Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2023 – 10:08 am GMT

PDB ID	:	2W01
Title	:	Crystal structure of the guanylyl cyclase Cya2
Authors	:	Rauch, A.; Leipelt, M.; Russwurm, M.; Steegborn, C.
Deposited on	:	2008-08-08
Resolution	:	2.31 Å(reported)

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

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

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

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

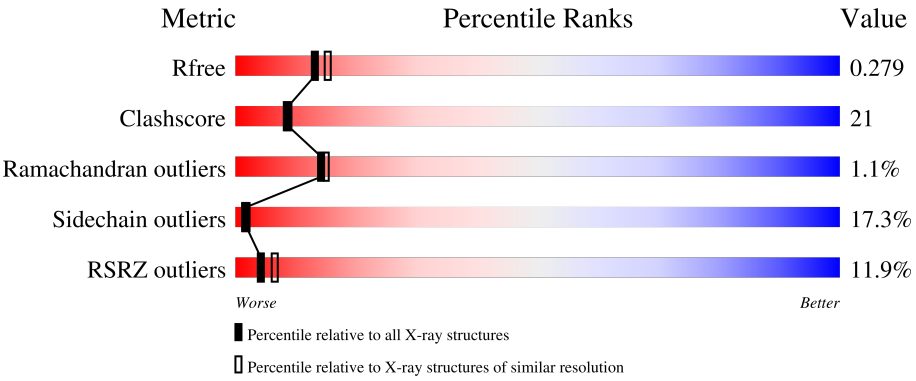
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.31 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.



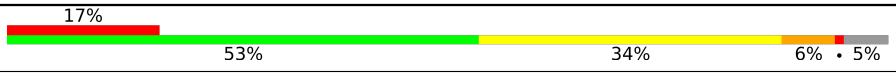
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	208	5% 64% 23% 10%
1	B	208	13% 59% 28% 7% 5%
1	C	208	9% 62% 29% 5%
1	D	208	10% 58% 29% 8%
1	E	208	14% 61% 29% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	208	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9379 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 ADENYLATE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1504	940	260	298	6			
1	B	197	Total	C	N	O	S	0	0	0
			1470	920	255	289	6			
1	C	200	Total	C	N	O	S	0	0	0
			1495	936	259	294	6			
1	D	199	Total	C	N	O	S	0	0	0
			1486	931	258	291	6			
1	E	199	Total	C	N	O	S	0	0	0
			1486	931	258	291	6			
1	F	197	Total	C	N	O	S	0	0	0
			1470	920	255	289	6			

- Molecule 2 is water.

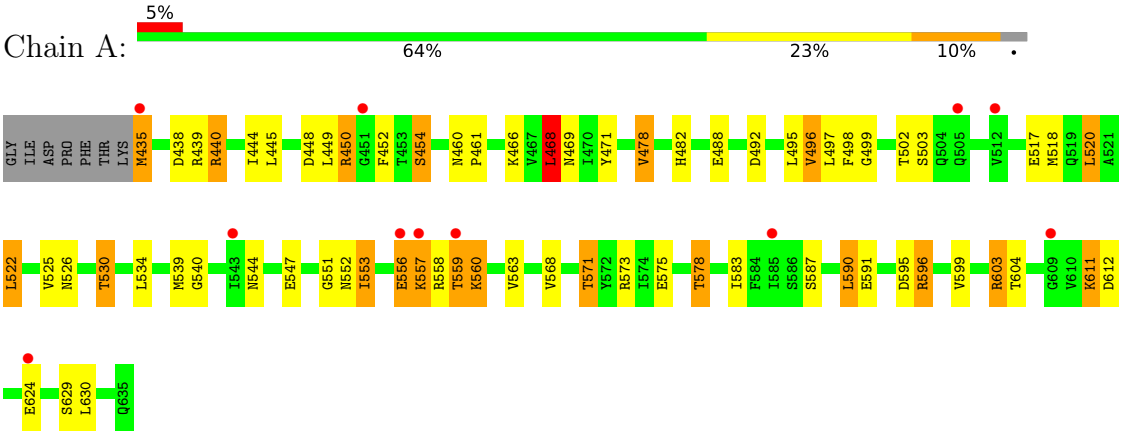
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	89	Total	O	0	0
			89	89		
2	C	84	Total	O	0	0
			84	84		
2	D	72	Total	O	0	0
			72	72		
2	E	66	Total	O	0	0
			66	66		
2	F	67	Total	O	0	0
			67	67		

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.

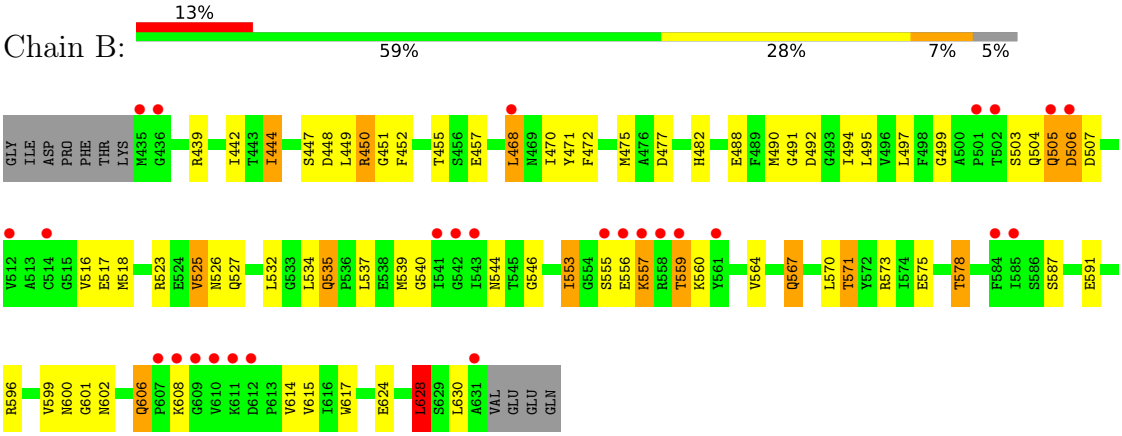
• Molecule 1: ADENYLATE CYCLASE

Chain A:



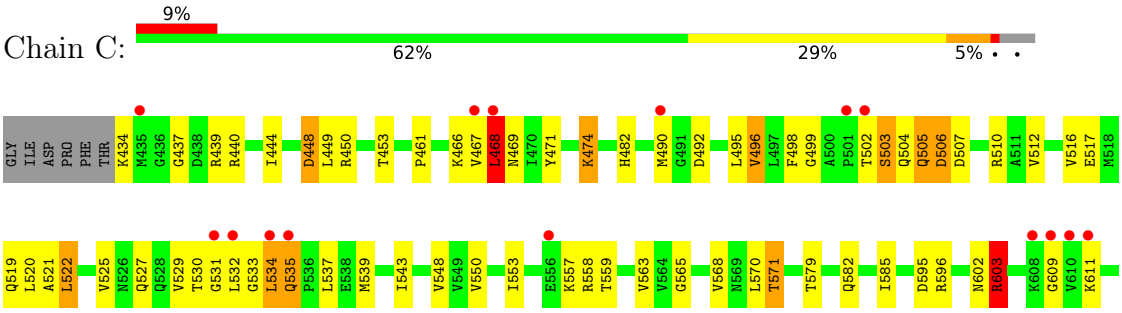
• Molecule 1: ADENYLATE CYCLASE

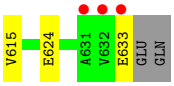
Chain B:



