Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2022 – 06:15 pm GMT

PDB ID	:	6QPO
Title	:	Adenovirus species D serotype 49 Fiber-Knob KO1 mutant
Authors	:	Baker, A.T.; Rizkallah, P.J.
Deposited on	:	2019-02-14
Resolution	:	2.45 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

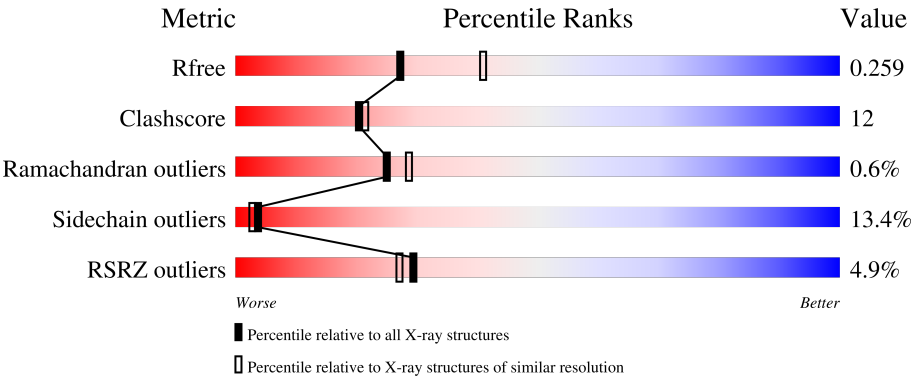
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.45 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.



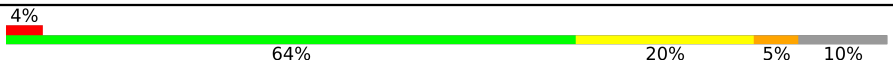
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	223	2% 62% 22% • 10%
1	B	223	9% 59% 25% 5% 10%
1	C	223	4% 62% 23% • 10%
1	D	223	6% 66% 18% • • 10%
1	E	223	2% 63% 22% • 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	223	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9346 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 Fiber.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	0	0
			1552	984	253	311	4			
1	B	200	Total	C	N	O	S	0	0	0
			1552	984	253	311	4			
1	C	200	Total	C	N	O	S	0	0	0
			1552	984	253	311	4			
1	D	200	Total	C	N	O	S	0	0	0
			1552	984	253	311	4			
1	E	200	Total	C	N	O	S	0	0	0
			1552	984	253	311	4			
1	F	200	Total	C	N	O	S	0	0	0
			1552	984	253	311	4			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	MET	-	initiating methionine	UNP Q09TX9
A	377	LYS	-	expression tag	UNP Q09TX9
A	378	ARG	-	expression tag	UNP Q09TX9
A	379	HIS	-	expression tag	UNP Q09TX9
A	380	HIS	-	expression tag	UNP Q09TX9
A	381	HIS	-	expression tag	UNP Q09TX9
A	382	HIS	-	expression tag	UNP Q09TX9
A	383	HIS	-	expression tag	UNP Q09TX9
A	384	HIS	-	expression tag	UNP Q09TX9
A	385	GLY	-	expression tag	UNP Q09TX9
A	386	SER	-	expression tag	UNP Q09TX9
A	408	GLU	SER	conflict	UNP Q09TX9
A	409	ALA	PRO	conflict	UNP Q09TX9
B	376	MET	-	initiating methionine	UNP Q09TX9
B	377	LYS	-	expression tag	UNP Q09TX9
B	378	ARG	-	expression tag	UNP Q09TX9
B	379	HIS	-	expression tag	UNP Q09TX9

Continued on next page...

Continued from previous page...

