0.42
1:D:616:SER:HA	1:D:617:PRO:HD3	1.82	0.42
1:D:644:LYS:HD2	1:D:667:ARG:HG3	2.01	0.42
1:B:330:ASP:O	1:B:334:SER:HB3	2.19	0.42
1:B:547:TYR:HD2	1:B:550:LEU:HD23	1.85	0.42
1:B:669:ASN:O	1:B:672:ILE:HB	2.19	0.42
1:D:661:PRO:CG	1:D:662:THR:H	2.32	0.42
1:B:286:GLN:O	1:B:287:GLU:HB2	2.19	0.42
1:B:308:HIS:CG	1:B:320:ILE:HG12	2.54	0.42
1:A:333:GLU:CG	1:B:376:LEU:HD13	2.42	0.42
1:A:644:LYS:HD2	1:A:667:ARG:HG3	2.01	0.42
1:B:423:LYS:H	1:B:423:LYS:HG3	1.55	0.42
1:B:494:LYS:HZ1	1:B:530:LEU:HD12	1.78	0.42
1:B:648:GLU:O	1:B:651:LEU:HB2	2.19	0.42
1:A:296:ILE:HA	1:A:296:ILE:HD13	1.62	0.42
1:D:335:LYS:HG2	1:D:337:LYS:HE3	2.02	0.42
1:A:414:PHE:O	1:A:415:GLU:C	2.60	0.42
1:B:533:THR:O	1:B:534:ASP:HB2	2.20	0.42
1:D:522:VAL:CG1	1:D:524:ILE:HG12	2.50	0.42
1:D:622:ILE:O	1:D:623:LYS:C	2.62	0.42
1:D:673:SER:O	1:D:677:ASN:HB2	2.19	0.42
1:B:302:ASP:HB3	1:B:303:PRO:CD	2.50	0.42
1:B:327:ALA:HA	1:B:328:PRO:HD2	1.90	0.42
1:B:644:LYS:HD2	1:B:667:ARG:CZ	2.50	0.42
1:B:432:ASP:OD1	1:B:432:ASP:C	2.62	0.42
1:B:465:PRO:HB2	1:B:467:HIS:CE1	2.55	0.42
1:A:461:VAL:HA	1:A:464:MET:HE2	2.01	0.41
1:A:526:LYS:HE2	1:A:612:THR:OG1	2.19	0.41
1:A:665:ALA:O	1:A:666:SER:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:ASN:O	1:B:673:SER:N	2.38	0.41
1:D:287:GLU:HA	1:D:290:ASN:HB2	2.00	0.41
1:D:548:GLU:O	1:D:551:THR:HB	2.20	0.41
1:D:632:GLY:C	1:D:634:ALA:H	2.28	0.41
1:A:471:ILE:HB	1:A:520:THR:HG22	2.02	0.41
1:B:629:VAL:C	1:B:631:GLU:N	2.77	0.41
1:D:335:LYS:CG	1:D:336:LYS:H	2.11	0.41
1:D:457:LEU:HA	1:D:457:LEU:HD23	1.75	0.41
1:D:466:GLU:HA	1:D:466:GLU:OE2	2.20	0.41
1:A:526:LYS:CB	1:A:582:GLN:HG2	2.41	0.41
1:A:531:GLU:C	1:A:533:THR:N	2.78	0.41
1:B:462:THR:C	1:B:464:MET:H	2.29	0.41
1:B:662:THR:HB	1:B:663:SER:H	1.54	0.41
1:D:558:LEU:HD13	1:D:562:VAL:HG21	2.03	0.41
1:B:605:SER:C	1:B:606:TYR:CD2	2.99	0.41
1:B:444:ARG:HG2	1:B:454:LEU:HB3	2.03	0.41
1:B:532:GLU:CG	1:B:540:ARG:HH21	2.33	0.41
1:B:670:ARG:HB2	1:B:670:ARG:NH1	2.35	0.41
1:D:467:HIS:O	1:D:530:LEU:HD11	2.20	0.41
1:D:536:GLU:HB3	1:D:540:ARG:CZ	2.51	0.41
1:A:548:GLU:O	1:A:551:THR:HB	2.20	0.41
1:B:460:TYR:C	1:B:460:TYR:CD2	2.98	0.41
1:D:430:HIS:HD2	1:D:431:GLU:OE1	2.04	0.41
1:A:281:PRO:C	1:A:283:ASP:H	2.28	0.41
1:A:531:GLU:CB	1:A:534:ASP:CG	2.94	0.41
1:A:607:MET:SD	1:A:608:SER:N	2.94	0.41
1:A:661:PRO:CG	1:A:662:THR:H	2.33	0.41
1:B:440:ALA:HA	1:B:443:LEU:CD1	2.50	0.41
1:B:607:MET:HE2	1:B:607:MET:O	2.21	0.41
1:A:382:MET:O	1:A:385:GLN:HG2	2.20	0.41
1:A:389:MET:HA	1:A:389:MET:HE3	2.02	0.41
1:A:435:ASN:O	1:A:436:ARG:C	2.64	0.41
1:A:501:LEU:HB3	1:A:506:ASP:CB	2.51	0.41
1:B:597:ALA:O	1:B:600:ASP:O	2.39	0.41
1:D:507:GLU:O	1:D:508:TYR:C	2.64	0.41
1:A:576:ALA:HA	1:A:614:GLU:O	2.20	0.40
1:D:335:LYS:O	1:D:336:LYS:HB2	2.20	0.40
