



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 05:04 AM UTC

PDB ID : 2W01 / pdb_00002w01
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	:	4-5-2 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

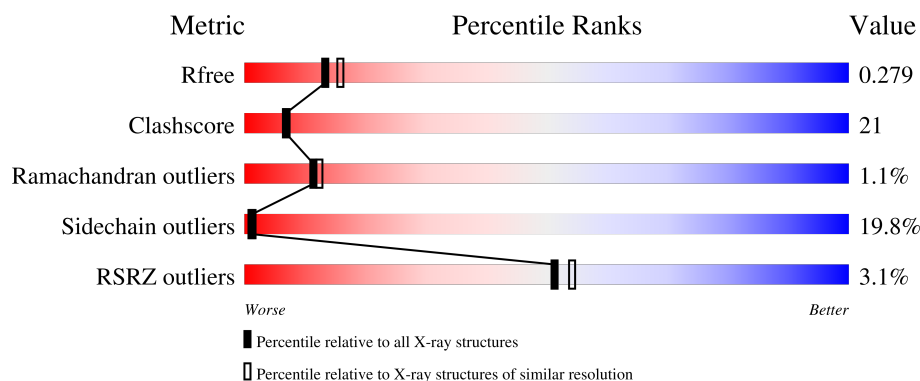
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (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 $\leq 5\%$. 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	208	 61% 24% 11% 4%
1	B	208	 58% 27% 9% 5%
1	C	208	 60% 29% 6% 5%
1	D	208	 55% 29% 11% 5%
1	E	208	 58% 29% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	208	7% 50% 34% 10% • 5%

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			

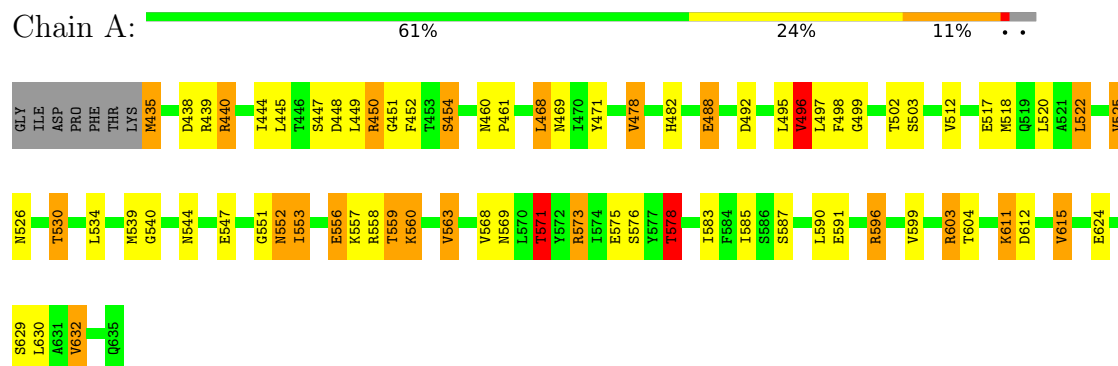
- Molecule 2 is water.

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		

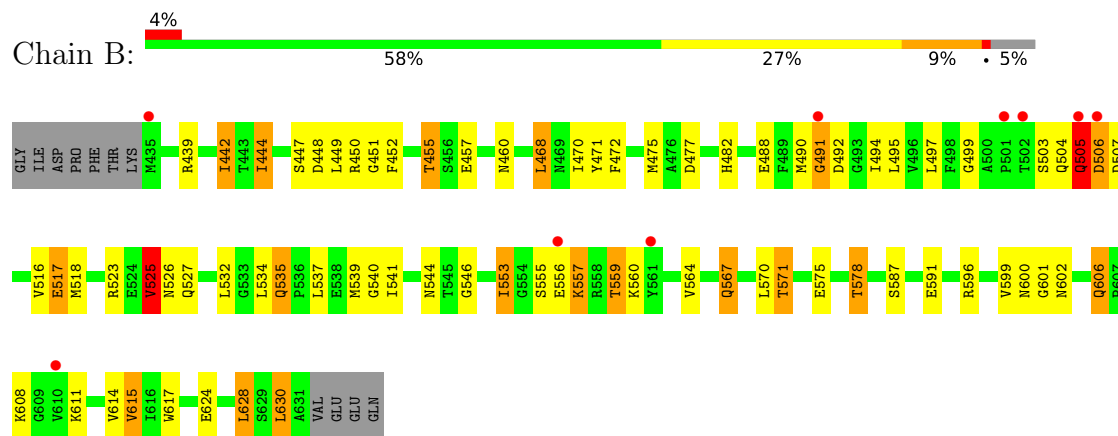
3 Residue-property plots

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.