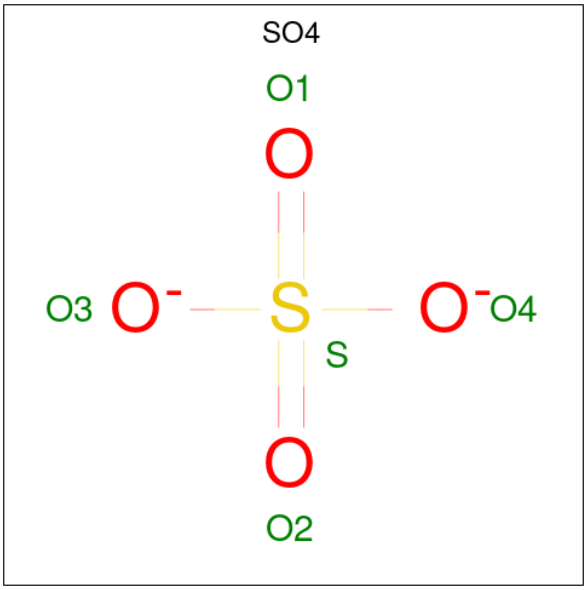
Chain	Residue	Modelled	Actual	Comment	Reference
B	380	HIS	-	expression tag	UNP Q09TX9
B	381	HIS	-	expression tag	UNP Q09TX9
B	382	HIS	-	expression tag	UNP Q09TX9
B	383	HIS	-	expression tag	UNP Q09TX9
B	384	HIS	-	expression tag	UNP Q09TX9
B	385	GLY	-	expression tag	UNP Q09TX9
B	386	SER	-	expression tag	UNP Q09TX9
B	408	GLU	SER	conflict	UNP Q09TX9
B	409	ALA	PRO	conflict	UNP Q09TX9
C	376	MET	-	initiating methionine	UNP Q09TX9
C	377	LYS	-	expression tag	UNP Q09TX9
C	378	ARG	-	expression tag	UNP Q09TX9
C	379	HIS	-	expression tag	UNP Q09TX9
C	380	HIS	-	expression tag	UNP Q09TX9
C	381	HIS	-	expression tag	UNP Q09TX9
C	382	HIS	-	expression tag	UNP Q09TX9
C	383	HIS	-	expression tag	UNP Q09TX9
C	384	HIS	-	expression tag	UNP Q09TX9
C	385	GLY	-	expression tag	UNP Q09TX9
C	386	SER	-	expression tag	UNP Q09TX9
C	408	GLU	SER	conflict	UNP Q09TX9
C	409	ALA	PRO	conflict	UNP Q09TX9
D	376	MET	-	initiating methionine	UNP Q09TX9
D	377	LYS	-	expression tag	UNP Q09TX9
D	378	ARG	-	expression tag	UNP Q09TX9
D	379	HIS	-	expression tag	UNP Q09TX9
D	380	HIS	-	expression tag	UNP Q09TX9
D	381	HIS	-	expression tag	UNP Q09TX9
D	382	HIS	-	expression tag	UNP Q09TX9
D	383	HIS	-	expression tag	UNP Q09TX9
D	384	HIS	-	expression tag	UNP Q09TX9
D	385	GLY	-	expression tag	UNP Q09TX9
D	386	SER	-	expression tag	UNP Q09TX9
D	408	GLU	SER	conflict	UNP Q09TX9
D	409	ALA	PRO	conflict	UNP Q09TX9
E	376	MET	-	initiating methionine	UNP Q09TX9
E	377	LYS	-	expression tag	UNP Q09TX9
E	378	ARG	-	expression tag	UNP Q09TX9
E	379	HIS	-	expression tag	UNP Q09TX9
E	380	HIS	-	expression tag	UNP Q09TX9
E	381	HIS	-	expression tag	UNP Q09TX9
E	382	HIS	-	expression tag	UNP Q09TX9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	383	HIS	-	expression tag	UNP Q09TX9
E	384	HIS	-	expression tag	UNP Q09TX9
E	385	GLY	-	expression tag	UNP Q09TX9
E	386	SER	-	expression tag	UNP Q09TX9
E	408	GLU	SER	conflict	UNP Q09TX9
E	409	ALA	PRO	conflict	UNP Q09TX9
F	376	MET	-	initiating methionine	UNP Q09TX9
F	377	LYS	-	expression tag	UNP Q09TX9
F	378	ARG	-	expression tag	UNP Q09TX9
F	379	HIS	-	expression tag	UNP Q09TX9
F	380	HIS	-	expression tag	UNP Q09TX9
F	381	HIS	-	expression tag	UNP Q09TX9
F	382	HIS	-	expression tag	UNP Q09TX9
F	383	HIS	-	expression tag	UNP Q09TX9
F	384	HIS	-	expression tag	UNP Q09TX9
F	385	GLY	-	expression tag	UNP Q09TX9
F	386	SER	-	expression tag	UNP Q09TX9
F	408	GLU	SER	conflict	UNP Q09TX9
F	409	ALA	PRO	conflict	UNP Q09TX9

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

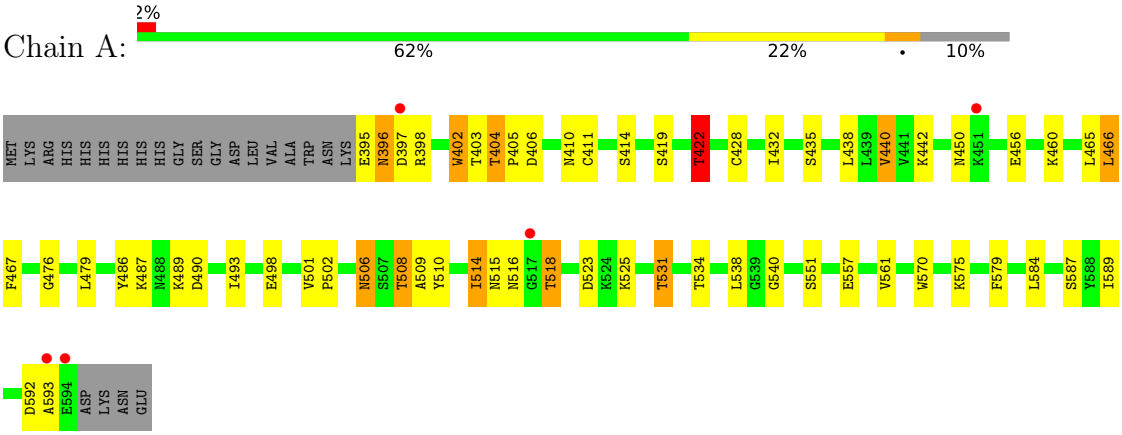
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	11	Total O 11 11	0	0
3	B	7	Total O 7 7	0	0
3	C	3	Total O 3 3	0	0
3	D	4	Total O 4 4	0	0
3	E	2	Total O 2 2	0	0
3	F	2	Total O 2 2	0	0

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.

