Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 06:52 AM EDT

PDB ID	:	1UK1
Title	:	Crystal structure of human poly(ADP-ribose) polymerase complexed with a potent inhibitor
Authors	:	Kinoshita, T.
Deposited on	:	2003-08-14
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:

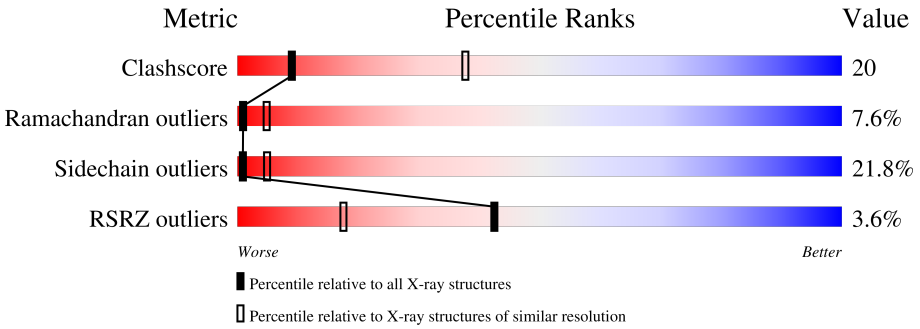
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 <=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	350	3%, 46%, 35%, 15%, .
1	B	350	5%, 39%, 37%, 18%, 6%

2 Entry composition (i)

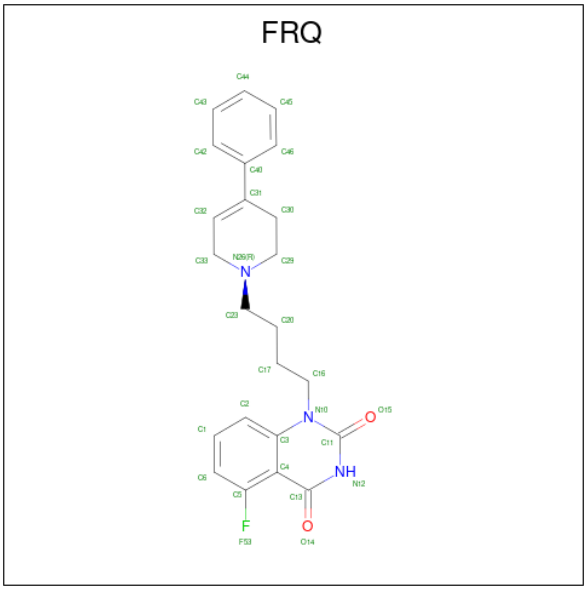
There are 3 unique types of molecules in this entry. The entry contains 5757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Poly [ADP-ribose] polymerase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2754	1752	465	526	11			
1	B	350	Total	C	N	O	S	0	0	0
			2754	1752	465	526	11			

- Molecule 2 is 5-FLUORO-1-[4-(4-PHENYL-3,6-DIHYDROPYRIDIN-1(2H)-YL)BUTYL]QUINAZOLINE-2,4(1H,3H)-DIONE (three-letter code: FRQ) (formula: $C_{23}H_{24}FN_3O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			29	23	1	3	2		
2	B	1	Total	C	F	N	O	0	0
			29	23	1	3	2		

- Molecule 3 is water.

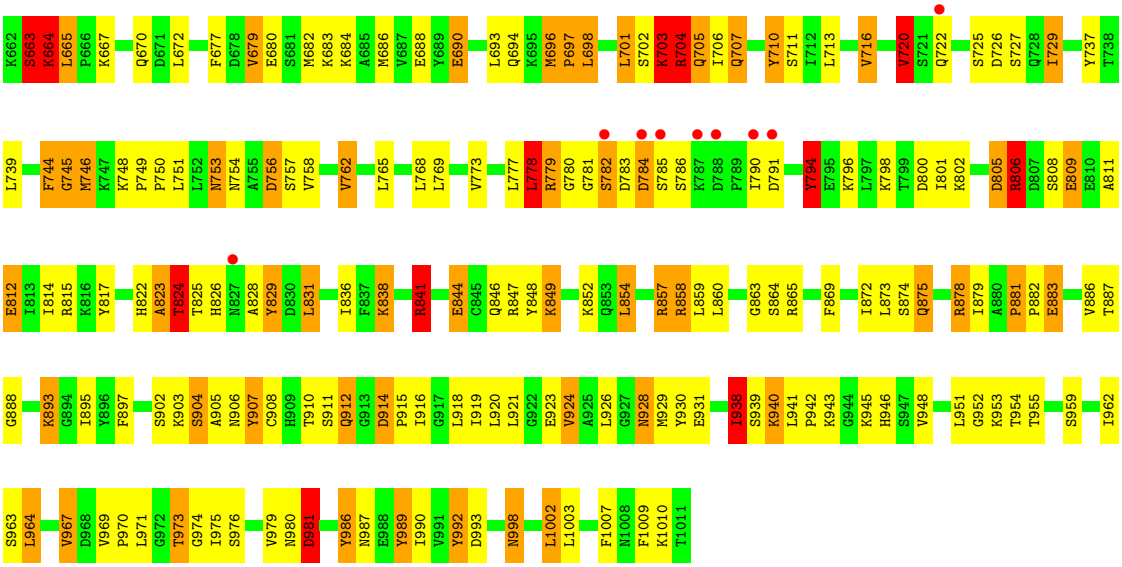
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	101	Total O 101 101	0	0
3	B	90	Total O 90 90	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

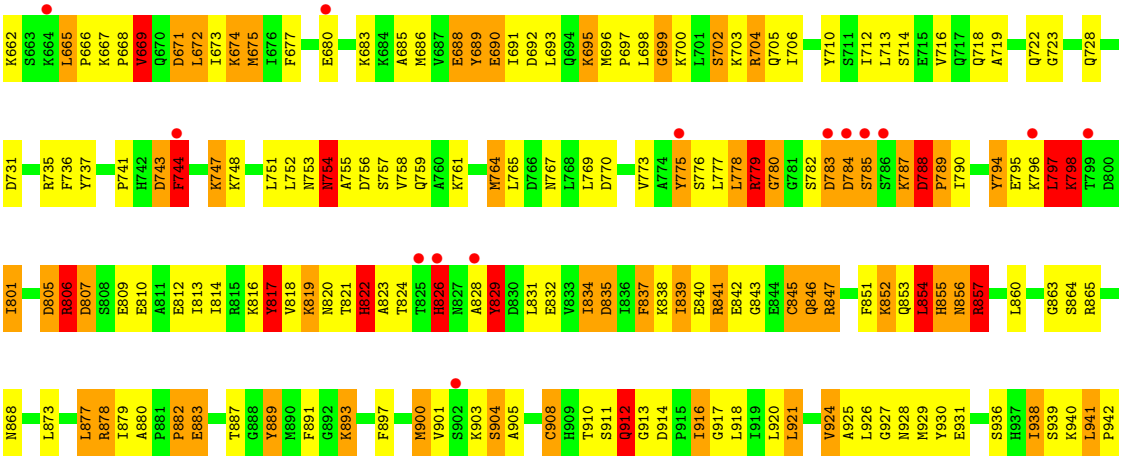
• Molecule 1: Poly [ADP-ribose] polymerase-1