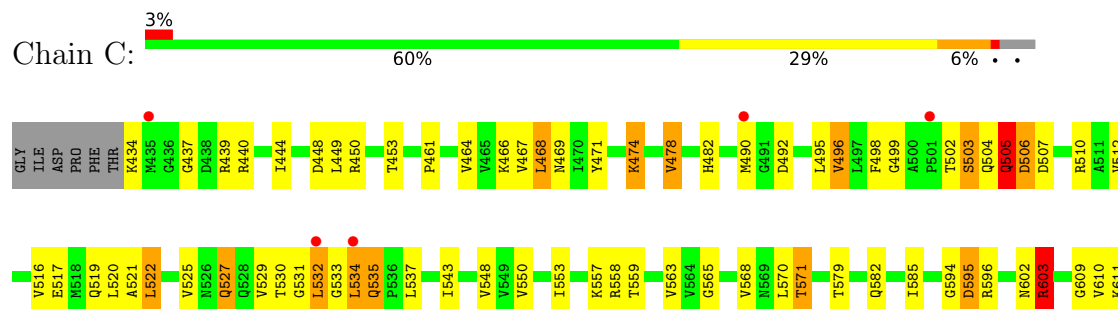
• Molecule 1: ADENYLATE CYCLASE

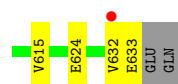


• Molecule 1: ADENYLATE CYCLASE

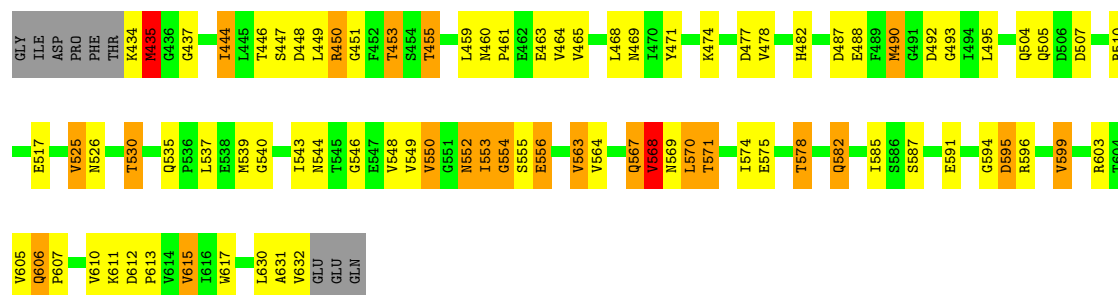


• Molecule 1: ADENYLATE CYCLASE

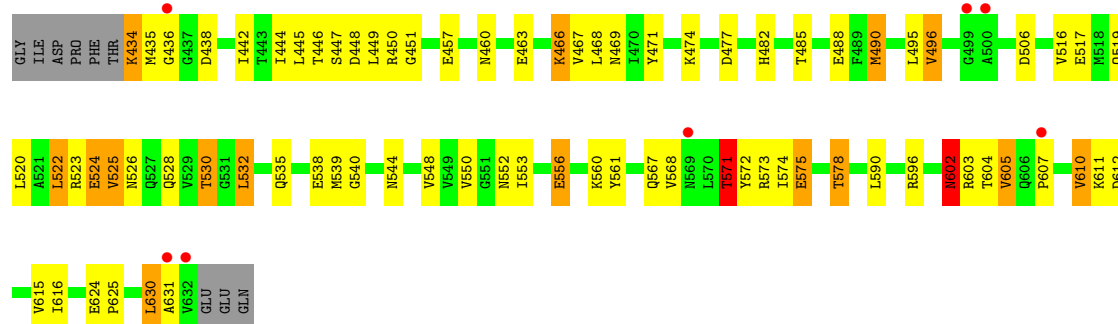




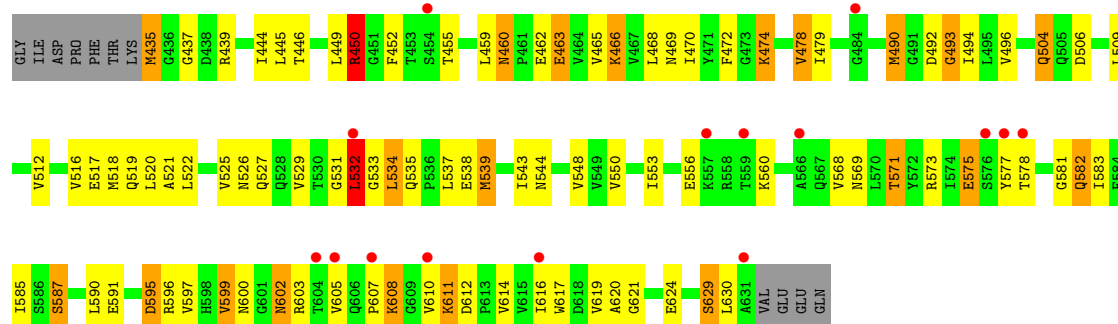
• Molecule 1: ADENYLATE CYCLASE



• Molecule 1: ADENYLATE CYCLASE



• Molecule 1: ADENYLATE CYCLASE



4 Data and refinement statistics

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) 97.1 (19.94-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (5.09%)	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 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

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	1.18	3/1525 (0.2%)	1.31	8/2069 (0.4%)
1	B	1.09	3/1491 (0.2%)	1.22	2/2023 (0.1%)
1	C	1.17	2/1516 (0.1%)	1.30	6/2056 (0.3%)
1	D	1.13	4/1507 (0.3%)	1.27	7/2044 (0.3%)
1	E	1.16	10/1507 (0.7%)	1.22	8/2044 (0.4%)
1	F	0.96	1/1491 (0.1%)	1.19	6/2023 (0.3%)
All	All	1.12	23/9037 (0.3%)	1.25	37/12259 (0.3%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	556	GLU	CD-OE1	8.21	1.41	1.25
1	F	603	ARG	CZ-NH1	7.93	1.43	1.32
1	E	438	ASP	CG-OD2	7.14	1.39	1.25
1	E	556	GLU	CG-CD	7.04	1.69	1.52
1	B	525	VAL	CA-CB	6.79	1.62	1.54
1	E	438	ASP	CG-OD1	6.27	1.37	1.25
1	E	556	GLU	CD-OE2	6.21	1.37	1.25
1	D	568	VAL	CA-CB	6.17	1.62	1.54
1	A	512	VAL	CA-CB	6.16	1.61	1.54
1	E	496	VAL	CA-CB	6.04	1.62	1.54
1	E	434	LYS	CG-CD	5.94	1.70	1.52
1	C	478	VAL	CA-CB	5.91	1.62	1.54
1	E	571	THR	CA-CB	5.66	1.62	1.53
1	B	541	ILE	CA-CB	5.60	1.62	1.54
1	D	549	VAL	CA-CB	5.54	1.61	1.54
1	E	434	LYS	N-CA	5.54	1.56	1.46
1	D	615	VAL	CA-CB	5.43	1.60	1.54
1	D	525	VAL	CA-CB	5.41	1.61	1.54