• Molecule 1: ADENYLATE CYCLASE

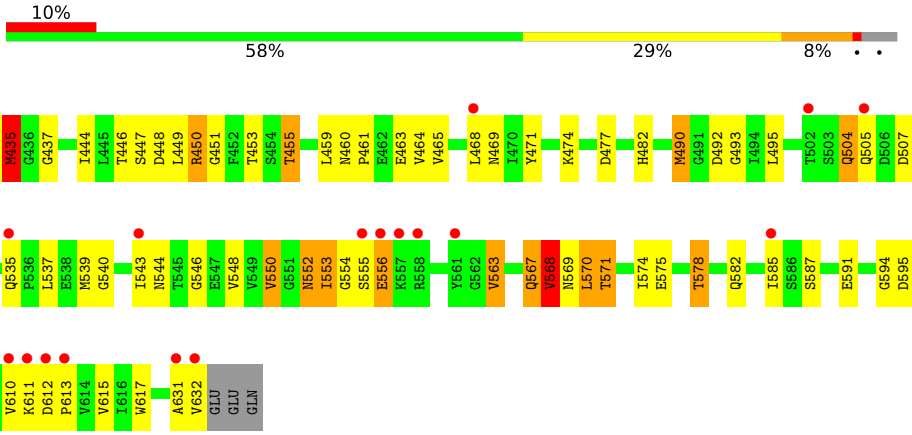
Chain C:

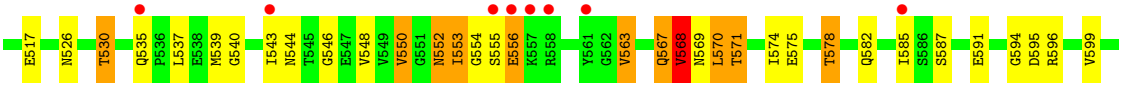


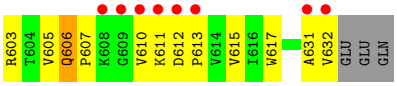


• Molecule 1: ADENYLATE CYCLASE

Chain D:

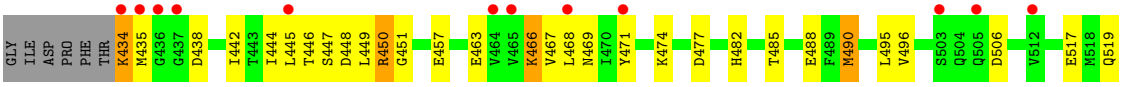


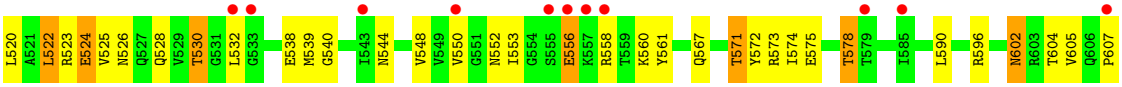


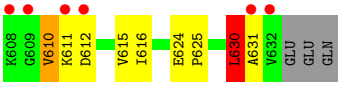


• Molecule 1: ADENYLATE CYCLASE

Chain E:

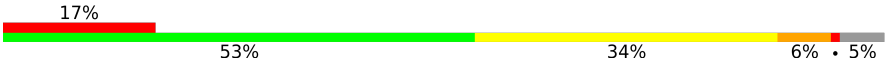


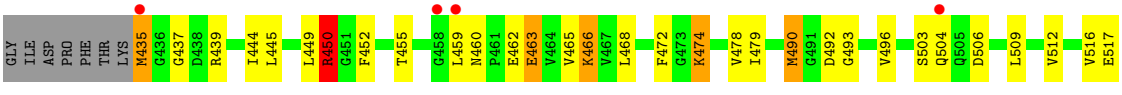


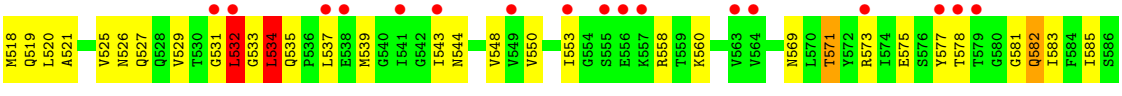


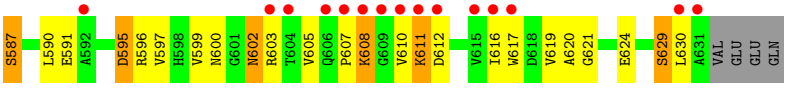
• Molecule 1: ADENYLATE CYCLASE

Chain F:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.45Å 84.09Å 115.33Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	19.94 – 2.31 19.94 – 2.31	Depositor EDS
% Data completeness (in resolution range)	97.0 (19.94-2.31) 97.0 (19.94-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.194 , 0.282 0.193 , 0.279	Depositor DCC
R_{free} test set	2597 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9379	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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

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	0.92	0/1525	0.96	5/2069 (0.2%)
1	B	0.85	0/1491	0.92	1/2023 (0.0%)
1	C	0.90	0/1516	1.02	4/2056 (0.2%)
1	D	0.89	1/1507 (0.1%)	0.97	4/2044 (0.2%)
1	E	1.05	7/1507 (0.5%)	0.87	1/2044 (0.0%)
1	F	0.77	1/1491 (0.1%)	0.85	2/2023 (0.1%)
All	All	0.90	9/9037 (0.1%)	0.93	17/12259 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	556	GLU	CD-OE1	13.90	1.41	1.25
1	E	556	GLU	CG-CD	11.79	1.69	1.51
1	E	556	GLU	CD-OE2	10.45	1.37	1.25
1	F	603	ARG	CZ-NH1	8.31	1.43	1.33
1	D	568	VAL	CB-CG1	-6.20	1.39	1.52
1	E	438	ASP	CG-OD2	5.90	1.39	1.25
1	E	434	LYS	CG-CD	5.24	1.70	1.52
1	E	434	LYS	N-CA	5.21	1.56	1.46
1	E	438	ASP	CG-OD1	5.18	1.37	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	510	ARG	NE-CZ-NH2	-9.60	115.50	120.30
1	F	603	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	D	510	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	C	448	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	520	LEU	CA-CB-CG	6.39	130.00	115.30
1	C	603	ARG	CB-CA-C	-6.04	98.32	110.40
1	F	534	LEU	CA-CB-CG	5.90	128.86	115.30
1	A	590	LEU	CB-CG-CD2	5.78	120.82	111.00
1	A	595	ASP	CB-CG-OD2	5.52	123.27	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	468	LEU	CB-CG-CD1	5.42	120.22	111.00
1	D	550	VAL	CB-CA-C	-5.19	101.54	111.40
1	D	594	GLY	C-N-CA	5.18	134.65	121.70
1	B	628	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	468	LEU	CA-CB-CG	5.12	127.09	115.30
1	E	630	LEU	CA-CB-CG	5.03	126.87	115.30
1	C	468	LEU	CB-CG-CD1	5.01	119.51	111.00
1	C	539	MET	CG-SD-CE	5.01	108.21	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1504	0	1500	59	0
1	B	1470	0	1471	75	0
1	C	1495	0	1499	48	0
1	D	1486	0	1493	61	0
1	E	1486	0	1493	59	0
1	F	1470	0	1471	82	0
2	A	90	0	0	3	0
2	B	89	0	0	7	0
2	C	84	0	0	6	0
2	D	72	0	0	8	0
2	E	66	0	0	2	0
2	F	67	0	0	13	0
All	All	9379	0	8927	366	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 21.