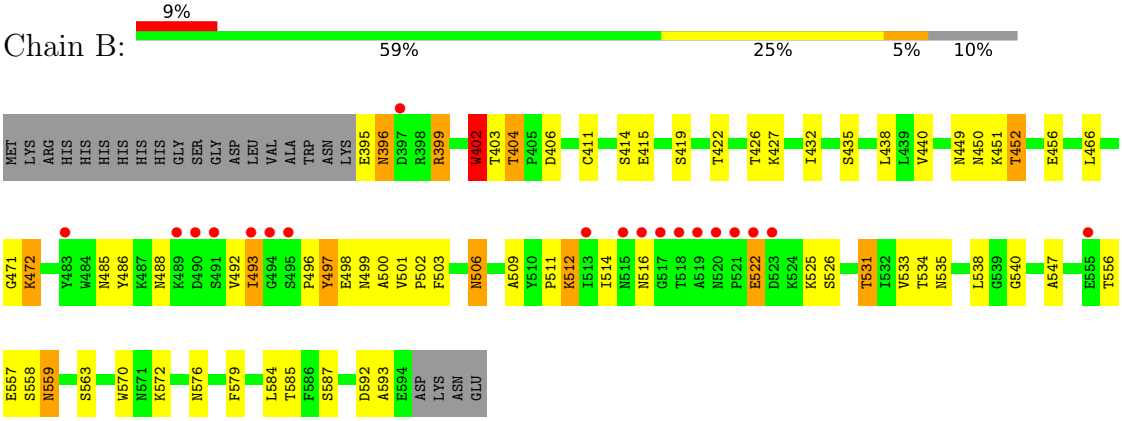
• Molecule 1: Fiber

Chain A:



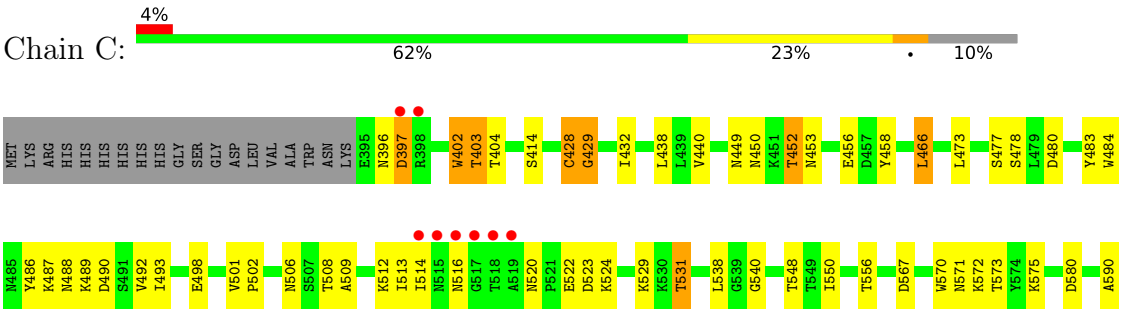
• Molecule 1: Fiber

Chain B:



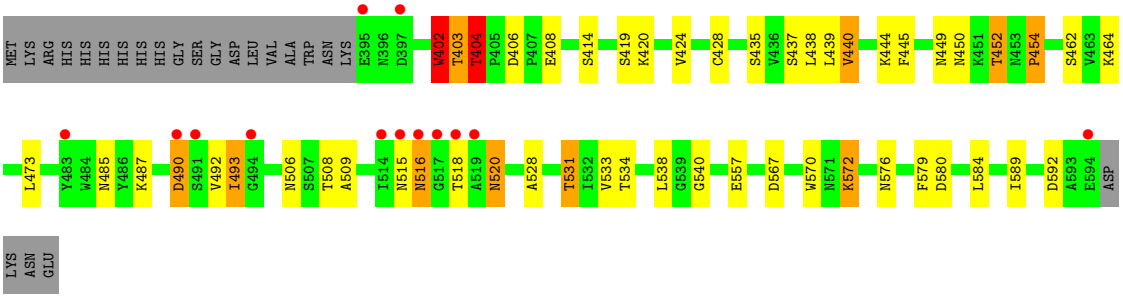
• Molecule 1: Fiber

Chain C:



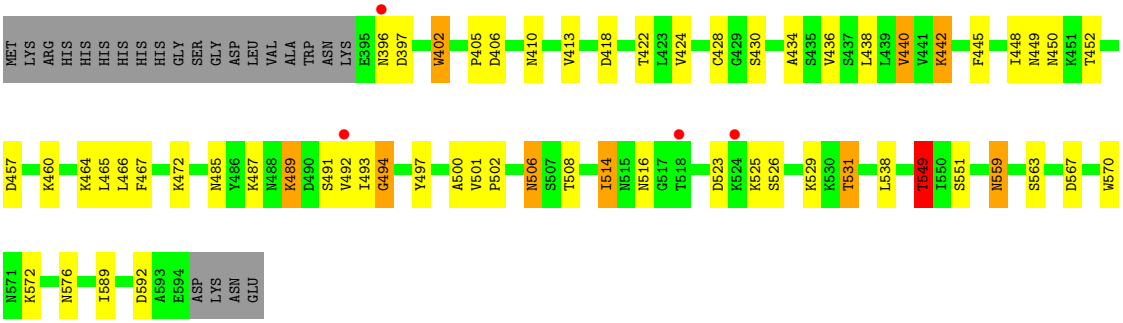
• Molecule 1: Fiber

Chain D:



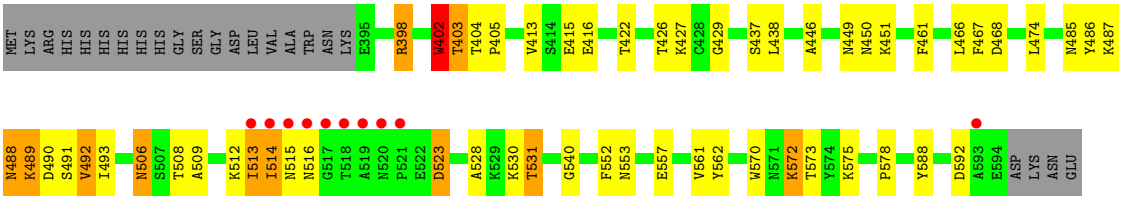
• Molecule 1: Fiber

Chain E:



• Molecule 1: Fiber

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	105.17Å 55.99Å 116.03Å 90.00° 112.47° 90.00°	Depositor
Resolution (Å)	57.06 – 2.45 57.06 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.0 (57.06-2.45) 99.0 (57.06-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.193 , 0.258 0.196 , 0.259	Depositor DCC
R_{free} test set	2225 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	60.0	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9346	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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: SO4

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	0.84	1/1585 (0.1%)	1.05	1/2152 (0.0%)
1	B	0.83	2/1585 (0.1%)	1.05	1/2152 (0.0%)
1	C	0.78	0/1585	1.00	1/2152 (0.0%)
1	D	0.83	0/1585	1.04	2/2152 (0.1%)
1	E	0.75	0/1585	1.00	1/2152 (0.0%)
1	F	0.79	0/1585	0.99	0/2152
All	All	0.81	3/9510 (0.0%)	1.02	6/12912 (0.0%)

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	B	0	3
1	D	0	1
1	F	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	415	GLU	CD-OE1	6.51	1.32	1.25
1	A	551	SER	CA-CB	-5.24	1.45	1.52
1	B	435	SER	CA-CB	-5.05	1.45	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	404	THR	CA-CB-OG1	-7.10	94.09	109.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	454	PRO	N-CA-C	-6.51	95.18	112.10
1	A	422	THR	CB-CA-C	6.13	128.17	111.60
1	E	549	THR	CB-CA-C	5.31	125.94	111.60
1	D	404	THR	CB-CA-C	5.07	125.28	111.60
1	C	428	CYS	CA-CB-SG	5.06	123.11	114.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	402	TRP	Peptide
1	B	496	PRO	Peptide
1	B	522	GLU	Peptide
1	D	402	TRP	Peptide
1	F	402	TRP	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	1552	0	1529	42	0
1	B	1552	0	1529	55	0
1	C	1552	0	1529	36	0
1	D	1552	0	1529	42	0
1	E	1552	0	1529	48	0
1	F	1552	0	1529	33	0
2	A	5	0	0	0	0
3	A	11	0	0	1	0
3	B	7	0	0	0	0
3	C	3	0	0	0	0
3	D	4	0	0	2	0
3	E	2	0	0	0	0
3	F	2	0	0	1	0
All	All	9346	0	9174	229	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 12.