1	B	455	THR	CA-CB	5.38	1.61	1.53
1	A	615	VAL	CA-CB	5.38	1.60	1.54
1	A	632	VAL	CA-CB	5.13	1.60	1.54
1	E	516	VAL	CA-CB	5.13	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	464	VAL	CA-CB	5.11	1.60	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	505	GLN	N-CA-C	11.38	123.25	111.07
1	E	568	VAL	N-CA-C	-7.02	103.93	110.53
1	D	594	GLY	CA-C-N	6.86	134.65	121.54
1	D	594	GLY	C-N-CA	6.86	134.65	121.54
1	F	538	GLU	N-CA-C	-6.21	99.59	109.59
1	F	493	GLY	N-CA-C	6.16	120.65	110.55
1	C	595	ASP	N-CA-C	6.14	119.61	111.75
1	D	550	VAL	CB-CA-C	-6.10	101.54	110.81
1	C	603	ARG	N-CA-C	-6.03	99.88	109.23
1	B	505	GLN	N-CA-C	5.99	118.60	111.71
1	E	460	ASN	CA-C-N	5.83	125.97	119.32
1	E	460	ASN	C-N-CA	5.83	125.97	119.32
1	E	436	GLY	N-CA-C	5.79	121.88	111.34
1	C	594	GLY	CA-C-N	5.77	128.81	120.38
1	C	594	GLY	C-N-CA	5.77	128.81	120.38
1	E	603	ARG	N-CA-C	-5.77	100.53	109.24
1	D	582	GLN	N-CA-C	5.70	119.34	110.17
1	A	488	GLU	N-CA-C	5.68	117.73	108.76
1	B	460	ASN	CB-CA-C	5.60	117.50	109.11
1	F	469	ASN	N-CA-C	5.53	119.20	112.23
1	F	470	ILE	N-CA-C	-5.51	105.13	110.42
1	A	451	GLY	N-CA-C	5.49	123.36	114.90
1	E	496	VAL	N-CA-C	5.47	116.36	108.48
1	A	578	THR	N-CA-CB	-5.43	102.04	110.29
1	E	571	THR	CB-CA-C	5.41	119.77	110.79
1	A	571	THR	CB-CA-C	5.38	119.40	110.90
1	D	554	GLY	N-CA-C	5.36	117.15	110.29
1	F	460	ASN	CA-C-N	5.31	126.47	119.84
1	F	460	ASN	C-N-CA	5.31	126.47	119.84
1	D	595	ASP	N-CA-C	5.29	122.07	110.80
1	A	496	VAL	CB-CA-C	5.23	118.56	110.50
1	A	569	ASN	N-CA-C	5.23	117.66	111.33
1	A	615	VAL	CB-CA-C	5.22	117.39	110.91
1	E	602	ASN	N-CA-C	5.16	117.03	109.24
1	C	603	ARG	CB-CA-C	-5.07	98.32	109.56
1	A	552	ASN	N-CA-C	5.06	116.73	108.63
1	D	453	THR	N-CA-CB	5.03	117.52	110.12