All (366) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:607:PRO:HD2	1:D:610:VAL:HG21	1.22	1.17
1:B:444:ILE:HG12	1:B:571:THR:HG21	1.20	1.11
1:B:540:GLY:HA3	1:B:578:THR:HG21	1.32	1.08
1:D:548:VAL:HG11	1:D:563:VAL:HG22	1.38	1.06
1:B:587:SER:O	1:B:591:GLU:HG2	1.59	1.03
1:E:552:ASN:ND2	1:E:561:TYR:HD1	1.58	0.99
1:B:471:TYR:OH	1:B:539:MET:HE3	1.62	0.97
1:B:475:MET:HE3	1:B:518:MET:HB3	1.51	0.93
1:E:540:GLY:HA3	1:E:578:THR:HG21	1.49	0.93
1:E:540:GLY:HA3	1:E:578:THR:CG2	1.98	0.92
1:B:540:GLY:HA3	1:B:578:THR:CG2	2.00	0.91
1:C:529:VAL:HG11	1:C:535:GLN:O	1.71	0.90
1:F:587:SER:O	1:F:591:GLU:HG2	1.71	0.89
1:B:444:ILE:HD12	1:B:495:LEU:HD11	1.56	0.88
1:A:603:ARG:HG2	1:A:603:ARG:HH21	1.37	0.88
1:B:444:ILE:HG12	1:B:571:THR:CG2	2.04	0.87
1:F:452:PHE:HB3	2:F:2005:HOH:O	1.75	0.85
1:F:492:ASP:HB3	2:F:2005:HOH:O	1.74	0.85
1:D:607:PRO:HD2	1:D:610:VAL:CG2	2.05	0.85
1:F:449:LEU:HB2	2:F:2005:HOH:O	1.78	0.84
1:F:611:LYS:HD2	1:F:611:LYS:H	1.42	0.84
1:C:529:VAL:CG1	1:C:535:GLN:O	2.25	0.83
1:F:460:ASN:OD1	1:F:463:GLU:HG3	1.78	0.83
1:F:492:ASP:CB	2:F:2005:HOH:O	2.27	0.83
1:E:471:TYR:OH	1:E:539:MET:CE	2.27	0.83
1:D:596:ARG:HG3	2:D:2047:HOH:O	1.78	0.82
1:C:469:ASN:HD21	1:D:553:ILE:HA	1.45	0.82
1:A:603:ARG:HH21	1:A:603:ARG:CG	1.91	0.82
1:C:603:ARG:HG3	1:C:603:ARG:HH11	1.44	0.82
1:B:452:PHE:HA	1:B:455:THR:CG2	2.09	0.82
1:C:579:THR:H	1:C:582:GLN:HE21	1.25	0.81
1:C:482:HIS:HE1	1:C:517:GLU:OE2	1.62	0.81
1:E:552:ASN:HD21	1:E:561:TYR:HD1	1.27	0.81
1:B:444:ILE:CD1	1:B:495:LEU:HD11	2.11	0.80
1:F:474:LYS:HD2	1:F:525:VAL:CG2	2.11	0.80
1:F:575:GLU:HG2	2:F:2006:HOH:O	1.81	0.80
1:F:578:THR:HB	1:F:582:GLN:HB2	1.63	0.80
1:A:553:ILE:HG23	1:B:472:PHE:HE2	1.48	0.79
1:B:540:GLY:CA	1:B:578:THR:HG21	2.12	0.79
1:E:573:ARG:HD2	1:E:607:PRO:HB2	1.63	0.78
1:B:451:GLY:O	1:B:455:THR:HG22	1.83	0.78
1:C:503:SER:HB2	2:C:2023:HOH:O	1.82	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LYS:HD2	1:A:612:ASP:H	1.47	0.78
1:B:526:ASN:HD21	1:B:537:LEU:H	1.31	0.78
1:C:469:ASN:ND2	1:D:554:GLY:H	1.82	0.78
1:A:553:ILE:HG23	1:B:472:PHE:CE2	2.19	0.77
1:F:532:LEU:HD23	2:F:2036:HOH:O	1.84	0.77
1:A:435:MET:CB	1:A:551:GLY:HA2	2.15	0.77
1:D:540:GLY:HA3	1:D:578:THR:HG21	1.66	0.76
1:B:599:VAL:HG11	1:B:617:TRP:HE3	1.49	0.76
1:C:505:GLN:HA	1:C:505:GLN:OE1	1.86	0.76
1:D:526:ASN:O	1:D:530:THR:HB	1.85	0.76
1:F:435:MET:N	2:F:2001:HOH:O	2.19	0.76
1:A:526:ASN:O	1:A:530:THR:HB	1.85	0.75
1:B:475:MET:HE1	1:B:539:MET:SD	2.27	0.75
1:F:474:LYS:HD2	1:F:525:VAL:HG23	1.68	0.75
1:F:478:VAL:HB	1:F:517:GLU:OE1	1.86	0.75
1:E:567:GLN:O	1:E:571:THR:HG22	1.86	0.75
1:A:435:MET:HB2	1:A:551:GLY:HA2	1.68	0.74
1:E:524:GLU:HA	1:E:524:GLU:OE1	1.87	0.74
1:E:490:MET:HE1	1:E:572:TYR:OH	1.88	0.74
1:D:471:TYR:OH	1:D:539:MET:CE	2.37	0.73
1:F:479:ILE:HG13	1:F:518:MET:HE3	1.69	0.73
1:C:474:LYS:HE2	1:C:521:ALA:HB1	1.70	0.73
1:E:552:ASN:ND2	1:E:561:TYR:CD1	2.50	0.73
1:B:471:TYR:OH	1:B:539:MET:CE	2.35	0.73
1:E:574:ILE:HD12	1:E:616:ILE:HG21	1.69	0.73
1:B:444:ILE:HD12	1:B:495:LEU:CD1	2.18	0.72
1:B:602:ASN:OD1	1:B:615:VAL:HG13	1.87	0.72
1:F:474:LYS:NZ	1:F:521:ALA:HB1	2.04	0.71
1:E:447:SER:HB2	1:E:539:MET:HE2	1.70	0.71
1:D:548:VAL:CG1	1:D:563:VAL:HG22	2.19	0.70
1:A:471:TYR:OH	1:A:539:MET:CE	2.40	0.70
1:E:469:ASN:HD21	1:F:553:ILE:HA	1.56	0.70
1:E:526:ASN:O	1:E:530:THR:HB	1.92	0.70
1:B:504:GLN:O	1:B:507:ASP:OD1	2.10	0.69
1:E:490:MET:CE	1:E:572:TYR:OH	2.39	0.69
1:F:596:ARG:HB2	2:F:2054:HOH:O	1.92	0.69
1:B:444:ILE:CG1	1:B:571:THR:HG21	2.13	0.69
1:B:447:SER:O	2:B:2007:HOH:O	2.11	0.69
1:B:599:VAL:HG12	1:B:601:GLY:H	1.56	0.69
1:A:482:HIS:HE1	1:A:517:GLU:OE1	1.76	0.68
1:A:482:HIS:HD2	2:A:2084:HOH:O	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:TYR:OH	1:D:539:MET:HE3	1.94	0.67
1:D:540:GLY:HA3	1:D:578:THR:CG2	2.23	0.67
1:A:603:ARG:HG2	1:A:603:ARG:NH2	2.10	0.67
1:D:612:ASP:HB3	1:D:613:PRO:HD2	1.77	0.67
1:E:474:LYS:HZ1	1:E:528:GLN:HE22	1.42	0.67
1:E:474:LYS:O	1:E:477:ASP:HB2	1.95	0.67
1:F:595:ASP:OD1	1:F:595:ASP:N	2.27	0.66
1:F:479:ILE:CG1	1:F:518:MET:CE	2.73	0.66
1:F:583:ILE:HB	1:F:619:VAL:HB	1.77	0.66
1:A:611:LYS:HD2	1:A:612:ASP:N	2.10	0.66
1:E:573:ARG:HH12	1:E:610:VAL:HB	1.61	0.66