1:D:503:ASP:O	1:D:506:ASP:HB2	2.21	0.40
1:D:644:LYS:C	1:D:644:LYS:HD3	2.47	0.40
1:A:523:ASP:O	1:A:579:ARG:NH1	2.55	0.40
1:B:275:PRO:HG2	1:B:278:THR:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:ARG:HG2	1:D:454:LEU:HB3	2.03	0.40
1:D:562:VAL:HG12	1:D:564:LYS:H	1.86	0.40
1:A:334:SER:H	1:B:350:ILE:HD12	1.86	0.40
1:A:339:ASN:ND2	1:A:341:ILE:H	2.20	0.40
1:D:330:ASP:OD2	1:D:334:SER:HB3	2.22	0.40
1:D:447:SER:OG	1:D:450:SER:N	2.54	0.40
1:A:465:PRO:HB2	1:A:467:HIS:CE1	2.57	0.40
1:A:533:THR:OG1	1:A:536:GLU:HG2	2.21	0.40
1:A:536:GLU:HB3	1:A:540:ARG:CZ	2.51	0.40
1:B:466:GLU:OE2	1:B:466:GLU:HA	2.22	0.40
1:B:534:ASP:O	1:B:537:LYS:HB3	2.21	0.40
1:B:540:ARG:CG	1:B:540:ARG:NH1	2.70	0.40
1:B:623:LYS:O	1:B:627:LYS:HG2	2.21	0.40
1:B:562:VAL:HG12	1:B:563:GLU:N	2.37	0.40
1:D:396:ILE:HG12	1:D:396:ILE:H	1.60	0.40
1:D:539:GLU:H	1:D:539:GLU:HG2	1.67	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	403/405 (100%)	350 (87%)	40 (10%)	13 (3%)	3	18
1	B	403/405 (100%)	353 (88%)	39 (10%)	11 (3%)	4	22
1	D	403/405 (100%)	342 (85%)	49 (12%)	12 (3%)	3	19
All	All	1209/1215 (100%)	1045 (86%)	128 (11%)	36 (3%)	3	19

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	534	ASP
1	A	662	THR
1	B	332	PHE
1	B	336	LYS
1	B	531	GLU
1	B	609	SER
1	B	662	THR
1	D	332	PHE
1	D	530	LEU
1	D	531	GLU
1	D	662	THR
1	A	531	GLU
1	A	661	PRO
1	B	606	TYR
1	B	661	PRO
1	D	336	LYS
1	D	661	PRO
1	A	336	LYS
1	A	530	LEU
1	A	591	ARG
1	B	602	SER
1	D	603	MET
1	D	607	MET
1	A	602	SER
1	B	526	LYS
1	B	528	PHE
1	D	533	THR
1	D	630	ASP
1	A	335	LYS
1	A	526	LYS
1	A	528	PHE
1	D	528	PHE
1	D	676	LEU
1	B	660	GLU
1	A	660	GLU

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	366/368 (100%)	307 (84%)	59 (16%)	2	12
1	B	366/368 (100%)	301 (82%)	65 (18%)	2	10
1	D	366/368 (100%)	305 (83%)	61 (17%)	2	12
All	All	1098/1104 (100%)	913 (83%)	185 (17%)	2	11

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	287	GLU
1	A	294	LYS
1	A	296	ILE
1	A	306	VAL
1	A	307	LYS
1	A	312	GLU
1	A	331	LEU
1	A	332	PHE
1	A	335	LYS
1	A	336	LYS
1	A	342	LYS
1	A	345	VAL
1	A	347	ARG
1	A	351	THR
1	A	355	GLU
1	A	358	ILE
1	A	368	VAL
1	A	391	VAL
1	A	398	LYS
1	A	406	GLU
1	A	413	GLN
1	A	416	LYS
1	A	423	LYS
1	A	427	LEU
1	A	444	ARG
1	A	452	ASP
1	A	453	GLU
1	A	458	THR
1	A	466	GLU
1	A	477	GLU
1	A	482	VAL
1	A	494	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	505	ILE
1	A	513	LEU
1	A	517	GLU
1	A	521	LEU
1	A	522	VAL
1	A	526	LYS
1	A	527	ASP
1	A	530	LEU
1	A	531	GLU
1	A	540	ARG
1	A	548	GLU
1	A	564	LYS
1	A	594	LYS
1	A	596	GLN
1	A	601	SER
1	A	607	MET
1	A	611	LYS
1	A	615	ILE
1	A	638	THR
1	A	640	LYS
1	A	652	LEU
1	A	660	GLU
1	A	662	THR
1	A	663	SER
1	A	670	ARG
1	A	671	LEU
1	A	677	ASN
1	B	287	GLU
1	B	294	LYS
1	B	296	ILE
1	B	301	GLU