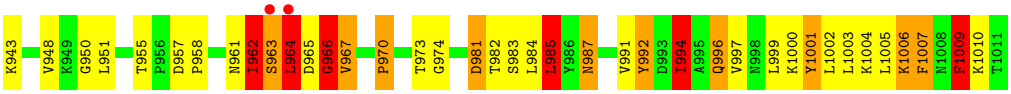
Chain A:



• Molecule 1: Poly [ADP-ribose] polymerase-1

Chain B:




K943
V948
K949
G950
L951
T955
P956
D957
P958
N961
I962
S963
L964
D965
G966
V967
P970
T973
G974
D981
T982
S983
L984
L985
Y986
N987
V991
Y992
D993
I994
A995
Q996
V997
N998
L999
K1000
Y1001
L1002
L1003
K1004
L1005
K1006
F1007
N1008
F1009
K1010
T1011

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	179.96Å 53.27Å 91.47Å 90.00° 113.80° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 49.54 – 2.97	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.00) 98.5 (49.54-2.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.96Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.242 , 0.274 0.281 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.0	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.0	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	0.86	EDS
Total number of atoms	5757	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.93	1/2806 (0.0%)	1.80	42/3786 (1.1%)
1	B	0.97	0/2806	1.88	51/3786 (1.3%)
All	All	0.95	1/5612 (0.0%)	1.84	93/7572 (1.2%)

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	14
1	B	0	28
All	All	0	42

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	806	ARG	NE-CZ	5.32	1.40	1.33

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	806	ARG	NE-CZ-NH1	11.55	126.07	120.30
1	B	889	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	A	847	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	B	689	TYR	CB-CG-CD2	-8.20	116.08	121.00
1	A	865	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	A	710	TYR	CB-CG-CD2	-8.00	116.20	121.00
1	A	828	ALA	C-N-CA	7.94	141.55	121.70
1	B	845	CYS	CA-CB-SG	-7.57	100.38	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	916	ILE	CA-CB-CG1	7.41	125.09	111.00
1	A	847	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	794	TYR	CB-CG-CD1	-7.07	116.76	121.00
1	A	829	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	B	829	TYR	CB-CG-CD1	-6.85	116.89	121.00
1	A	989	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	B	782	SER	N-CA-C	6.61	128.84	111.00
1	B	737	TYR	CB-CG-CD2	-6.57	117.06	121.00
1	A	945	LYS	CA-CB-CG	-6.55	98.98	113.40
1	B	754	ASN	N-CA-CB	-6.46	98.97	110.60
1	B	817	TYR	CB-CG-CD2	-6.34	117.19	121.00
1	B	788	ASP	N-CA-C	6.29	127.97	111.00
1	B	764	MET	CA-CB-CG	6.26	123.95	113.30
1	B	710	TYR	CB-CG-CD2	-6.24	117.26	121.00
1	B	822	HIS	CA-CB-CG	-6.24	102.99	113.60
1	A	914	ASP	N-CA-CB	6.21	121.78	110.60
1	B	705	GLN	CB-CA-C	-6.20	98.00	110.40
1	B	856	ASN	C-N-CA	6.19	137.18	121.70
1	B	883	GLU	N-CA-C	6.19	127.71	111.00
1	A	704	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	848	TYR	CB-CG-CD1	-6.16	117.30	121.00
1	B	854	LEU	CA-CB-CG	6.13	129.40	115.30
1	B	784	ASP	N-CA-C	6.11	127.51	111.00
1	A	737	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	B	735	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	B	847	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	B	857	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	A	930	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	B	775	TYR	CB-CG-CD2	-5.98	117.41	121.00
1	A	963	SER	C-N-CA	-5.98	106.76	121.70
1	A	841	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	983	SER	N-CA-CB	5.92	119.38	110.50
1	B	780	GLY	N-CA-C	5.91	127.88	113.10
1	A	720	VAL	CG1-CB-CG2	-5.91	101.44	110.90
1	B	994	ILE	CA-CB-CG1	5.89	122.19	111.00
1	B	853	GLN	C-N-CA	-5.87	107.02	121.70
1	B	1001	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	A	698	LEU	CB-CA-C	5.81	121.24	110.20
1	A	729	ILE	CA-CB-CG1	-5.81	99.97	111.00
1	B	985	LEU	CB-CG-CD1	5.77	120.80	111.00
1	A	858	ARG	CD-NE-CZ	-5.75	115.55	123.60
1	B	806	ARG	N-CA-C	5.75	126.53	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	779	ARG	CD-NE-CZ	-5.73	115.58	123.60
1	B	847	ARG	CD-NE-CZ	-5.71	115.61	123.60
1	A	779	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	964	LEU	CB-CA-C	5.68	121.00	110.20
1	A	924	VAL	CA-CB-CG2	5.68	119.42	110.90
1	A	938	ILE	CA-C-N	-5.67	104.74	117.20
1	A	907	TYR	CB-CG-CD2	-5.64	117.62	121.00
1	B	983	SER	CB-CA-C	-5.63	99.41	110.10
1	A	757	SER	N-CA-CB	5.58	118.86	110.50
1	A	993	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	782	SER	C-N-CA	-5.56	107.81	121.70
1	A	939	SER	N-CA-CB	-5.56	102.16	110.50
1	B	669	VAL	CA-CB-CG2	5.48	119.12	110.90
1	A	878	ARG	C-N-CA	-5.48	108.01	121.70
1	A	778	LEU	CB-CA-C	5.45	120.55	110.20
1	B	753	ASN	CA-C-O	5.42	131.47	120.10
1	A	992	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	A	981	ASP	N-CA-C	5.36	125.48	111.00
1	B	665	LEU	CB-CA-C	-5.36	100.02	110.20
1	A	806	ARG	CD-NE-CZ	5.36	131.10	123.60
1	B	928	ASN	N-CA-CB	-5.35	100.97	110.60
1	A	756	ASP	C-N-CA	-5.34	108.35	121.70
1	B	691	ILE	C-N-CA	-5.31	108.43	121.70
1	B	921	LEU	CB-CA-C	-5.29	100.14	110.20
1	B	857	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	B	787	LYS	N-CA-C	5.27	125.23	111.00
1	B	1010	LYS	CA-CB-CG	5.25	124.96	113.40
1	A	704	ARG	CB-CG-CD	5.22	125.17	111.60
1	A	963	SER	N-CA-CB	5.22	118.33	110.50
1	A	791	ASP	N-CA-C	5.20	125.03	111.00
1	B	908	CYS	CA-CB-SG	5.18	123.33	114.00
1	B	1009	PHE	CB-CG-CD2	-5.13	117.21	120.80
1	B	1009	PHE	N-CA-C	5.11	124.81	111.00
1	B	912	GLN	C-N-CA	5.10	133.01	122.30
1	B	1010	LYS	N-CA-CB	-5.10	101.42	110.60
1	A	829	TYR	N-CA-C	5.09	124.73	111.00
1	A	697	PRO	C-N-CA	-5.07	109.02	121.70
1	B	992	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	744	PHE	N-CA-C	5.02	124.55	111.00
1	B	966	GLY	C-N-CA	5.02	134.25	121.70
1	A	794	TYR	C-N-CA	-5.01	109.19	121.70
1	B	829	TYR	N-CA-CB	5.01	119.61	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	907	TYR	CG-CD2-CE2	-5.00	117.30	121.30