All (229) 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:485:ASN:CG	1:B:493:ILE:HD11	1.59	1.22
1:B:471:GLY:O	1:B:497:TYR:OH	1.66	1.13
1:B:485:ASN:ND2	1:B:493:ILE:HD11	1.78	0.99
1:E:396:ASN:OD1	1:F:429:GLY:HA2	1.68	0.94
1:E:397:ASP:HB2	1:E:487:LYS:O	1.68	0.94
1:A:508:THR:HG23	1:B:406:ASP:HB2	1.49	0.92
1:B:485:ASN:HB3	1:B:492:VAL:CG2	2.00	0.91
1:B:485:ASN:CG	1:B:493:ILE:CD1	2.39	0.90
1:A:514:ILE:HD13	1:A:514:ILE:O	1.71	0.89
1:A:422:THR:HG21	1:C:529:LYS:HZ1	1.38	0.86
1:D:515:ASN:HD21	1:D:518:THR:HG23	1.40	0.86
1:A:428:CYS:SG	3:A:706:HOH:O	2.34	0.85
1:B:485:ASN:OD1	1:B:493:ILE:HD11	1.76	0.84
1:B:526:SER:OG	1:C:580:ASP:OD1	1.94	0.84
1:A:540:GLY:HA3	1:C:531:THR:HG21	1.58	0.84
1:E:449:ASN:HD22	1:E:576:ASN:HD21	1.28	0.81
1:B:511:PRO:HA	1:B:512:LYS:NZ	1.96	0.80
1:B:485:ASN:ND2	1:B:493:ILE:CD1	2.45	0.79
1:B:403:THR:HG21	1:B:422:THR:HA	1.64	0.78
1:C:403:THR:OG1	1:C:404:THR:N	2.14	0.77
1:A:450:ASN:HD21	1:A:570:TRP:HE1	1.35	0.73
1:C:506:ASN:HD22	1:C:509:ALA:H	1.37	0.73
1:E:449:ASN:HD22	1:E:576:ASN:ND2	1.85	0.72
1:E:514:ILE:HD13	1:E:514:ILE:O	1.89	0.72
1:A:422:THR:HG21	1:C:529:LYS:NZ	2.04	0.71
1:A:516:ASN:HD21	1:A:525:LYS:H	1.39	0.70
1:D:506:ASN:HD22	1:D:509:ALA:H	1.38	0.70
1:E:450:ASN:HD21	1:E:570:TRP:HE1	1.40	0.70
1:B:450:ASN:HD21	1:B:570:TRP:HE1	1.40	0.70
1:D:516:ASN:HD22	1:D:516:ASN:H	1.40	0.69
1:D:516:ASN:HD22	1:D:516:ASN:N	1.89	0.69
1:D:506:ASN:ND2	1:D:508:THR:H	1.90	0.69
1:D:580:ASP:OD1	1:E:526:SER:OG	2.12	0.68
1:A:531:THR:HG21	1:B:540:GLY:HA3	1.75	0.67
1:B:485:ASN:HB3	1:B:492:VAL:HG23	1.75	0.67
1:D:440:VAL:HG13	1:D:579:PHE:HB3	1.75	0.67
1:F:450:ASN:HD21	1:F:570:TRP:HE1	1.41	0.67
1:C:402:TRP:CZ2	1:C:487:LYS:HG3	2.31	0.66
1:B:449:ASN:HD22	1:B:576:ASN:ND2	1.94	0.66
1:F:403:THR:HG22	1:F:404:THR:O	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:540:GLY:HA3	1:E:531:THR:HG21	1.78	0.65
1:B:531:THR:HG21	1:C:540:GLY:HA3	1.80	0.64
1:A:506:ASN:HD21	1:A:508:THR:HB	1.62	0.63
1:A:396:ASN:ND2	1:C:429:GLY:HA2	2.13	0.63
1:A:428:CYS:O	1:B:426:THR:HG21	1.98	0.63
1:A:502:PRO:HG3	1:A:593:ALA:HB2	1.81	0.62
1:C:397:ASP:HB2	1:C:487:LYS:O	1.99	0.62
1:B:472:LYS:HG3	1:B:498:GLU:O	2.00	0.62
1:B:511:PRO:HA	1:B:512:LYS:HZ3	1.62	0.62
1:A:403:THR:O	1:A:404:THR:HB	2.00	0.61
1:B:485:ASN:OD1	1:B:497:TYR:HB3	2.01	0.61
1:B:399:ARG:HG3	1:B:427:LYS:HB2	1.83	0.61
1:B:531:THR:HG23	1:B:533:VAL:HG23	1.82	0.61
1:C:506:ASN:HD21	1:C:508:THR:HB	1.65	0.61
1:A:404:THR:HG23	1:A:405:PRO:HD2	1.81	0.60
1:D:450:ASN:HD21	1:D:570:TRP:HE1	1.50	0.60
1:F:403:THR:HG21	1:F:422:THR:HA	1.83	0.60
1:A:440:VAL:HG13	1:A:579:PHE:HB3	1.85	0.59
1:E:406:ASP:HB2	1:F:508:THR:HG22	1.83	0.59
1:E:449:ASN:ND2	1:E:576:ASN:ND2	2.50	0.59
1:F:467:PHE:HB2	1:F:562:TYR:HB2	1.84	0.58
1:E:525:LYS:O	1:E:525:LYS:HD3	2.03	0.58
1:B:486:TYR:OH	1:B:500:ALA:HA	2.03	0.58
1:D:462:SER:HB3	1:D:567:ASP:OD1	2.03	0.58