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	1504	0	1500	62	0
1	B	1470	0	1471	78	0
1	C	1495	0	1499	51	0
1	D	1486	0	1493	64	0
1	E	1486	0	1493	59	0
1	F	1470	0	1471	84	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	380	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 (380) 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:447:SER:HB2	1:B:539:MET:HE2	1.34	1.10
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:E:490:MET:HE1	1:E:572:TYR:OH	1.62	0.98
1:D:471:TYR:OH	1:D:539:MET:HE3	1.63	0.97
1:B:475:MET:HE3	1:B:518:MET:HE3	1.49	0.93
1:E:540:GLY:HA3	1:E:578:THR:HG21	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:447:SER:HB2	1:D:539:MET:HE2	1.53	0.88
1:A:603:ARG:HG2	1:A:603:ARG:HH21	1.37	0.88
1:B:475:MET:HE3	1:B:518:MET:CE	2.03	0.88
1:B:475:MET:HE1	1:B:518:MET:HB3	1.56	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:B:447:SER:CB	1:B:539:MET:HE2	2.07	0.84
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:D:447:SER:CB	1:D:539:MET:HE2	2.10	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:474:LYS:HD2	1:F:525:VAL:HG23	1.68	0.75
1:F:522:LEU:HD22	1:F:539:MET:HE2	1.67	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:B:471:TYR:OH	1:B:539:MET:CE	2.35	0.74
1:D:471:TYR:OH	1:D:539:MET:CE	2.37	0.73
1:E:524:GLU:HA	1:E:524:GLU:OE1	1.87	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:E:574:ILE:HD12	1:E:616:ILE:HG21	1.69	0.73
1:E:447:SER:HB2	1:E:539:MET:HE2	1.70	0.73
1:E:474:LYS:HZ1	1:E:528:GLN:HE22	1.37	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:F:479:ILE:HG13	1:F:518:MET:HE3	1.71	0.71
1:D:548:VAL:CG1	1:D:563:VAL:HG22	2.19	0.70
1:B:475:MET:HE2	1:B:539:MET:HE1	1.73	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:A:471:TYR:CE1	1:A:539:MET:HE3	2.26	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: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:E:490:MET:CE	1:E:572:TYR:OH	2.39	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
1:D:540:GLY:HA3	1:D:578:THR:CG2	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:471:TYR:OH	1:B:539:MET:HE3	1.95	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:F:479:ILE:CG1	1:F:518:MET:HE3	2.26	0.64
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:E:490:MET:HE3	1:E:495:LEU:HB2	1.80	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: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:471:TYR:OH	1:B:539:MET:HE1	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:471:TYR:HE1	1:A:539:MET:HE3	1.68	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: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: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:B:475:MET:HE3	1:B:518:MET:HE2	1.87	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
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:A:522:LEU:HA	1:A:525:VAL:HG13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:475:MET:CE	1:B:518:MET:HB3	2.31	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:F:577:TYR:CE1	1:F:605:VAL:HG11	2.42	0.55
1:D:555:SER:O	1:D:556:GLU:C	2.50	0.54
1:F:569:ASN:HB3	1:F:573:ARG:HH21	1.72	0.54
1:A:471:TYR:OH	1:A:539:MET:HE3	2.06	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: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:C:504:GLN:CD	1:C:505:GLN:H	2.16	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:F:602:ASN:C	1:F:602:ASN:HD22	2.17	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:CZ	1:A:539:MET:HE3	2.45	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:471:TYR:CE1	1:E:539:MET:HE3	2.45	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:466:LYS:HA	1:F:466:LYS:HZ3	1.76	0.50
1:A:449:LEU:O	1:A:450:ARG:C	2.55	0.50
1:D:599:VAL:HG11	1:D:617:TRP:CE3	2.46	0.50