There are no chirality outliers.

All (42) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	663	SER	Peptide
1	A	694	GLN	Peptide
1	A	703	LYS	Peptide
1	A	744	PHE	Sidechain
1	A	745	GLY	Peptide
1	A	746	MET	Peptide
1	A	782	SER	Peptide
1	A	784	ASP	Peptide
1	A	786	SER	Peptide
1	A	794	TYR	Sidechain
1	A	805	ASP	Peptide
1	A	823	ALA	Peptide
1	A	938	ILE	Peptide
1	A	986	TYR	Sidechain
1	B	1009	PHE	Peptide
1	B	671	ASP	Peptide
1	B	680	GLU	Peptide
1	B	718	GLN	Peptide
1	B	743	ASP	Peptide
1	B	775	TYR	Sidechain
1	B	778	LEU	Peptide
1	B	779	ARG	Sidechain
1	B	783	ASP	Peptide
1	B	787	LYS	Peptide
1	B	797	LEU	Peptide
1	B	798	LYS	Peptide
1	B	806	ARG	Sidechain
1	B	828	ALA	Peptide
1	B	837	PHE	Sidechain
1	B	841	ARG	Sidechain
1	B	854	LEU	Peptide
1	B	857	ARG	Sidechain
1	B	865	ARG	Sidechain
1	B	878	ARG	Sidechain
1	B	882	PRO	Peptide
1	B	920	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	940	LYS	Peptide
1	B	963	SER	Peptide
1	B	964	LEU	Peptide
1	B	966	GLY	Peptide
1	B	981	ASP	Peptide
1	B	984	LEU	Peptide

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	2754	0	2795	96	0
1	B	2754	0	2795	130	0
2	A	29	0	24	1	0
2	B	29	0	24	2	0
3	A	101	0	0	3	0
3	B	90	0	0	2	0
All	All	5757	0	5638	226	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 20.