1:F:512:LYS:HG2	1:F:553:ASN:HB3	1.86	0.57
1:A:506:ASN:ND2	1:A:508:THR:H	2.03	0.57
1:B:485:ASN:CB	1:B:492:VAL:CG2	2.80	0.57
1:C:397:ASP:HB3	1:C:487:LYS:HB3	1.86	0.57
1:E:506:ASN:HD21	1:E:508:THR:HB	1.70	0.57
1:C:403:THR:HA	1:C:483:TYR:O	2.05	0.56
1:D:506:ASN:ND2	1:D:509:ALA:H	2.04	0.56
1:E:549:THR:HG23	1:E:567:ASP:HB2	1.86	0.56
1:D:572:LYS:CE	3:D:603:HOH:O	2.53	0.56
1:E:465:LEU:HD12	1:E:465:LEU:N	2.21	0.56
1:C:403:THR:HG22	1:C:484:TRP:HE3	1.70	0.56
1:B:466:LEU:HD21	1:B:557:GLU:HB3	1.88	0.56
1:E:464:LYS:C	1:E:465:LEU:HD12	2.27	0.55
1:B:440:VAL:HG13	1:B:579:PHE:HB3	1.89	0.55
1:C:488:ASN:HB2	1:C:493:ILE:HD13	1.89	0.55
1:A:489:LYS:O	1:A:490:ASP:HB2	2.07	0.55
1:F:488:ASN:HB3	1:F:489:LYS:HE2	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572:LYS:HE2	3:D:603:HOH:O	2.06	0.54
1:A:508:THR:CG2	1:B:406:ASP:HB2	2.29	0.54
1:A:587:SER:OG	1:B:585:THR:HG23	2.08	0.54
1:C:449:ASN:CG	1:C:452:THR:HG23	2.28	0.54
1:A:508:THR:HG23	1:B:406:ASP:CB	2.29	0.54
1:B:450:ASN:ND2	1:B:570:TRP:HE1	2.06	0.54
1:C:486:TYR:O	1:C:492:VAL:HA	2.07	0.54
1:B:449:ASN:HD22	1:B:576:ASN:HD21	1.56	0.54
1:C:403:THR:HG22	1:C:484:TRP:CE3	2.43	0.53
1:E:418:ASP:HB2	1:E:442:LYS:O	2.08	0.53
1:B:501:VAL:N	1:B:502:PRO:CD	2.71	0.53
1:B:403:THR:HG22	1:B:404:THR:O	2.09	0.53
1:C:397:ASP:OD1	1:C:397:ASP:N	2.42	0.52
1:F:486:TYR:HB2	1:F:493:ILE:HD12	1.91	0.52
1:A:575:LYS:HG3	1:A:575:LYS:O	2.09	0.52
1:D:528:ALA:O	1:D:531:THR:HB	2.09	0.52
1:E:506:ASN:ND2	1:E:508:THR:H	2.07	0.52
1:F:528:ALA:O	1:F:531:THR:HB	2.10	0.52
1:D:428:CYS:O	1:F:426:THR:HG21	2.10	0.52
1:D:515:ASN:HD21	1:D:518:THR:CG2	2.17	0.52
1:A:534:THR:HG21	1:A:584:LEU:HD11	1.90	0.52
1:C:520:ASN:HD21	1:C:522:GLU:HB3	1.74	0.52
1:E:450:ASN:ND2	1:E:570:TRP:HE1	2.08	0.51
1:B:472:LYS:HA	1:B:497:TYR:CZ	2.46	0.51
1:E:485:ASN:HB3	1:E:492:VAL:HB	1.93	0.50
1:B:516:ASN:HD21	1:B:525:LYS:HB2	1.77	0.50
1:D:516:ASN:N	1:D:516:ASN:ND2	2.60	0.50
1:B:486:TYR:HE1	1:B:503:PHE:CE1	2.30	0.50
1:F:506:ASN:HD22	1:F:509:ALA:H	1.60	0.49
1:A:466:LEU:HD21	1:A:557:GLU:HB3	1.94	0.49
1:D:449:ASN:HB3	1:D:452:THR:HG23	1.94	0.49
1:D:506:ASN:HD22	1:D:508:THR:H	1.58	0.49
1:B:486:TYR:OH	1:B:500:ALA:CB	2.61	0.49
1:E:449:ASN:ND2	1:E:576:ASN:HD21	2.01	0.49
1:F:488:ASN:CB	1:F:489:LYS:HE2	2.43	0.49
1:F:572:LYS:NZ	3:F:601:HOH:O	2.37	0.48
1:B:396:ASN:O	1:B:399:ARG:HB2	2.13	0.48
1:D:520:ASN:OD1	1:D:520:ASN:N	2.45	0.48
1:C:506:ASN:ND2	1:C:508:THR:HB	2.28	0.48
1:C:594:GLU:OE2	1:C:594:GLU:HA	2.13	0.48
1:E:506:ASN:HD22	1:E:508:THR:N	2.11	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:ASP:HB3	1:F:474:LEU:HD21	1.94	0.48
1:A:514:ILE:O	1:A:514:ILE:CD1	2.55	0.48
1:B:472:LYS:CG	1:B:498:GLU:O	2.60	0.47
1:C:450:ASN:HD21	1:C:570:TRP:HE1	1.61	0.47
1:C:466:LEU:HB2	1:C:477:SER:OG	2.14	0.47
1:D:462:SER:CB	1:D:567:ASP:OD1	2.61	0.47
1:E:506:ASN:HD22	1:E:506:ASN:C	2.17	0.47
1:F:489:LYS:HB2	1:F:490:ASP:H	1.53	0.47