1:B:596:ARG:HD2	1:B:624:GLU:O	1.95	0.66
1:B:475:MET:HE3	1:B:518:MET:CE	2.26	0.66
1:E:482:HIS:HE1	1:E:517:GLU:OE1	1.79	0.66
1:C:550:VAL:HG12	1:C:563:VAL:HG22	1.78	0.65
1:E:540:GLY:HA3	1:E:578:THR:HG23	1.78	0.65
1:F:466:LYS:HA	1:F:466:LYS:NZ	2.12	0.65
1:A:596:ARG:HG3	1:A:596:ARG:NH1	2.10	0.65
1:D:507:ASP:OD1	1:D:510:ARG:NH2	2.30	0.64
1:A:482:HIS:CE1	1:A:517:GLU:OE1	2.51	0.64
1:F:465:VAL:HG23	1:F:466:LYS:HE2	1.80	0.64
1:A:469:ASN:HD21	1:B:553:ILE:HA	1.61	0.63
1:F:630:LEU:HG	2:F:2060:HOH:O	1.99	0.63
1:E:444:ILE:HB	1:E:571:THR:HG21	1.79	0.63
1:A:596:ARG:HG3	1:A:596:ARG:HH11	1.62	0.63
1:A:596:ARG:HD2	1:A:624:GLU:O	1.98	0.63
1:C:579:THR:H	1:C:582:GLN:NE2	1.95	0.62
1:E:474:LYS:NZ	1:E:528:GLN:HE22	1.98	0.62
1:A:596:ARG:CD	1:A:624:GLU:O	2.47	0.62
1:B:457:GLU:OE2	2:B:2013:HOH:O	2.16	0.62
1:B:452:PHE:HA	1:B:455:THR:HG22	1.82	0.62
1:B:447:SER:HB2	1:B:539:MET:CE	2.30	0.61
1:C:434:LYS:HA	1:D:469:ASN:HD22	1.64	0.61
1:F:474:LYS:HZ2	1:F:521:ALA:HB1	1.64	0.61
1:F:519:GLN:OE1	1:F:581:GLY:HA2	2.01	0.61
1:B:608:LYS:H	1:B:608:LYS:HD2	1.66	0.61
1:D:575:GLU:O	1:D:578:THR:HB	2.01	0.61
1:B:475:MET:HE3	1:B:518:MET:HE2	1.84	0.60
1:D:546:GLY:HA3	1:D:567:GLN:HG3	1.84	0.60
1:D:607:PRO:O	1:D:610:VAL:HG22	2.02	0.60
1:A:471:TYR:OH	1:A:539:MET:HE3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:505:GLN:OE1	1:C:505:GLN:CA	2.49	0.60
1:A:444:ILE:HB	1:A:571:THR:HG21	1.84	0.60
1:F:479:ILE:HG13	1:F:518:MET:CE	2.31	0.59
1:F:529:VAL:O	1:F:534:LEU:HD13	2.01	0.59
1:F:590:LEU:HD23	1:F:590:LEU:O	2.03	0.59
1:A:575:GLU:O	1:A:578:THR:HB	2.03	0.59
1:A:556:GLU:HB3	1:A:557:LYS:HD2	1.83	0.59
1:C:502:THR:HG22	2:C:2019:HOH:O	2.01	0.59
1:F:600:ASN:ND2	1:F:620:ALA:HB2	2.18	0.59
1:B:447:SER:CB	1:B:539:MET:HE1	2.33	0.59
1:B:544:ASN:OD1	1:B:567:GLN:HG3	2.02	0.59
1:C:482:HIS:CE1	1:C:517:GLU:OE2	2.50	0.59
1:C:510:ARG:NH2	2:C:2029:HOH:O	2.35	0.58
1:F:519:GLN:HG3	1:F:583:ILE:HD11	1.85	0.58
1:C:596:ARG:HD2	1:C:624:GLU:O	2.04	0.58
1:D:474:LYS:HE3	2:D:2011:HOH:O	2.02	0.58
1:A:435:MET:HB3	1:A:551:GLY:HA2	1.85	0.58
1:B:546:GLY:HA3	1:B:567:GLN:HG2	1.84	0.58
1:F:520:LEU:HD21	1:F:629:SER:O	2.03	0.58
1:A:553:ILE:CG2	1:B:472:PHE:HE2	2.16	0.58
1:F:611:LYS:H	1:F:611:LYS:CD	2.13	0.58
1:E:611:LYS:HD3	1:E:612:ASP:OD2	2.04	0.58
1:F:435:MET:HB3	1:F:437:GLY:H	1.68	0.58
1:A:449:LEU:HD12	1:A:492:ASP:HB2	1.85	0.57
1:F:526:ASN:ND2	1:F:537:LEU:H	2.02	0.57
1:B:471:TYR:CZ	1:B:539:MET:HE3	2.38	0.57
1:D:546:GLY:HA3	1:D:567:GLN:CG	2.35	0.56
1:A:435:MET:N	1:A:552:ASN:H	2.04	0.56
1:E:540:GLY:CA	1:E:578:THR:HG21	2.31	0.56
1:E:596:ARG:HH21	1:E:625:PRO:HD3	1.70	0.56
1:C:548:VAL:HG21	1:C:563:VAL:HG13	1.86	0.56
1:D:444:ILE:HB	1:D:571:THR:HG21	1.87	0.56
1:A:471:TYR:CE1	1:A:539:MET:HE1	2.40	0.56
1:B:447:SER:HB2	1:B:539:MET:HE1	1.86	0.56
1:B:452:PHE:HA	1:B:455:THR:HG23	1.85	0.56
1:F:512:VAL:HG11	1:F:597:VAL:HG13	1.86	0.56
1:E:488:GLU:HG3	1:E:490:MET:HG2	1.88	0.56
1:A:611:LYS:HG3	2:A:2076:HOH:O	2.06	0.56
1:D:544:ASN:HB3	1:D:571:THR:HB	1.88	0.56
1:B:455:THR:HG21	2:B:2010:HOH:O	2.06	0.56
1:B:449:LEU:HD21	1:B:471:TYR:CE1	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:522:LEU:HD22	1:C:525:VAL:CG2	2.35	0.55
1:B:599:VAL:HG11	1:B:617:TRP:CE3	2.38	0.55
1:E:575:GLU:O	1:E:578:THR:HB	2.05	0.55
1:F:460:ASN:OD1	1:F:463:GLU:CG	2.54	0.55
1:D:471:TYR:OH	1:D:539:MET:HE1	2.05	0.55
1:A:522:LEU:HA	1:A:525:VAL:HG13	1.88	0.55
1:A:596:ARG:HH11	1:A:596:ARG:CG	2.19	0.55
1:C:522:LEU:HA	1:C:525:VAL:HG22	1.88	0.55
1:E:471:TYR:CE1	1:E:539:MET:CE	2.89	0.55
1:C:506:ASP:HA	2:C:2026:HOH:O	2.06	0.55
1:B:475:MET:CE	1:B:518:MET:HB3	2.31	0.55
1:F:577:TYR:CE1	1:F:605:VAL:HG11	2.42	0.55
1:F:569:ASN:HB3	1:F:573:ARG:HH21	1.72	0.54
1:B:490:MET:O	1:B:492:ASP:N	2.41	0.54
1:D:540:GLY:CA	1:D:578:THR:HG21	2.37	0.54
1:E:471:TYR:CE1	1:E:539:MET:HE1	2.43	0.54
1:B:526:ASN:ND2	1:B:537:LEU:H	2.03	0.54
1:C:527:GLN:O	1:C:531:GLY:N	2.39	0.54
1:D:570:LEU:O	1:D:574:ILE:HG13	2.07	0.54
1:D:451:GLY:O	1:D:455:THR:HG23	2.08	0.53
1:B:482:HIS:HE1	1:B:517:GLU:OE1	1.92	0.53
1:D:492:ASP:OD1	2:D:2018:HOH:O	2.18	0.53
1:A:587:SER:O	1:A:591:GLU:HG3	2.09	0.52
1:C:453:THR:HG21	1:D:569:ASN:ND2	2.24	0.52