All (226) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:831:LEU:HG	1:B:1005:LEU:HD21	1.57	0.87
1:B:822:HIS:HE2	1:B:831:LEU:HD22	1.40	0.86
1:B:692:ASP:HB3	1:B:743:ASP:HB2	1.58	0.83
1:B:665:LEU:HB3	1:B:669:VAL:HG13	1.65	0.78
1:A:923:GLU:HG3	1:A:967:VAL:HG11	1.66	0.78
1:B:863:GLY:HA3	1:B:904:SER:O	1.83	0.77
1:B:857:ARG:H	1:B:926:LEU:HB2	1.50	0.76
1:B:686:MET:HB2	1:B:693:LEU:HD11	1.70	0.74
1:B:930:TYR:HB3	1:B:948:VAL:HG22	1.70	0.73
1:A:784:ASP:HA	1:A:785:SER:HB2	1.72	0.72
1:A:684:LYS:O	1:A:688:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:HIS:HE1	1:B:831:LEU:HD13	1.56	0.70
1:A:716:VAL:O	1:A:720:VAL:HG23	1.91	0.69
1:B:702:SER:O	1:B:706:ILE:HG12	1.91	0.69
1:B:822:HIS:CE1	1:B:831:LEU:HD13	2.27	0.69
1:B:770:ASP:HA	1:B:773:VAL:HG12	1.73	0.69
1:B:941:LEU:HD22	1:B:992:TYR:CD1	2.29	0.68
1:A:941:LEU:HD22	1:A:992:TYR:CD1	2.29	0.67
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	1.75	0.67
1:B:822:HIS:NE2	1:B:831:LEU:HD22	2.10	0.67
1:B:879:ILE:HG13	1:B:994:ILE:HG21	1.77	0.66
1:B:829:TYR:HD1	1:B:1007:PHE:HB3	1.61	0.65
1:B:770:ASP:HB2	1:B:868:ASN:OD1	1.94	0.65
1:B:829:TYR:CE1	1:B:1007:PHE:HD2	2.14	0.65
1:A:701:LEU:HD21	1:A:768:LEU:HD13	1.78	0.65
1:A:682:MET:O	1:A:686:MET:HG3	1.96	0.64
1:B:798:LYS:HG3	1:B:842:GLU:CD	2.18	0.64
1:A:941:LEU:HD22	1:A:992:TYR:HD1	1.62	0.64
1:A:710:TYR:CE2	1:A:881:PRO:HG2	2.33	0.63
1:B:672:LEU:HA	1:B:675:MET:HB3	1.81	0.63
1:B:770:ASP:HB3	1:B:868:ASN:HA	1.81	0.63
1:B:941:LEU:HD12	1:B:942:PRO:HD2	1.81	0.62
1:B:685:ALA:HA	1:B:688:GLU:OE2	1.99	0.62
1:B:925:ALA:HB3	1:B:996:GLN:HG2	1.80	0.61
1:B:666:PRO:HB2	1:B:668:PRO:HD2	1.82	0.61
1:B:829:TYR:CD1	1:B:831:LEU:HD11	2.35	0.61
1:A:849:LYS:O	1:A:852:LYS:HB2	2.01	0.61
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.84	0.60
1:A:954:THR:HB	1:A:986:TYR:CD1	2.36	0.60
1:B:897:PHE:HZ	1:B:997:VAL:HG11	1.65	0.60
1:B:911:SER:O	1:B:913:GLY:HA2	2.01	0.60
1:A:706:ILE:HG23	1:A:765:LEU:HD22	1.84	0.60
1:A:777:LEU:HD13	1:A:796:LYS:HG3	1.84	0.60
1:B:712:ILE:HG21	1:B:736:PHE:HB2	1.85	0.58
1:B:857:ARG:HD2	1:B:967:VAL:HG22	1.85	0.58
1:B:936:SER:HB3	1:B:938:ILE:HD12	1.86	0.58
1:B:917:GLY:HA3	1:B:1007:PHE:CE1	2.38	0.58
1:B:837:PHE:HD2	1:B:1002:LEU:O	1.87	0.57
1:B:856:ASN:HA	1:B:857:ARG:CB	2.34	0.57
1:A:918:LEU:HD13	1:A:1002:LEU:HD11	1.86	0.57
1:B:914:ASP:HB2	1:B:916:ILE:HG12	1.86	0.57
1:A:910:THR:HG21	1:A:1007:PHE:CD1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:HIS:CD2	1:A:902:SER:HB2	2.41	0.56
1:A:875:GLN:HB2	1:A:878:ARG:HD3	1.88	0.56
1:B:810:GLU:O	1:B:814:ILE:HG13	2.06	0.56
1:B:829:TYR:CD1	1:B:1007:PHE:HD2	2.23	0.56
1:B:834:ILE:HD11	1:B:1006:LYS:CB	2.35	0.56
1:A:863:GLY:H	1:A:904:SER:HB3	1.72	0.55
1:B:699:GLY:O	1:B:700:LYS:HG2	2.06	0.55
1:B:852:LYS:HD2	1:B:857:ARG:HH12	1.70	0.55
1:B:728:GLN:HB3	3:B:2:HOH:O	2.07	0.55
1:B:1007:PHE:CD1	1:B:1007:PHE:N	2.73	0.55
1:B:843:GLY:O	1:B:846:GLN:HB2	2.07	0.54
1:A:941:LEU:HD12	1:A:942:PRO:HD2	1.90	0.54
1:B:855:HIS:HB3	1:B:927:GLY:HA2	1.88	0.54
1:A:882:PRO:O	1:A:883:GLU:HG3	2.08	0.54
1:B:798:LYS:O	1:B:842:GLU:HG2	2.07	0.54
1:B:673:ILE:CD1	1:B:794:TYR:HD1	2.21	0.54
1:B:693:LEU:HA	1:B:696:MET:O	2.08	0.54
1:A:720:VAL:HG21	1:A:753:ASN:HA	1.89	0.53
1:B:829:TYR:CE1	1:B:831:LEU:HD11	2.44	0.53
1:A:931:GLU:HB3	1:A:951:LEU:HD11	1.89	0.53
1:B:770:ASP:CB	1:B:868:ASN:HA	2.38	0.53
1:A:859:LEU:HG	1:A:921:LEU:HD22	1.91	0.53
1:A:869:PHE:HE2	1:A:920:LEU:HG	1.74	0.53
1:B:685:ALA:O	1:B:688:GLU:HG2	2.09	0.53
1:A:822:HIS:CD2	1:A:831:LEU:HB2	2.44	0.53
1:A:702:SER:OG	1:A:705:GLN:HB3	2.08	0.52
1:B:831:LEU:CG	1:B:1005:LEU:HD21	2.34	0.52
1:B:880:ALA:HB3	1:B:893:LYS:HG2	1.91	0.52
1:A:846:GLN:O	1:A:849:LYS:HB2	2.08	0.52
1:A:948:VAL:HG23	1:A:992:TYR:HE1	1.74	0.52
1:A:663:SER:HB2	1:A:665:LEU:HB2	1.91	0.52
1:B:689:TYR:CG	1:B:764:MET:HG2	2.44	0.52
1:B:835:ASP:H	1:B:1004:LYS:HB3	1.74	0.52
1:B:860:LEU:HD12	1:B:924:VAL:CG1	2.40	0.51
1:B:832:GLU:O	1:B:1005:LEU:HA	2.10	0.51
1:A:919:ILE:HG22	1:A:1003:LEU:HB2	1.92	0.51
1:B:851:PHE:CD1	1:B:996:GLN:HG3	2.46	0.51
1:B:835:ASP:HB2	1:B:837:PHE:CE2	2.45	0.51
1:B:926:LEU:HB3	1:B:929:MET:CE	2.41	0.51
1:B:704:ARG:H	1:B:704:ARG:HD3	1.75	0.51
1:B:917:GLY:HA3	1:B:1007:PHE:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:THR:HB	1:A:986:TYR:CE1	2.46	0.50
1:B:696:MET:HG3	1:B:741:PRO:HD2	1.94	0.50
1:B:801:ILE:HG22	1:B:837:PHE:CD1	2.46	0.50
1:A:702:SER:HB2	1:A:704:ARG:HB2	1.93	0.50
1:B:860:LEU:HD12	1:B:924:VAL:HG13	1.94	0.50
1:A:809:GLU:HA	1:A:812:GLU:HG2	1.92	0.49
1:B:841:ARG:HD2	1:B:999:LEU:HD12	1.94	0.49
1:B:839:ILE:HD12	1:B:999:LEU:HB3	1.94	0.49
1:A:915:PRO:O	1:A:916:ILE:HD13	2.12	0.49
1:B:897:PHE:CZ	1:B:997:VAL:HG11	2.47	0.49
1:A:822:HIS:HD2	1:A:831:LEU:HB2	1.77	0.49
1:A:903:LYS:O	1:A:907:TYR:CE2	2.66	0.49
1:B:864:SER:O	1:B:908:CYS:HA	2.13	0.48
1:A:665:LEU:HD21	1:A:794:TYR:CD1	2.48	0.48
1:B:662:LYS:HA	1:B:788:ASP:OD1	2.13	0.48
1:B:818:VAL:O	1:B:901:VAL:HG11	2.14	0.48
1:B:797:LEU:HD22	1:B:873:LEU:HB2	1.96	0.48
1:A:953:LYS:HB3	1:A:979:VAL:O	2.12	0.48
1:A:903:LYS:HD3	1:A:986:TYR:HD2	1.78	0.48
1:B:839:ILE:HG13	1:B:1000:LYS:O	2.14	0.48
1:A:886:VAL:HA	1:A:893:LYS:HD3	1.96	0.48