1:B:411:CYS:HB3	1:B:419:SER:OG	2.13	0.47
1:A:510:TYR:OH	1:A:589:ILE:HD12	2.14	0.47
1:D:408:GLU:OE2	1:D:408:GLU:HA	2.14	0.47
1:E:506:ASN:HD21	1:E:508:THR:CB	2.28	0.47
1:A:486:TYR:HB2	1:A:493:ILE:HD12	1.96	0.47
1:A:506:ASN:HD22	1:A:508:THR:H	1.63	0.47
1:B:485:ASN:OD1	1:B:497:TYR:CB	2.63	0.46
1:C:531:THR:HA	1:C:550:ILE:O	2.15	0.46
1:D:506:ASN:HB2	1:D:589:ILE:HG22	1.97	0.46
1:D:490:ASP:OD1	1:D:490:ASP:N	2.48	0.46
1:B:531:THR:HG21	1:C:540:GLY:CA	2.44	0.46
1:D:534:THR:HG21	1:D:584:LEU:HD11	1.97	0.46
1:E:467:PHE:HA	1:E:472:LYS:O	2.15	0.46
1:C:432:ILE:HG12	1:C:590:ALA:HB2	1.97	0.46
1:E:465:LEU:N	1:E:465:LEU:CD1	2.78	0.46
1:D:439:LEU:HD22	1:E:525:LYS:O	2.15	0.46
1:F:552:PHE:CZ	1:F:588:TYR:HB3	2.50	0.46
1:A:501:VAL:N	1:A:502:PRO:CD	2.79	0.46
1:C:453:ASN:HB3	1:C:458:TYR:CD2	2.51	0.46
1:D:485:ASN:HB3	1:D:492:VAL:HB	1.98	0.45
1:A:404:THR:HG22	1:A:406:ASP:H	1.81	0.45
1:F:530:LYS:HE3	1:F:552:PHE:O	2.16	0.45
1:A:506:ASN:ND2	1:A:508:THR:HB	2.29	0.45
1:F:513:ILE:HG22	1:F:515:ASN:H	1.80	0.45
1:F:449:ASN:ND2	1:F:575:LYS:O	2.50	0.45
1:A:506:ASN:HD22	1:A:509:ALA:H	1.63	0.45
1:C:501:VAL:N	1:C:502:PRO:CD	2.80	0.45
1:E:402:TRP:CH2	1:E:487:LYS:HD2	2.52	0.45
1:E:506:ASN:ND2	1:E:508:THR:N	2.65	0.45
1:A:411:CYS:HB3	1:A:419:SER:OG	2.17	0.44
1:D:464:LYS:HE3	1:D:557:GLU:OE2	2.17	0.44
1:E:526:SER:HB3	1:E:529:LYS:HB2	2.00	0.44
1:F:402:TRP:CZ2	1:F:487:LYS:HG3	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASN:ND2	1:C:429:GLY:CA	2.81	0.44
1:D:420:LYS:HE3	1:E:523:ASP:O	2.17	0.44
1:B:511:PRO:HA	1:B:512:LYS:HZ2	1.76	0.44
1:F:446:ALA:O	1:F:578:PRO:HA	2.18	0.44
1:D:506:ASN:HD22	1:D:508:THR:N	2.14	0.44
1:E:506:ASN:HD22	1:E:508:THR:H	1.65	0.44
1:B:493:ILE:N	1:B:493:ILE:HD13	2.32	0.43
1:D:449:ASN:HD22	1:D:576:ASN:HD21	1.66	0.43
1:E:440:VAL:HG21	1:E:445:PHE:C	2.38	0.43
1:D:402:TRP:C	1:D:403:THR:O	2.54	0.43
1:E:402:TRP:CZ2	1:E:487:LYS:HD2	2.53	0.43
1:E:422:THR:O	1:E:436:VAL:HA	2.19	0.43
1:D:402:TRP:CG	1:D:403:THR:O	2.71	0.43
1:B:506:ASN:HD22	1:B:509:ALA:H	1.66	0.43
1:D:449:ASN:HD22	1:D:576:ASN:ND2	2.16	0.43
1:E:497:TYR:CE2	1:E:500:ALA:HB2	2.54	0.43
1:E:506:ASN:ND2	1:E:508:THR:HB	2.33	0.43
1:F:398:ARG:HA	1:F:398:ARG:HD3	1.90	0.43
1:B:449:ASN:CG	1:B:452:THR:HG23	2.40	0.42
1:C:514:ILE:HG22	1:C:516:ASN:HD21	1.83	0.42
1:E:424:VAL:O	1:E:434:ALA:HA	2.19	0.42
1:F:523:ASP:CG	1:F:523:ASP:O	2.57	0.42
1:F:485:ASN:HB3	1:F:492:VAL:CG1	2.48	0.42
1:F:512:LYS:HE3	1:F:512:LYS:HB3	1.83	0.42
1:D:404:THR:HG23	1:D:406:ASP:H	1.84	0.42
1:C:397:ASP:CB	1:C:487:LYS:O	2.66	0.42
1:D:531:THR:HG21	1:F:540:GLY:HA3	2.01	0.42
1:B:535:ASN:HD22	1:B:547:ALA:HA	1.84	0.42
1:D:424:VAL:HG21	1:E:589:ILE:HG12	2.01	0.42
1:D:506:ASN:ND2	1:D:508:THR:N	2.63	0.42
1:B:502:PRO:HG3	1:B:593:ALA:HB2	2.02	0.42
1:B:522:GLU:O	1:B:522:GLU:HG3	2.19	0.42
1:E:410:ASN:OD1	1:E:410:ASN:N	2.52	0.42
1:E:514:ILE:HD13	1:E:514:ILE:C	2.40	0.42