1:F:460:ASN:CG	1:F:463:GLU:HG3	2.36	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:447:SER:HB2	1:A:539:MET:HE2	1.93	0.50
1:A:471:TYR:CE1	1:A:539:MET:CE	2.92	0.50
1:A:544:ASN:HB3	1:A:571:THR:HB	1.93	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: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:C:461:PRO:HB2	1:D:437:GLY:C	2.38	0.49
1:E:490:MET:CE	1:E:495:LEU:HB2	2.41	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:E:471:TYR:CE1	1:E:539:MET:HE1	2.48	0.49
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:C:531:GLY:C	1:C:533:GLY:H	2.20	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:B:475:MET:HE2	1:B:539:MET:CE	2.42	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:B:475:MET:CE	1:B:539:MET:HE1	2.43	0.48
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
1:D:631:ALA:HB2	2:D:2071:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:471:TYR:HE1	1:A:539:MET:CE	2.27	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: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:F:531:GLY:C	1:F:533:GLY:H	2.24	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:A:568:VAL:O	1:A:571:THR:HG23	2.16	0.45
1:E:530:THR:C	1:E:532:LEU:H	2.23	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:487:ASP:C	1:D:487:ASP:OD1	2.60	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:F:602:ASN:C	1:F:602:ASN:ND2	2.74	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: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
1:E:471:TYR:OH	1:E:539:MET:HE1	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:445:LEU:C	1:F:445:LEU:HD23	2.42	0.44
1:A:488:GLU:CD	1:A:560:LYS:HZ1	2.26	0.44
1:B:475:MET:HE2	1:B:539:MET:SD	2.58	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:B:504:GLN:O	1:B:507:ASP:CG	2.61	0.43
1:C:532:LEU:C	1:C:534:LEU:HD13	2.43	0.43
1:D:490:MET:HE2	1:D:490:MET:HB3	1.83	0.43
1:B:444:ILE:CD1	1:B:495:LEU:CD1	2.85	0.43
1:B:475:MET:CE	1:B:539:MET:SD	3.06	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: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:E:471:TYR:OH	1:E:539:MET:HE3	2.12	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:A:573:ARG:O	1:A:576:SER:OG	2.32	0.42
1:D:630:LEU:O	1:D:631:ALA:C	2.62	0.42
1:F:519:GLN:HG3	1:F:583:ILE:CD1	2.50	0.42
1:C:531:GLY:C	1:C:533:GLY:N	2.78	0.42
1:D:490:MET:HG2	1:D:490:MET:H	1.72	0.42
1:B:490:MET:C	1:B:492:ASP:N	2.78	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:D:447:SER:OG	1:D:539:MET:HE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:GLU:HG3	1:D:490:MET:HE3	2.01	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
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: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:C:504:GLN:CD	1:C:505:GLN:N	2.78	0.41
1:D:482:HIS:CE1	1:D:517:GLU:OE1	2.73	0.41
1:E:474:LYS:HZ1	1:E:528:GLN:NE2	2.13	0.41
1:F:455:THR:O	1:F:459:LEU:HG	2.20	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:F:544:ASN:HB3	1:F:571:THR:CG2	2.50	0.41
1:B:475:MET:CE	1:B:518:MET:HE2	2.51	0.41
1:D:606:GLN:HE21	1:D:606:GLN:HB3	1.72	0.41
1:E:474:LYS:HG3	1:E:525:VAL:HG12	2.02	0.40
1:B:490:MET:O	1:B:491:GLY:C	2.64	0.40
1:B:602:ASN:OD1	1:B:615:VAL:CG1	2.65	0.40
1:F:479:ILE:HD11	1:F:518:MET:HE1	2.03	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 [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	199/208 (96%)	184 (92%)	12 (6%)	3 (2%)	8	7
1	B	195/208 (94%)	190 (97%)	4 (2%)	1 (0%)	24	30
1	C	198/208 (95%)	183 (92%)	12 (6%)	3 (2%)	8	7
1	D	197/208 (95%)	188 (95%)	6 (3%)	3 (2%)	8	7
1	E	197/208 (95%)	184 (93%)	12 (6%)	1 (0%)	24	30
1	F	195/208 (94%)	182 (93%)	11 (6%)	2 (1%)	12	14
All	All	1181/1248 (95%)	1111 (94%)	57 (5%)	13 (1%)	11	12