1:B:706:ILE:HG23	1:B:765:LEU:HD22	1.95	0.47
1:A:702:SER:O	1:A:706:ILE:HG13	2.15	0.47
1:B:795:GLU:O	1:B:798:LYS:HB3	2.15	0.47
1:B:903:LYS:HZ2	2:B:502:FRQ:H6	1.78	0.47
1:B:950:GLY:O	1:B:987:ASN:HA	2.14	0.47
1:A:948:VAL:HB	1:A:990:ILE:HD13	1.96	0.47
1:B:891:PHE:HA	1:B:936:SER:O	2.15	0.47
1:B:910:THR:O	1:B:1009:PHE:HZ	1.98	0.47
1:A:859:LEU:HD12	1:A:859:LEU:HA	1.75	0.46
1:A:805:ASP:OD1	1:A:806:ARG:HD2	2.15	0.46
1:B:852:LYS:HD2	1:B:857:ARG:NH1	2.30	0.46
1:B:673:ILE:HD11	1:B:794:TYR:HD1	1.81	0.46
1:A:663:SER:CB	1:A:665:LEU:HB2	2.46	0.46
1:A:762:VAL:HG11	1:A:888:GLY:HA3	1.98	0.46
1:A:952:GLY:H	1:A:987:ASN:HD22	1.62	0.46
1:B:776:SER:O	1:B:779:ARG:HG3	2.16	0.46
1:B:921:LEU:HD12	1:B:1001:TYR:HB2	1.98	0.46
1:A:858:ARG:HD2	1:A:860:LEU:HD21	1.98	0.46
1:A:895:ILE:HG22	1:A:897:PHE:CE1	2.51	0.46
1:A:864:SER:HB3	1:A:869:PHE:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:SER:HB3	2:A:501:FRQ:O14	2.17	0.45
1:B:744:PHE:HD1	1:B:744:PHE:O	1.99	0.45
1:B:905:ALA:HB1	1:B:1007:PHE:HE2	1.80	0.45
1:A:703:LYS:O	1:A:707:GLN:HG3	2.16	0.45
1:A:749:PRO:O	1:A:751:LEU:HD22	2.16	0.45
1:A:749:PRO:HA	1:A:750:PRO:HD3	1.80	0.45
1:A:841:ARG:HD2	1:A:873:LEU:O	2.17	0.45
1:B:962:ILE:HG23	1:B:963:SER:H	1.81	0.45
1:A:677:PHE:HB3	1:A:778:LEU:HD12	1.99	0.45
1:B:963:SER:OG	1:B:966:GLY:N	2.49	0.45
1:A:748:LYS:HA	1:A:749:PRO:HD3	1.74	0.45
1:A:769:LEU:O	1:A:773:VAL:HG23	2.16	0.45
1:A:969:VAL:HA	1:A:970:PRO:HD3	1.79	0.45
1:A:696:MET:HA	1:A:697:PRO:HD3	1.82	0.45
1:B:879:ILE:CG1	1:B:994:ILE:HG21	2.46	0.45
1:B:889:TYR:HA	3:B:24:HOH:O	2.17	0.44
1:A:739:LEU:HA	1:A:739:LEU:HD12	1.57	0.44
1:B:695:LYS:HE3	1:B:695:LYS:HB3	1.75	0.44
1:A:928:ASN:HD21	1:A:946:HIS:CE1	2.36	0.44
1:B:777:LEU:HD12	1:B:796:LYS:HB3	2.00	0.44
1:A:809:GLU:HA	1:A:812:GLU:CG	2.47	0.44
1:B:809:GLU:HA	1:B:812:GLU:HG3	1.99	0.44
1:B:931:GLU:HB3	1:B:951:LEU:HD11	2.00	0.44
1:B:703:LYS:HB2	1:B:704:ARG:HH11	1.82	0.44
1:A:703:LYS:H	1:A:703:LYS:HD3	1.83	0.44
1:A:746:MET:SD	1:A:746:MET:N	2.90	0.44
1:A:973:THR:O	1:A:975:ILE:HG12	2.18	0.44
1:B:755:ALA:HA	1:B:758:VAL:HG22	1.99	0.44
1:B:821:THR:O	1:B:900:MET:HG3	2.17	0.44
1:B:957:ASP:HA	1:B:958:PRO:HD3	1.70	0.44
1:B:665:LEU:HD23	1:B:669:VAL:HG22	2.01	0.43
1:A:754:ASN:HB3	3:A:190:HOH:O	2.17	0.43
1:A:808:SER:HA	3:A:157:HOH:O	2.18	0.43
1:A:745:GLY:O	1:A:746:MET:SD	2.76	0.43
1:B:822:HIS:CD2	1:B:901:VAL:HG13	2.53	0.43
1:A:696:MET:O	1:A:696:MET:HG3	2.17	0.43
1:A:852:LYS:O	1:A:857:ARG:CZ	2.66	0.43
1:B:829:TYR:CE1	1:B:1007:PHE:CD2	3.02	0.43
1:A:769:LEU:HD11	1:A:881:PRO:HG3	2.00	0.43
1:A:915:PRO:HB2	1:A:1007:PHE:O	2.19	0.43
1:A:948:VAL:HG23	1:A:992:TYR:CE1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:LYS:HA	1:B:816:LYS:HD3	1.82	0.43
1:B:817:TYR:OH	1:B:970:PRO:HD2	2.19	0.43
1:B:814:ILE:HG22	1:B:1003:LEU:HD21	2.01	0.43
1:B:840:GLU:HG3	1:B:845:CYS:SG	2.59	0.43
1:A:663:SER:HA	1:A:664:LYS:NZ	2.33	0.42
1:A:713:LEU:O	1:A:716:VAL:HG12	2.20	0.42
1:B:754:ASN:HB3	1:B:757:SER:H	1.84	0.42
1:B:713:LEU:HD12	1:B:765:LEU:HD12	2.00	0.42
1:A:811:ALA:O	1:A:815:ARG:HG3	2.19	0.42
1:A:928:ASN:ND2	1:A:946:HIS:CE1	2.88	0.42
1:B:673:ILE:HG21	1:B:790:ILE:O	2.20	0.42
1:B:697:PRO:O	1:B:698:LEU:C	2.56	0.42
1:B:672:LEU:HD11	1:B:918:LEU:HD21	2.02	0.42
1:B:912:GLN:HG3	1:B:1009:PHE:CD2	2.55	0.42
1:A:844:GLU:OE2	1:A:998:ASN:HB2	2.20	0.42
1:A:1010:LYS:HA	1:A:1010:LYS:HD2	1.82	0.42
1:B:689:TYR:O	1:B:690:GLU:HG2	2.19	0.42
1:A:895:ILE:HG22	1:A:897:PHE:CZ	2.55	0.42
1:B:813:ILE:HD12	1:B:964:LEU:HD13	2.01	0.42
1:A:679:VAL:HG13	1:A:682:MET:HE3	2.01	0.41
1:B:788:ASP:O	1:B:789:PRO:C	2.59	0.41
1:A:781:GLY:H	1:A:796:LYS:NZ	2.19	0.41
1:A:823:ALA:O	1:A:825:THR:N	2.54	0.41
1:A:860:LEU:HD13	1:A:989:TYR:CD1	2.55	0.41
1:A:670:GLN:HG2	1:A:790:ILE:HG21	2.02	0.41
1:B:769:LEU:HD23	1:B:769:LEU:HA	1.89	0.41
1:A:926:LEU:HD13	1:A:929:MET:HE2	2.03	0.41
1:B:877:LEU:HD23	1:B:877:LEU:HA	1.81	0.41
1:B:889:TYR:HE2	2:B:502:FRQ:H292	1.86	0.41
1:A:874:SER:C	1:A:875:GLN:HG2	2.41	0.41
1:A:938:ILE:HB	1:A:940:LYS:H	1.85	0.41
1:B:674:LYS:HB3	1:B:790:ILE:HD11	2.02	0.41
1:B:829:TYR:HE1	1:B:1007:PHE:HD2	1.63	0.41
1:B:797:LEU:HD23	1:B:797:LEU:HA	1.86	0.41
1:B:823:ALA:HB3	1:B:826:HIS:HE1	1.85	0.41
1:B:917:GLY:O	1:B:918:LEU:HD12	2.21	0.41
1:A:928:ASN:ND2	1:A:946:HIS:ND1	2.68	0.41
1:B:716:VAL:O	1:B:719:ALA:HB3	2.21	0.41
1:B:903:LYS:HE2	1:B:985:LEU:HD13	2.02	0.41
1:B:962:ILE:HG23	1:B:963:SER:N	2.35	0.41
1:A:854:LEU:HD22	1:A:854:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:SER:HA	1:A:905:ALA:HB3	2.01	0.41
1:B:752:LEU:CD2	1:B:757:SER:HB3	2.51	0.40
1:B:814:ILE:HD13	1:B:814:ILE:HG21	1.90	0.40
1:B:841:ARG:CZ	1:B:841:ARG:HB3	2.50	0.40
1:A:811:ALA:HB1	1:A:836:ILE:HD13	2.03	0.40
1:A:824:THR:HA	3:A:169:HOH:O	2.20	0.40
1:B:805:ASP:O	1:B:807:ASP:N	2.54	0.40
1:B:941:LEU:HD22	1:B:992:TYR:HD1	1.80	0.40
1:A:802:LYS:HB3	1:A:838:LYS:HG2	2.03	0.40
1:B:829:TYR:HE1	1:B:1007:PHE:CD2	2.39	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	348/350 (99%)	271 (78%)	56 (16%)	21 (6%)	1	9
1	B	348/350 (99%)	259 (74%)	57 (16%)	32 (9%)	1	3
All	All	696/700 (99%)	530 (76%)	113 (16%)	53 (8%)	1	5