1	B	306	VAL
1	B	307	LYS
1	B	312	GLU
1	B	331	LEU
1	B	332	PHE
1	B	335	LYS
1	B	336	LYS
1	B	342	LYS
1	B	345	VAL
1	B	347	ARG
1	B	351	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	355	GLU
1	B	358	ILE
1	B	368	VAL
1	B	378	LEU
1	B	380	ARG
1	B	391	VAL
1	B	398	LYS
1	B	406	GLU
1	B	413	GLN
1	B	416	LYS
1	B	423	LYS
1	B	427	LEU
1	B	444	ARG
1	B	452	ASP
1	B	453	GLU
1	B	466	GLU
1	B	477	GLU
1	B	479	LEU
1	B	482	VAL
1	B	494	LYS
1	B	505	ILE
1	B	513	LEU
1	B	517	GLU
1	B	521	LEU
1	B	522	VAL
1	B	526	LYS
1	B	527	ASP
1	B	530	LEU
1	B	531	GLU
1	B	532	GLU
1	B	540	ARG
1	B	548	GLU
1	B	564	LYS
1	B	594	LYS
1	B	596	GLN
1	B	600	ASP
1	B	605	SER
1	B	606	TYR
1	B	607	MET
1	B	609	SER
1	B	611	LYS
1	B	615	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	638	THR
1	B	640	LYS
1	B	642	LEU
1	B	652	LEU
1	B	662	THR
1	B	663	SER
1	B	670	ARG
1	B	673	SER
1	D	287	GLU
1	D	294	LYS
1	D	296	ILE
1	D	306	VAL
1	D	307	LYS
1	D	331	LEU
1	D	332	PHE
1	D	333	GLU
1	D	336	LYS
1	D	342	LYS
1	D	345	VAL
1	D	347	ARG
1	D	351	THR
1	D	355	GLU
1	D	358	ILE
1	D	368	VAL
1	D	380	ARG
1	D	391	VAL
1	D	396	ILE
1	D	398	LYS
1	D	406	GLU
1	D	413	GLN
1	D	416	LYS
1	D	423	LYS
1	D	427	LEU
1	D	444	ARG
1	D	452	ASP
1	D	453	GLU
1	D	466	GLU
1	D	474	ILE
1	D	482	VAL
1	D	489	ASP
1	D	501	LEU
1	D	513	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	517	GLU
1	D	519	LYS
1	D	521	LEU
1	D	522	VAL
1	D	526	LYS
1	D	527	ASP
1	D	531	GLU
1	D	540	ARG
1	D	548	GLU
1	D	564	LYS
1	D	594	LYS
1	D	596	GLN
1	D	603	MET
1	D	606	TYR
1	D	609	SER
1	D	611	LYS
1	D	615	ILE
1	D	637	LYS
1	D	638	THR
1	D	640	LYS
1	D	642	LEU
1	D	652	LEU
1	D	662	THR
1	D	663	SER
1	D	670	ARG
1	D	672	ILE
1	D	677	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	290	ASN
1	A	339	ASN
1	A	385	GLN
1	A	386	ASN
1	A	413	GLN
1	A	424	ASN
1	A	430	HIS
1	A	470	ASN
1	A	596	GLN
1	B	290	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	339	ASN
1	B	385	GLN
1	B	386	ASN
1	B	413	GLN
1	B	446	ASN
1	D	286	GLN
1	D	290	ASN
1	D	339	ASN
1	D	385	GLN
1	D	386	ASN
1	D	395	ASN
1	D	413	GLN
1	D	424	ASN
1	D	596	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	405/405 (100%)	0.04	8 (1%) 65 41	49, 80, 140, 193	6 (1%)
1	B	405/405 (100%)	0.03	4 (0%) 79 59	47, 80, 148, 177	6 (1%)
1	D	405/405 (100%)	-0.01	6 (1%) 72 49	55, 79, 113, 153	6 (1%)
All	All	1215/1215 (100%)	0.02	18 (1%) 72 49	47, 80, 139, 193	18 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	606	TYR	3.9
1	D	607	MET	3.3
1	D	593	MET	2.9
1	D	286	GLN	2.7
1	B	384	GLN	2.6
1	B	607	MET	2.6
1	A	600	ASP	2.3
1	A	599	ARG	2.3
1	A	607	MET	2.3
1	B	533	THR	2.2
1	A	593	MET	2.2
1	B	585	TRP	2.2
1	A	287	GLU	2.2
1	A	601	SER	2.1
1	A	653	THR	2.1
1	D	536	GLU	2.1
1	D	604	SER	2.0
1	A	598	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.