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%)	130 (80%)	33 (20%)	1	1
1	B	159/169 (94%)	129 (81%)	30 (19%)	1	1
1	C	162/169 (96%)	128 (79%)	34 (21%)	1	1
1	D	161/169 (95%)	129 (80%)	32 (20%)	1	1
1	E	161/169 (95%)	131 (81%)	30 (19%)	1	1
1	F	159/169 (94%)	127 (80%)	32 (20%)	1	1
All	All	965/1014 (95%)	774 (80%)	191 (20%)	1	1

All (191) 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	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	525	VAL
1	A	530	THR
1	A	534	LEU
1	A	553	ILE
1	A	556	GLU
1	A	559	THR
1	A	560	LYS
1	A	563	VAL
1	A	571	THR
1	A	573	ARG

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Mol	Chain	Res	Type
1	A	578	THR
1	A	585	ILE
1	A	590	LEU
1	A	596	ARG
1	A	599	VAL
1	A	603	ARG
1	A	604	THR
1	A	611	LYS
1	A	615	VAL
1	A	629	SER
1	A	632	VAL
1	B	442	ILE
1	B	444	ILE
1	B	468	LEU
1	B	477	ASP
1	B	494	ILE
1	B	505	GLN
1	B	506	ASP
1	B	517	GLU
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	578	THR
1	B	600	ASN
1	B	606	GLN
1	B	611	LYS
1	B	614	VAL
1	B	615	VAL
1	B	628	LEU
1	B	630	LEU
1	C	440	ARG

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Mol	Chain	Res	Type
1	C	448	ASP
1	C	466	LYS
1	C	468	LEU
1	C	474	LYS
1	C	478	VAL
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
1	C	520	LEU
1	C	522	LEU
1	C	527	GLN
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	610	VAL
1	C	611	LYS
1	C	615	VAL
1	C	632	VAL
1	C	633	GLU
1	D	434	LYS
1	D	435	MET
1	D	444	ILE
1	D	448	ASP
1	D	450	ARG
1	D	453	THR
1	D	455	THR
1	D	464	VAL
1	D	468	LEU

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Mol	Chain	Res	Type
1	D	478	VAL
1	D	490	MET
1	D	505	GLN
1	D	525	VAL
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	564	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
1	D	599	VAL
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	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	525	VAL
1	E	530	THR
1	E	532	LEU
1	E	535	GLN
1	E	538	GLU
1	E	550	VAL
1	E	556	GLU