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	664	LYS
1	A	690	GLU
1	A	809	GLU
1	A	824	THR
1	A	829	TYR
1	A	981	ASP
1	A	1009	PHE
1	B	747	LYS

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Mol	Chain	Res	Type
1	B	789	PRO
1	B	797	LEU
1	B	829	TYR
1	B	855	HIS
1	B	883	GLU
1	B	943	LYS
1	B	964	LEU
1	A	701	LEU
1	A	704	ARG
1	A	725	SER
1	A	806	ARG
1	A	883	GLU
1	A	962	ILE
1	A	974	GLY
1	B	671	ASP
1	B	699	GLY
1	B	723	GLY
1	B	778	LEU
1	B	785	SER
1	B	805	ASP
1	B	806	ARG
1	B	826	HIS
1	B	857	ARG
1	B	877	LEU
1	B	974	GLY
1	B	987	ASN
1	A	780	GLY
1	B	722	GLN
1	B	788	ASP
1	B	973	THR
1	B	985	LEU
1	A	729	ILE
1	A	798	LYS
1	A	912	GLN
1	A	914	ASP
1	B	819	LYS
1	A	881	PRO
1	B	962	ILE
1	B	967	VAL
1	A	959	SER
1	B	846	GLN
1	B	882	PRO

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Mol	Chain	Res	Type
1	B	970	PRO
1	B	667	LYS
1	B	780	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	308/308 (100%)	241 (78%)	67 (22%)	1 5
1	B	308/308 (100%)	241 (78%)	67 (22%)	1 5
All	All	616/616 (100%)	482 (78%)	134 (22%)	1 5

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	663	SER
1	A	664	LYS
1	A	665	LEU
1	A	667	LYS
1	A	672	LEU
1	A	679	VAL
1	A	680	GLU
1	A	683	LYS
1	A	690	GLU
1	A	693	LEU
1	A	696	MET
1	A	698	LEU
1	A	703	LYS
1	A	704	ARG
1	A	705	GLN
1	A	707	GLN
1	A	711	SER
1	A	716	VAL
1	A	720	VAL
1	A	722	GLN

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Mol	Chain	Res	Type
1	A	726	ASP
1	A	727	SER
1	A	744	PHE
1	A	753	ASN
1	A	756	ASP
1	A	758	VAL
1	A	762	VAL
1	A	778	LEU
1	A	779	ARG
1	A	783	ASP
1	A	800	ASP
1	A	801	ILE
1	A	806	ARG
1	A	812	GLU
1	A	814	ILE
1	A	817	TYR
1	A	824	THR
1	A	831	LEU
1	A	838	LYS
1	A	841	ARG
1	A	844	GLU
1	A	849	LYS
1	A	854	LEU
1	A	857	ARG
1	A	875	GLN
1	A	879	ILE
1	A	887	THR
1	A	893	LYS
1	A	904	SER
1	A	906	ASN
1	A	908	CYS
1	A	911	SER
1	A	912	GLN
1	A	924	VAL
1	A	928	ASN
1	A	940	LYS
1	A	943	LYS
1	A	955	THR
1	A	964	LEU
1	A	967	VAL
1	A	971	LEU
1	A	973	THR

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Mol	Chain	Res	Type
1	A	976	SER
1	A	980	ASN
1	A	981	ASP
1	A	998	ASN
1	A	1002	LEU
1	B	669	VAL
1	B	672	LEU
1	B	674	LYS
1	B	675	MET
1	B	677	PHE
1	B	683	LYS
1	B	688	GLU
1	B	690	GLU
1	B	695	LYS
1	B	702	SER
1	B	704	ARG
1	B	714	SER
1	B	731	ASP
1	B	744	PHE
1	B	747	LYS
1	B	748	LYS
1	B	751	LEU
1	B	754	ASN
1	B	756	ASP
1	B	759	GLN
1	B	761	LYS
1	B	767	ASN
1	B	779	ARG
1	B	783	ASP
1	B	784	ASP
1	B	785	SER
1	B	798	LYS
1	B	801	ILE
1	B	806	ARG
1	B	807	ASP
1	B	817	TYR
1	B	819	LYS
1	B	820	ASN
1	B	822	HIS
1	B	824	THR
1	B	826	HIS
1	B	829	TYR