1:F:607:PRO:HD2	1:F:610:VAL:HB	1.89	0.52
1:A:471:TYR:CE1	1:A:539:MET:CE	2.92	0.52
1:D:482:HIS:HD2	2:D:2066:HOH:O	1.92	0.52
1:D:482:HIS:HE1	1:D:517:GLU:OE1	1.92	0.52
1:E:552:ASN:HD22	1:E:561:TYR:HD1	1.48	0.52
1:A:553:ILE:CG2	1:B:472:PHE:CE2	2.90	0.51
1:B:505:GLN:NE2	1:B:506:ASP:H	2.07	0.51
1:C:505:GLN:OE1	1:C:505:GLN:O	2.28	0.51
1:E:605:VAL:HG13	1:E:607:PRO:HD3	1.91	0.51
1:A:471:TYR:HE1	1:A:539:MET:HE1	1.73	0.51
1:C:449:LEU:HD12	1:C:492:ASP:HB2	1.93	0.51
1:F:444:ILE:HB	1:F:571:THR:HG21	1.92	0.51
1:D:567:GLN:O	1:D:571:THR:HG22	2.11	0.51
1:E:602:ASN:HD22	1:E:602:ASN:H	1.58	0.51
1:B:535:GLN:HG3	2:B:2041:HOH:O	2.11	0.51
1:C:603:ARG:HG3	1:C:603:ARG:NH1	2.20	0.51
1:F:543:ILE:HB	1:F:585:ILE:HG22	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:490:MET:HE1	1:E:495:LEU:HB2	1.93	0.51
1:F:544:ASN:HB3	1:F:571:THR:HG22	1.93	0.51
1:B:504:GLN:NE2	2:B:2028:HOH:O	2.43	0.50
1:E:602:ASN:HD22	1:E:602:ASN:N	2.09	0.50
1:D:599:VAL:HG11	1:D:617:TRP:CE3	2.46	0.50
1:F:590:LEU:CD1	1:F:599:VAL:HG21	2.41	0.50
1:C:468:LEU:HD23	1:D:553:ILE:HD11	1.94	0.50
1:A:544:ASN:HB3	1:A:571:THR:HB	1.93	0.50
1:D:447:SER:CB	1:D:539:MET:HE2	2.40	0.50
1:E:490:MET:CE	1:E:495:LEU:HB2	2.41	0.50
1:F:462:GLU:O	1:F:465:VAL:HG22	2.12	0.50
1:D:568:VAL:O	1:D:571:THR:HG23	2.12	0.49
1:D:544:ASN:CB	1:D:571:THR:HB	2.42	0.49
1:F:608:LYS:HD3	2:F:2049:HOH:O	2.12	0.49
1:D:446:THR:HG22	1:D:495:LEU:HD13	1.94	0.49
1:D:555:SER:O	1:D:556:GLU:C	2.50	0.49
1:E:463:GLU:O	1:E:467:VAL:HG23	2.11	0.49
1:A:553:ILE:O	1:A:560:LYS:N	2.40	0.49
1:C:444:ILE:HB	1:C:571:THR:HG21	1.94	0.49
1:C:543:ILE:HB	1:C:585:ILE:HG22	1.94	0.49
1:A:540:GLY:HA3	1:A:578:THR:CG2	2.42	0.49
1:B:499:GLY:HA2	1:B:503:SER:HA	1.95	0.49
1:E:442:ILE:HG12	1:E:548:VAL:HG22	1.95	0.49
1:B:475:MET:HE3	1:B:518:MET:CB	2.33	0.48
1:B:535:GLN:CG	2:B:2041:HOH:O	2.61	0.48
1:F:587:SER:HA	1:F:617:TRP:HE1	1.78	0.48
1:B:475:MET:CE	1:B:518:MET:CE	2.91	0.48
1:B:517:GLU:HG3	1:B:628:LEU:HD21	1.95	0.48
1:E:471:TYR:HE1	1:E:539:MET:CE	2.27	0.48
1:D:449:LEU:HD21	1:D:471:TYR:CE1	2.49	0.48
1:F:512:VAL:HG11	1:F:597:VAL:CG1	2.43	0.48
1:F:449:LEU:HG	1:F:492:ASP:O	2.14	0.48
1:F:527:GLN:HB3	2:F:2034:HOH:O	2.12	0.48
1:A:596:ARG:HD3	1:A:624:GLU:O	2.13	0.48
1:F:439:ARG:HA	1:F:548:VAL:O	2.14	0.48
1:A:471:TYR:HE1	1:A:539:MET:CE	2.27	0.47
1:F:602:ASN:C	1:F:602:ASN:HD22	2.17	0.47
1:C:504:GLN:CD	1:C:505:GLN:H	2.16	0.47
1:E:553:ILE:CG2	1:F:472:PHE:HE2	2.28	0.47
1:D:543:ILE:HB	1:D:585:ILE:HG22	1.96	0.47
1:B:471:TYR:O	1:B:475:MET:HG2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:631:ALA:HB2	2:D:2071:HOH:O	2.13	0.47
1:E:490:MET:HE2	1:E:572:TYR:OH	2.12	0.47
1:A:468:LEU:HD21	1:B:564:VAL:HG21	1.95	0.47
1:F:445:LEU:HB3	1:F:496:VAL:HB	1.97	0.47
1:F:600:ASN:HD21	1:F:620:ALA:HB2	1.80	0.47
1:F:616:ILE:HG22	1:F:617:TRP:N	2.29	0.47
1:A:439:ARG:CG	1:A:547:GLU:HG2	2.45	0.47
1:A:497:LEU:HD11	1:A:563:VAL:HG21	1.97	0.47
1:A:552:ASN:ND2	1:A:559:THR:OG1	2.48	0.47
1:F:474:LYS:HZ3	1:F:521:ALA:HB1	1.79	0.47
1:C:449:LEU:HD21	1:C:471:TYR:CE1	2.50	0.46
1:B:567:GLN:O	1:B:571:THR:HG22	2.16	0.46
1:D:477:ASP:OD2	2:D:2011:HOH:O	2.21	0.46
1:E:471:TYR:CZ	1:E:539:MET:CE	2.98	0.46
1:E:471:TYR:CE1	1:E:539:MET:HE3	2.50	0.46
1:C:474:LYS:HE2	1:C:521:ALA:CB	2.43	0.46
1:E:624:GLU:HG3	1:E:625:PRO:HA	1.98	0.46
1:A:449:LEU:O	1:A:450:ARG:C	2.55	0.46
1:B:447:SER:HB2	1:B:539:MET:HE2	1.98	0.46
1:B:471:TYR:CE1	1:B:539:MET:HE3	2.51	0.46
1:A:461:PRO:HG3	1:B:439:ARG:HB2	1.97	0.45
1:B:517:GLU:CG	1:B:628:LEU:HD21	2.46	0.45
1:D:612:ASP:HB3	1:D:613:PRO:CD	2.46	0.45
1:F:460:ASN:CG	1:F:463:GLU:HG3	2.36	0.45
1:A:568:VAL:O	1:A:571:THR:HG23	2.16	0.45
1:A:583:ILE:HD12	1:A:630:LEU:HD11	1.97	0.45
1:D:603:ARG:NH1	2:D:2055:HOH:O	2.50	0.45
1:F:621:GLY:HA2	2:F:2060:HOH:O	2.17	0.45
1:F:479:ILE:HD11	1:F:518:MET:CE	2.47	0.45
1:F:450:ARG:NH1	1:F:578:THR:O	2.49	0.45
1:F:587:SER:HA	1:F:617:TRP:NE1	2.32	0.45
1:D:447:SER:HB2	1:D:539:MET:HE2	1.99	0.45
1:E:471:TYR:OH	1:E:539:MET:HE1	2.14	0.45
1:E:506:ASP:HA	2:E:2042:HOH:O	2.17	0.45
1:B:555:SER:O	1:B:559:THR:HG22	2.17	0.44
1:E:522:LEU:HA	1:E:525:VAL:HG13	1.99	0.44
1:E:519:GLN:HB2	1:E:630:LEU:HD11	1.99	0.44
1:D:490:MET:HG2	1:D:493:GLY:O	2.17	0.44