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Mol	Chain	Res	Type
1	E	560	LYS
1	E	571	THR
1	E	575	GLU
1	E	578	THR
1	E	590	LEU
1	E	602	ASN
1	E	604	THR
1	E	605	VAL
1	E	610	VAL
1	E	615	VAL
1	E	630	LEU
1	F	435	MET
1	F	446	THR
1	F	450	ARG
1	F	463	GLU
1	F	466	LYS
1	F	468	LEU
1	F	474	LYS
1	F	478	VAL
1	F	490	MET
1	F	494	ILE
1	F	504	GLN
1	F	509	LEU
1	F	532	LEU
1	F	534	LEU
1	F	535	GLN
1	F	539	MET
1	F	550	VAL
1	F	556	GLU
1	F	560	LYS
1	F	568	VAL
1	F	571	THR
1	F	575	GLU
1	F	582	GLN
1	F	587	SER
1	F	595	ASP
1	F	599	VAL
1	F	602	ASN
1	F	608	LYS
1	F	611	LYS
1	F	612	ASP
1	F	614	VAL

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Mol	Chain	Res	Type
1	F	629	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	ASN
1	A	481	HIS
1	A	482	HIS
1	A	552	ASN
1	A	600	ASN
1	B	482	HIS
1	B	505	GLN
1	B	526	ASN
1	B	567	GLN
1	B	606	GLN
1	C	469	ASN
1	C	482	HIS
1	C	535	GLN
1	C	544	ASN
1	C	567	GLN
1	C	569	ASN
1	C	582	GLN
1	C	602	ASN
1	D	460	ASN
1	D	482	HIS
1	D	504	GLN
1	D	535	GLN
1	D	552	ASN
1	D	600	ASN
1	D	606	GLN
1	D	627	ASN
1	E	460	ASN
1	E	481	HIS
1	E	482	HIS
1	E	527	GLN
1	E	528	GLN
1	E	569	ASN
1	E	602	ASN
1	F	526	ASN
1	F	535	GLN
1	F	552	ASN
1	F	600	ASN

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Mol	Chain	Res	Type
1	F	602	ASN
1	F	627	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 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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	201/208 (96%)	-0.18	0 100 100	27, 37, 54, 63	0
1	B	197/208 (94%)	0.20	9 (4%) 37 40	26, 38, 63, 72	0
1	C	200/208 (96%)	-0.02	6 (3%) 52 55	26, 36, 57, 61	0
1	D	199/208 (95%)	0.03	0 100 100	27, 38, 56, 72	0
1	E	199/208 (95%)	0.33	7 (3%) 47 50	28, 39, 61, 68	0
1	F	197/208 (94%)	0.76	15 (7%) 20 22	33, 42, 64, 75	0
All	All	1193/1248 (95%)	0.19	37 (3%) 51 54	26, 38, 59, 75	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	505	GLN	3.7
1	E	631	ALA	3.6
1	F	610	VAL	3.2
1	C	435	MET	3.1
1	C	534	LEU	3.1
1	C	501	PRO	3.1
1	F	607	PRO	3.0
1	B	610	VAL	3.0
1	E	632	VAL	2.9
1	E	499	GLY	2.8
1	F	532	LEU	2.8
1	E	607	PRO	2.8
1	F	605	VAL	2.8
1	F	578	THR	2.7
1	E	500	ALA	2.7
1	B	561	TYR	2.6
1	C	490	MET	2.6
1	B	491	GLY	2.6
1	B	502	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	632	VAL	2.5
1	F	576	SER	2.5
1	F	577	TYR	2.4
1	F	604	THR	2.4
1	B	435	MET	2.4
1	F	631	ALA	2.4
1	B	506	ASP	2.3
1	B	501	PRO	2.3
1	E	569	ASN	2.3
1	F	559	THR	2.3
1	F	484	GLY	2.2
1	F	566	ALA	2.2
1	F	557	LYS	2.1
1	C	532	LEU	2.1
1	F	616	ILE	2.1
1	F	454	SER	2.0
1	B	556	GLU	2.0
1	E	436	GLY	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.