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Mol	Chain	Res	Type
1	B	834	ILE
1	B	835	ASP
1	B	838	LYS
1	B	839	ILE
1	B	847	ARG
1	B	852	LYS
1	B	854	LEU
1	B	878	ARG
1	B	887	THR
1	B	893	LYS
1	B	900	MET
1	B	904	SER
1	B	912	GLN
1	B	924	VAL
1	B	938	ILE
1	B	939	SER
1	B	941	LEU
1	B	955	THR
1	B	961	ASN
1	B	962	ILE
1	B	965	ASP
1	B	981	ASP
1	B	982	THR
1	B	985	LEU
1	B	991	VAL
1	B	994	ILE
1	B	996	GLN
1	B	1006	LYS
1	B	1007	PHE
1	B	1009	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	718	GLN
1	A	722	GLN
1	A	822	HIS
1	A	912	GLN
1	A	928	ASN
1	A	934	HIS
1	B	717	GLN
1	B	728	GLN

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Mol	Chain	Res	Type
1	B	820	ASN
1	B	826	HIS
1	B	827	ASN
1	B	996	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FRQ	A	501	-	28,32,32	2.22	7 (25%)	33,44,44	3.06	9 (27%)
2	FRQ	B	502	-	28,32,32	2.12	9 (32%)	33,44,44	2.63	8 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRQ	A	501	-	-	2/11/21/21	0/4/4/4
2	FRQ	B	502	-	-	4/11/21/21	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FRQ	C30-C31	-5.22	1.34	1.50
2	A	501	FRQ	C5-C4	-5.04	1.36	1.42
2	B	502	FRQ	C4-C3	-4.93	1.37	1.42
2	B	502	FRQ	C5-C4	-4.62	1.36	1.42
2	A	501	FRQ	C4-C3	-4.61	1.37	1.42
2	B	502	FRQ	C30-C31	-4.25	1.37	1.50
2	B	502	FRQ	C32-C31	3.97	1.50	1.35
2	A	501	FRQ	C32-C31	3.91	1.50	1.35
2	A	501	FRQ	C11-N12	-3.87	1.28	1.37
2	A	501	FRQ	C3-N10	-3.76	1.35	1.40
2	B	502	FRQ	C3-N10	-3.56	1.36	1.40
2	A	501	FRQ	F53-C5	-3.02	1.31	1.36
2	B	502	FRQ	C11-N12	-2.86	1.31	1.37
2	B	502	FRQ	C6-C5	2.33	1.39	1.36
2	B	502	FRQ	C33-N26	-2.21	1.44	1.46
2	B	502	FRQ	F53-C5	-2.00	1.32	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	FRQ	C11-N12-C13	11.71	124.98	115.09
2	B	502	FRQ	C11-N12-C13	10.53	123.99	115.09
2	A	501	FRQ	C33-N26-C29	7.51	117.23	109.78
2	B	502	FRQ	C33-N26-C29	5.78	115.52	109.78
2	A	501	FRQ	C29-C30-C31	5.16	126.16	112.38
2	A	501	FRQ	C33-C32-C31	-4.69	110.55	123.88
2	A	501	FRQ	C32-C33-N26	-4.47	109.36	112.89
2	B	502	FRQ	C29-C30-C31	4.47	124.31	112.38
2	A	501	FRQ	C4-C3-N10	-3.43	116.76	118.87
2	B	502	FRQ	C33-C32-C31	-3.37	114.30	123.88
2	A	501	FRQ	C23-N26-C29	3.08	119.45	111.24
2	B	502	FRQ	C23-N26-C29	3.04	119.33	111.24
2	B	502	FRQ	C6-C5-C4	-2.95	121.33	123.99
2	A	501	FRQ	C6-C5-C4	-2.39	121.84	123.99
2	A	501	FRQ	C2-C3-N10	2.35	123.56	121.43
2	B	502	FRQ	C32-C33-N26	-2.19	111.16	112.89
2	B	502	FRQ	C30-C31-C32	-2.09	118.89	120.63

There are no chirality outliers.

All (6) torsion outliers are listed below:

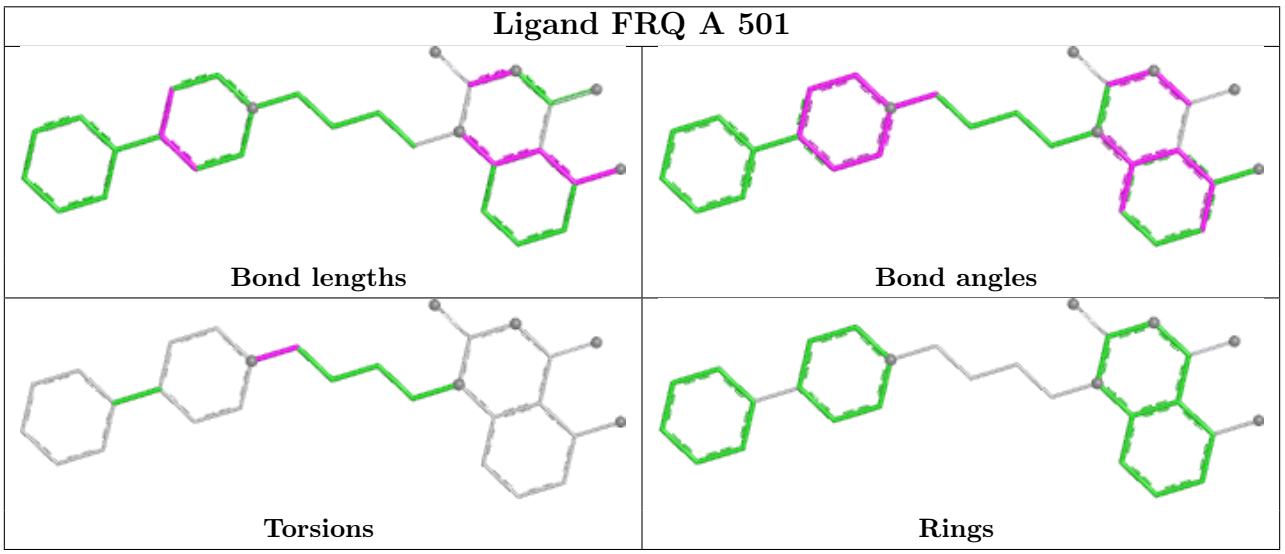
Mol	Chain	Res	Type	Atoms
2	B	502	FRQ	N10-C16-C17-C20
2	A	501	FRQ	C20-C23-N26-C29
2	A	501	FRQ	C20-C23-N26-C33
2	B	502	FRQ	C17-C20-C23-N26
2	B	502	FRQ	C16-C17-C20-C23
2	B	502	FRQ	C20-C23-N26-C29

There are no ring outliers.