1:C:461:PRO:HB2	1:D:437:GLY:C	2.38	0.44
1:C:512:VAL:O	1:C:516:VAL:HG23	2.17	0.44
1:C:563:VAL:HG12	1:C:568:VAL:CG2	2.48	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:SER:HB2	1:D:539:MET:CE	2.48	0.44
1:E:451:GLY:HA2	2:E:2010:HOH:O	2.16	0.44
1:E:573:ARG:HD2	1:E:607:PRO:CB	2.40	0.44
1:D:556:GLU:OE1	1:D:556:GLU:HA	2.17	0.44
1:E:523:ARG:HH22	1:E:631:ALA:HB3	1.82	0.44
1:C:531:GLY:C	1:C:533:GLY:H	2.20	0.44
1:F:450:ARG:NH1	1:F:578:THR:OG1	2.50	0.44
1:F:577:TYR:HD1	1:F:616:ILE:HD11	1.81	0.44
2:A:2046:HOH:O	1:B:488:GLU:HB2	2.17	0.44
1:D:504:GLN:HG3	2:D:2023:HOH:O	2.16	0.44
1:F:479:ILE:CG1	1:F:518:MET:HE1	2.48	0.43
1:B:444:ILE:CD1	1:B:495:LEU:CD1	2.85	0.43
1:F:466:LYS:HA	1:F:466:LYS:HZ3	1.84	0.43
1:F:602:ASN:ND2	1:F:602:ASN:O	2.51	0.43
1:B:470:ILE:HG22	1:B:525:VAL:HB	2.00	0.43
1:B:575:GLU:O	1:B:578:THR:HB	2.18	0.43
1:D:435:MET:HB3	1:D:552:ASN:H	1.84	0.43
1:B:475:MET:CE	1:B:518:MET:HE3	2.49	0.43
1:F:526:ASN:HD21	1:F:537:LEU:H	1.66	0.43
1:C:522:LEU:CD2	1:C:525:VAL:CG2	2.97	0.43
1:F:583:ILE:HG22	1:F:585:ILE:HG23	2.01	0.43
1:B:468:LEU:HD12	1:B:468:LEU:HA	1.90	0.43
1:D:446:THR:HG22	1:D:495:LEU:CD1	2.49	0.43
1:F:435:MET:CB	1:F:437:GLY:H	2.31	0.43
1:A:540:GLY:HA3	1:A:578:THR:HG21	2.00	0.43
1:A:445:LEU:HD22	1:A:496:VAL:HG13	2.00	0.43
1:A:478:VAL:CG2	1:A:518:MET:HG2	2.49	0.43
1:B:442:ILE:HD12	1:B:497:LEU:HB3	2.01	0.43
1:C:496:VAL:CG2	1:C:498:PHE:CE1	3.01	0.43
1:E:553:ILE:CG2	1:F:472:PHE:CE2	3.02	0.43
1:E:466:LYS:HD2	1:E:466:LYS:N	2.34	0.42
1:D:587:SER:O	1:D:591:GLU:HG2	2.19	0.42
1:F:519:GLN:HG3	1:F:583:ILE:CD1	2.50	0.42
1:D:490:MET:HG2	1:D:490:MET:H	1.72	0.42
1:B:557:LYS:HD3	1:B:557:LYS:HA	1.89	0.42
1:E:482:HIS:CE1	1:E:517:GLU:OE1	2.64	0.42
1:C:467:VAL:HG22	1:C:534:LEU:HD23	2.02	0.42
1:E:449:LEU:HD21	1:E:471:TYR:CE1	2.54	0.42
1:F:504:GLN:HB3	1:F:506:ASP:OD1	2.20	0.42
1:A:450:ARG:NH2	1:A:578:THR:O	2.53	0.42
1:A:496:VAL:HG22	1:A:498:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:SER:O	1:A:591:GLU:CG	2.68	0.41
1:B:516:VAL:HG13	1:B:630:LEU:HD13	2.02	0.41
1:D:450:ARG:H	1:D:450:ARG:HG2	1.65	0.41
1:E:544:ASN:ND2	1:E:567:GLN:OE1	2.38	0.41
1:F:590:LEU:HD12	1:F:599:VAL:HG21	2.02	0.41
1:F:490:MET:N	1:F:493:GLY:O	2.46	0.41
1:F:516:VAL:HG13	2:F:2060:HOH:O	2.20	0.41
1:B:448:ASP:OD1	1:B:450:ARG:NH2	2.39	0.41
1:E:471:TYR:OH	1:E:539:MET:HE3	2.13	0.41
1:A:438:ASP:OD1	1:A:440:ARG:HD2	2.19	0.41
1:A:499:GLY:HA2	1:A:503:SER:HB3	2.01	0.41
1:C:499:GLY:CA	1:C:507:ASP:OD1	2.68	0.41
1:C:503:SER:CB	2:C:2023:HOH:O	2.52	0.41
1:D:459:LEU:HD21	1:D:535:GLN:HE22	1.85	0.41
1:A:452:PHE:CE2	1:A:468:LEU:HD13	2.55	0.41
1:C:496:VAL:HG22	1:C:498:PHE:CE1	2.55	0.41
1:A:522:LEU:HD13	1:A:526:ASN:HD21	1.86	0.41
1:B:606:GLN:HB2	2:B:2075:HOH:O	2.21	0.41
1:C:437:GLY:HA3	1:D:465:VAL:HG21	2.03	0.41
1:C:439:ARG:NH1	1:D:461:PRO:HD3	2.36	0.41
1:D:482:HIS:CE1	1:D:517:GLU:OE1	2.73	0.41
1:F:455:THR:O	1:F:459:LEU:HG	2.20	0.41
1:F:531:GLY:C	1:F:533:GLY:H	2.24	0.41
1:A:488:GLU:CD	1:A:560:LYS:HZ1	2.24	0.41
1:C:522:LEU:O	1:C:525:VAL:HG22	2.21	0.41
1:D:460:ASN:HB3	1:D:463:GLU:OE2	2.21	0.41
1:E:530:THR:C	1:E:532:LEU:H	2.23	0.41
1:F:479:ILE:CG1	1:F:518:MET:HE3	2.35	0.41
1:F:544:ASN:HB3	1:F:571:THR:CG2	2.50	0.41
1:D:606:GLN:HE21	1:D:606:GLN:HB3	1.72	0.41
1:F:602:ASN:C	1:F:602:ASN:ND2	2.74	0.41
1:E:474:LYS:HG3	1:E:525:VAL:HG12	2.02	0.40
1:B:602:ASN:OD1	1:B:615:VAL:CG1	2.65	0.40
1:C:499:GLY:HA2	1:C:507:ASP:OD1	2.21	0.40
1:C:565:GLY:HA3	2:C:2038:HOH:O	2.21	0.40
1:E:445:LEU:HD23	1:E:446:THR:N	2.36	0.40
1:F:596:ARG:HD2	1:F:624:GLU:O	2.22	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	199/208 (96%)	184 (92%)	12 (6%)	3 (2%)	10 9
1	B	195/208 (94%)	190 (97%)	4 (2%)	1 (0%)	29 35
1	C	198/208 (95%)	183 (92%)	12 (6%)	3 (2%)	10 9
1	D	197/208 (95%)	188 (95%)	6 (3%)	3 (2%)	10 9
1	E	197/208 (95%)	184 (93%)	12 (6%)	1 (0%)	29 35
1	F	195/208 (94%)	182 (93%)	11 (6%)	2 (1%)	15 17
All	All	1181/1248 (95%)	1111 (94%)	57 (5%)	13 (1%)	14 15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	611	LYS
1	A	450	ARG
1	C	609	GLY
1	D	595	ASP
1	E	450	ARG
1	B	491	GLY
1	D	435	MET
1	F	450	ARG
1	F	532	LEU
1	C	450	ARG
1	A	454	SER
1	C	532	LEU
1	A	558	ARG

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	163/169 (96%)	133 (82%)	30 (18%)	1	1
1	B	159/169 (94%)	132 (83%)	27 (17%)	2	2
1	C	162/169 (96%)	132 (82%)	30 (18%)	1	1
1	D	161/169 (95%)	133 (83%)	28 (17%)	2	1
1	E	161/169 (95%)	134 (83%)	27 (17%)	2	2
1	F	159/169 (94%)	134 (84%)	25 (16%)	2	2
All	All	965/1014 (95%)	798 (83%)	167 (17%)	2	1

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	435	MET
1	A	440	ARG
1	A	448	ASP
1	A	454	SER
1	A	460	ASN
1	A	466	LYS
1	A	468	LEU
1	A	478	VAL
1	A	495	LEU
1	A	496	VAL
1	A	502	THR
1	A	520	LEU
1	A	522	LEU
1	A	530	THR
1	A	534	LEU
1	A	553	ILE
1	A	556	GLU
1	A	557	LYS
1	A	559	THR
1	A	560	LYS
1	A	571	THR
1	A	573	ARG
1	A	578	THR
1	A	590	LEU
1	A	596	ARG
1	A	599	VAL
1	A	603	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	604	THR
1	A	611	LYS
1	A	629	SER
1	B	444	ILE
1	B	450	ARG
1	B	468	LEU
1	B	477	ASP
1	B	494	ILE
1	B	505	GLN
1	B	506	ASP
1	B	523	ARG
1	B	525	VAL
1	B	527	GLN
1	B	532	LEU
1	B	534	LEU
1	B	535	GLN
1	B	553	ILE
1	B	556	GLU
1	B	557	LYS
1	B	559	THR
1	B	560	LYS
1	B	567	GLN
1	B	570	LEU
1	B	571	THR
1	B	573	ARG
1	B	578	THR
1	B	600	ASN
1	B	606	GLN
1	B	614	VAL
1	B	628	LEU
1	C	440	ARG
1	C	448	ASP
1	C	466	LYS
1	C	468	LEU
1	C	474	LYS
1	C	490	MET
1	C	495	LEU
1	C	496	VAL
1	C	503	SER
1	C	505	GLN
1	C	506	ASP
1	C	519	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	520	LEU
1	C	522	LEU
1	C	530	THR
1	C	534	LEU
1	C	535	GLN
1	C	537	LEU
1	C	553	ILE
1	C	557	LYS
1	C	558	ARG
1	C	559	THR
1	C	570	LEU
1	C	571	THR
1	C	595	ASP
1	C	602	ASN
1	C	603	ARG
1	C	611	LYS
1	C	615	VAL
1	C	633	GLU
1	D	434	LYS
1	D	435	MET
1	D	448	ASP
1	D	450	ARG
1	D	453	THR
1	D	455	THR
1	D	464	VAL
1	D	468	LEU
1	D	490	MET
1	D	504	GLN
1	D	505	GLN
1	D	530	THR
1	D	537	LEU
1	D	550	VAL
1	D	552	ASN
1	D	553	ILE
1	D	556	GLU
1	D	563	VAL
1	D	567	GLN
1	D	568	VAL
1	D	570	LEU
1	D	571	THR
1	D	578	THR
1	D	582	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	605	VAL
1	D	606	GLN
1	D	615	VAL
1	D	632	VAL
1	E	434	LYS
1	E	435	MET
1	E	448	ASP
1	E	450	ARG
1	E	457	GLU
1	E	466	LYS
1	E	468	LEU
1	E	485	THR
1	E	490	MET
1	E	496	VAL
1	E	520	LEU
1	E	522	LEU
1	E	524	GLU
1	E	530	THR
1	E	538	GLU
1	E	550	VAL
1	E	556	GLU
1	E	558	ARG
1	E	560	LYS
1	E	571	THR
1	E	578	THR
1	E	590	LEU
1	E	602	ASN
1	E	604	THR
1	E	610	VAL
1	E	615	VAL
1	E	630	LEU
1	F	435	MET
1	F	450	ARG
1	F	463	GLU
1	F	466	LYS
1	F	468	LEU
1	F	474	LYS
1	F	490	MET
1	F	503	SER
1	F	509	LEU
1	F	532	LEU
1	F	534	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	535	GLN
1	F	539	MET
1	F	550	VAL
1	F	558	ARG
1	F	560	LYS
1	F	571	THR
1	F	582	GLN
1	F	587	SER
1	F	595	ASP
1	F	602	ASN
1	F	608	LYS
1	F	611	LYS
1	F	612	ASP
1	F	629	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	ASN
1	A	481	HIS
1	A	482	HIS
1	A	544	ASN
1	A	552	ASN
1	A	600	ASN
1	A	635	GLN
1	B	460	ASN
1	B	482	HIS
1	B	505	GLN
1	B	526	ASN
1	C	469	ASN
1	C	482	HIS
1	C	535	GLN
1	C	582	GLN
1	D	460	ASN
1	D	482	HIS
1	D	535	GLN
1	D	552	ASN
1	D	600	ASN
1	D	606	GLN
1	E	460	ASN
1	E	482	HIS
1	E	527	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	528	GLN
1	E	552	ASN
1	E	602	ASN
1	F	526	ASN
1	F	535	GLN