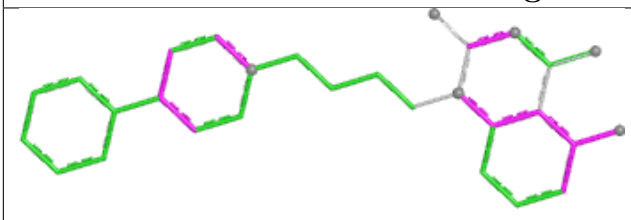
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	FRQ	1	0
2	B	502	FRQ	2	0

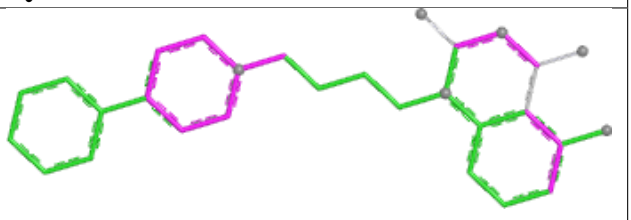
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



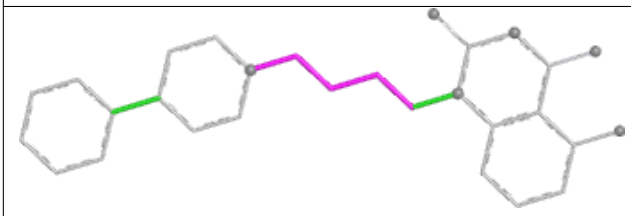
Ligand FRQ B 502



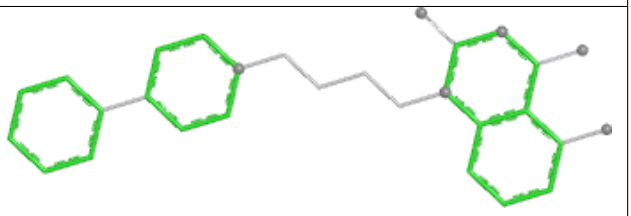
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	350/350 (100%)	0.07	9 (2%)	56	27	2, 15, 31, 42	0
1	B	350/350 (100%)	0.21	16 (4%)	32	12	2, 17, 33, 44	0
All	All	700/700 (100%)	0.14	25 (3%)	42	17	2, 16, 32, 44	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	783	ASP	5.1
1	B	785	SER	5.0
1	B	784	ASP	4.7
1	B	825	THR	3.8
1	A	782	SER	3.4
1	B	826	HIS	3.3
1	A	790	ILE	3.3
1	B	775	TYR	3.1
1	B	799	THR	3.0
1	A	827	ASN	2.9
1	B	786	SER	2.9
1	B	744	PHE	2.7
1	B	664	LYS	2.7
1	B	902	SER	2.5
1	A	791	ASP	2.4
1	A	785	SER	2.4
1	A	722	GLN	2.3
1	B	963	SER	2.3
1	A	784	ASP	2.2
1	A	788	ASP	2.2
1	A	787	LYS	2.2
1	B	796	LYS	2.2
1	B	828	ALA	2.2
1	B	680	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	964	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 monosaccharides in this entry.

6.4 Ligands (i)

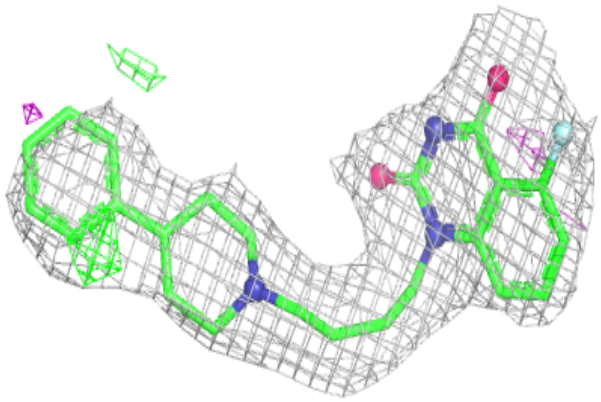
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

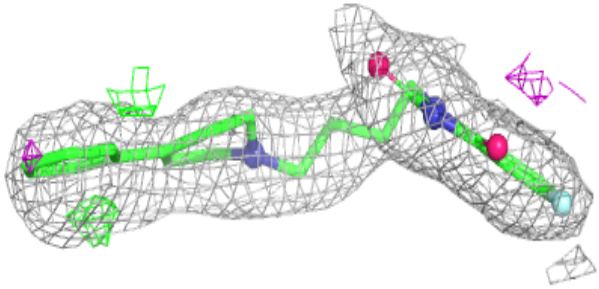
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FRQ	B	502	29/29	0.90	0.25	2,10,16,17	0
2	FRQ	A	501	29/29	0.92	0.25	3,11,19,20	0

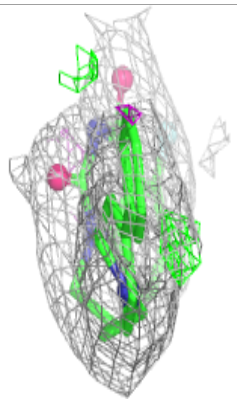
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FRQ B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

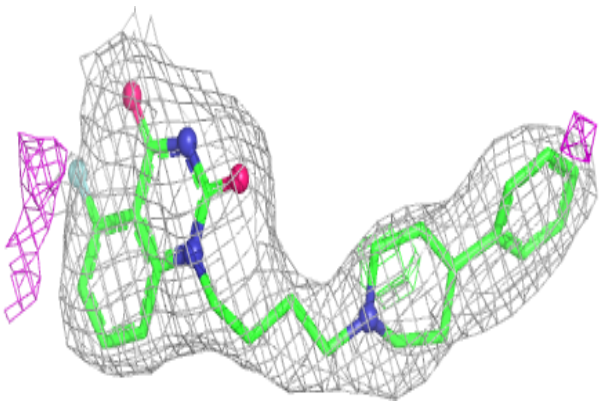


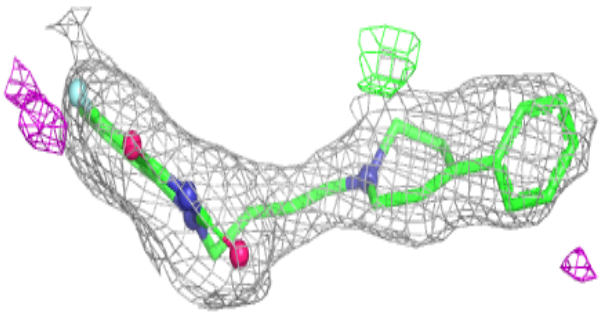


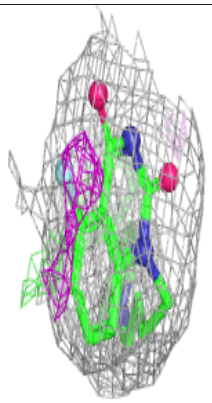


Electron density around FRQ A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.