1	F	600	ASN
1	F	602	ASN
1	F	627	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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	201/208 (96%)	0.23	11 (5%) 25 31	27, 37, 54, 63	0
1	B	197/208 (94%)	0.64	27 (13%) 3 4	26, 38, 63, 72	0
1	C	200/208 (96%)	0.42	18 (9%) 9 13	26, 36, 57, 61	0
1	D	199/208 (95%)	0.52	21 (10%) 6 9	27, 38, 56, 72	0
1	E	199/208 (95%)	0.80	29 (14%) 2 3	28, 39, 61, 68	0
1	F	197/208 (94%)	1.11	36 (18%) 1 1	33, 42, 64, 75	0
All	All	1193/1248 (95%)	0.62	142 (11%) 4 6	26, 38, 59, 75	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	502	THR	8.3
1	B	435	MET	8.0
1	B	610	VAL	7.8
1	E	631	ALA	7.7
1	F	610	VAL	7.3
1	E	434	LYS	6.7
1	B	631	ALA	6.6
1	B	558	ARG	6.5
1	B	611	LYS	6.3
1	D	632	VAL	6.2
1	F	607	PRO	6.2
1	E	632	VAL	5.9
1	F	604	THR	5.9
1	F	631	ALA	5.7
1	F	435	MET	5.7
1	F	611	LYS	5.6
1	B	556	GLU	5.5
1	B	505	GLN	5.5
1	C	633	GLU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	608	LYS	5.5
1	D	609	GLY	5.3
1	C	435	MET	5.1
1	F	556	GLU	5.0
1	F	543	ILE	4.9
1	E	557	LYS	4.9
1	F	608	LYS	4.9
1	D	557	LYS	4.9
1	B	501	PRO	4.8
1	E	505	GLN	4.7
1	E	558	ARG	4.5
1	E	607	PRO	4.4
1	C	534	LEU	4.4
1	E	435	MET	4.3
1	B	609	GLY	4.3
1	F	541	ILE	4.3
1	B	557	LYS	4.2
1	C	502	THR	4.2
1	D	434	LYS	4.1
1	F	578	THR	4.1
1	D	556	GLU	4.0
1	C	632	VAL	4.0
1	F	557	LYS	3.8
1	C	501	PRO	3.8
1	D	558	ARG	3.7
1	E	543	ILE	3.7
1	B	608	LYS	3.6
1	D	611	LYS	3.6
1	E	579	THR	3.6
1	F	609	GLY	3.5
1	D	631	ALA	3.5
1	B	555	SER	3.5
1	F	564	VAL	3.4
1	A	557	LYS	3.4
1	F	606	GLN	3.4
1	B	612	ASP	3.4
1	F	458	GLY	3.4
1	C	610	VAL	3.3
1	C	468	LEU	3.3
1	A	435	MET	3.3
1	E	555	SER	3.3
1	E	550	VAL	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	608	LYS	3.3
1	B	607	PRO	3.3
1	F	630	LEU	3.2
1	D	612	ASP	3.2
1	A	543	ILE	3.2
1	E	436	GLY	3.2
1	B	585	ILE	3.2
1	F	532	LEU	3.2
1	F	459	LEU	3.1
1	B	543	ILE	3.1
1	E	468	LEU	3.0
1	E	437	GLY	3.0
1	F	579	THR	3.0
1	E	532	LEU	3.0
1	B	541	ILE	3.0
1	E	512	VAL	2.9
1	A	559	THR	2.9
1	F	612	ASP	2.9
1	E	585	ILE	2.8
1	E	503	SER	2.8
1	C	531	GLY	2.8
1	F	537	LEU	2.8
1	D	512	VAL	2.8
1	A	609	GLY	2.8
1	F	603	ARG	2.8
1	A	556	GLU	2.8
1	C	611	LYS	2.8
1	C	609	GLY	2.7
1	F	615	VAL	2.7
1	C	490	MET	2.7
1	B	559	THR	2.7
1	E	609	GLY	2.7
1	F	616	ILE	2.7
1	B	561	TYR	2.6
1	D	585	ILE	2.6
1	C	532	LEU	2.6
1	F	573	ARG	2.5
1	F	577	TYR	2.5
1	B	512	VAL	2.5
1	F	563	VAL	2.4
1	D	543	ILE	2.4
1	E	556	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	538	GLU	2.4
1	F	553	ILE	2.4
1	D	555	SER	2.4
1	D	561	TYR	2.4
1	E	533	GLY	2.4
1	F	549	VAL	2.4
1	F	555	SER	2.4
1	A	512	VAL	2.4
1	E	612	ASP	2.3
1	C	631	ALA	2.3
1	E	445	LEU	2.3
1	A	505	GLN	2.3
1	E	611	LYS	2.2
1	B	542	GLY	2.2
1	D	502	THR	2.2
1	B	506	ASP	2.2
1	F	617	TRP	2.2
1	D	613	PRO	2.2
1	D	608	LYS	2.2
1	D	468	LEU	2.2
1	C	467	VAL	2.1
1	E	464	VAL	2.1
1	D	610	VAL	2.1
1	D	535	GLN	2.1
1	A	624	GLU	2.1
1	E	471	TYR	2.1
1	C	535	GLN	2.1
1	D	505	GLN	2.1
1	A	585	ILE	2.1
1	F	504	GLN	2.1
1	B	514	CYS	2.1
1	B	436	GLY	2.1
1	B	584	PHE	2.1
1	F	531	GLY	2.1
1	A	451	GLY	2.0
1	C	556	GLU	2.0
1	E	465	VAL	2.0
1	B	468	LEU	2.0
1	F	592	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.