1:B:559:ASN:HD21	1:D:493:ILE:HD11	1.86	0.41
1:A:506:ASN:HD22	1:A:508:THR:N	2.19	0.41
1:C:498:GLU:OE1	1:C:498:GLU:HA	2.20	0.41
1:A:402:TRP:CH2	1:A:487:LYS:HD2	2.55	0.41
1:A:518:THR:O	1:A:518:THR:OG1	2.31	0.41
1:B:432:ILE:O	1:B:587:SER:HA	2.20	0.41
1:F:514:ILE:O	1:F:514:ILE:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:487:LYS:HE2	1:C:489:LYS:O	2.21	0.41
1:A:397:ASP:HB3	1:A:487:LYS:O	2.21	0.41
1:B:402:TRP:O	1:B:402:TRP:CD1	2.74	0.41
1:E:501:VAL:N	1:E:502:PRO:CD	2.84	0.41
1:E:406:ASP:CB	1:F:508:THR:HG22	2.47	0.41
1:F:413:VAL:HG13	1:F:461:PHE:CD1	2.56	0.41
1:A:410:ASN:O	1:A:479:LEU:HD12	2.21	0.41
1:A:465:LEU:HB3	1:A:467:PHE:CE1	2.56	0.41
1:B:534:THR:HG21	1:B:584:LEU:HD11	2.03	0.41
1:D:440:VAL:HG21	1:D:445:PHE:C	2.41	0.41
1:D:487:LYS:NZ	1:E:592:ASP:OD1	2.39	0.41
1:F:402:TRP:CH2	1:F:405:PRO:HD3	2.56	0.41
1:F:449:ASN:OD1	1:F:451:LYS:HB3	2.21	0.41
1:A:406:ASP:HB2	1:C:508:THR:HG22	2.03	0.41
1:E:402:TRP:CH2	1:E:405:PRO:HD3	2.56	0.41
1:E:559:ASN:HD22	1:E:559:ASN:HA	1.56	0.41
1:B:497:TYR:CD1	1:B:497:TYR:C	2.95	0.40
1:D:531:THR:HG23	1:D:533:VAL:HG23	2.02	0.40
1:E:445:PHE:HD1	1:E:448:ILE:CD1	2.35	0.40
1:B:485:ASN:HB3	1:B:492:VAL:HG22	1.93	0.40
1:C:548:THR:HA	1:C:567:ASP:O	2.22	0.40
1:E:491:SER:OG	1:E:492:VAL:N	2.53	0.40
1:F:514:ILE:HD12	1:F:514:ILE:HA	1.91	0.40
1:A:432:ILE:O	1:A:587:SER:HA	2.20	0.40
1:E:493:ILE:O	1:E:494:GLY:C	2.59	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	198/223 (89%)	180 (91%)	16 (8%)	2 (1%)	15 16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	198/223 (89%)	181 (91%)	17 (9%)	0	100	100
1	C	198/223 (89%)	178 (90%)	19 (10%)	1 (0%)	29	34
1	D	198/223 (89%)	181 (91%)	16 (8%)	1 (0%)	29	34
1	E	198/223 (89%)	179 (90%)	17 (9%)	2 (1%)	15	16
1	F	198/223 (89%)	182 (92%)	15 (8%)	1 (0%)	29	34
All	All	1188/1338 (89%)	1081 (91%)	100 (8%)	7 (1%)	25	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	GLY
1	E	494	GLY
1	E	489	LYS
1	A	404	THR
1	D	403	THR
1	F	514	ILE
1	C	429	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	175/195 (90%)	151 (86%)	24 (14%)	3	3
1	B	175/195 (90%)	150 (86%)	25 (14%)	3	2
1	C	175/195 (90%)	148 (85%)	27 (15%)	2	2
1	D	175/195 (90%)	155 (89%)	20 (11%)	5	5
1	E	175/195 (90%)	153 (87%)	22 (13%)	4	3
1	F	175/195 (90%)	152 (87%)	23 (13%)	4	3
All	All	1050/1170 (90%)	909 (87%)	141 (13%)	4	3

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	GLU
1	A	396	ASN
1	A	398	ARG
1	A	402	TRP
1	A	414	SER
1	A	422	THR
1	A	435	SER
1	A	438	LEU
1	A	440	VAL
1	A	442	LYS
1	A	456	GLU
1	A	460	LYS
1	A	466	LEU
1	A	498	GLU
1	A	506	ASN
1	A	508	THR
1	A	514	ILE
1	A	515	ASN
1	A	518	THR
1	A	523	ASP
1	A	531	THR
1	A	538	LEU
1	A	561	VAL
1	A	592	ASP
1	B	395	GLU
1	B	396	ASN
1	B	399	ARG
1	B	402	TRP
1	B	414	SER
1	B	438	LEU
1	B	451	LYS
1	B	452	THR
1	B	456	GLU
1	B	472	LYS
1	B	488	ASN
1	B	493	ILE
1	B	497	TYR
1	B	499	ASN
1	B	506	ASN
1	B	512	LYS
1	B	514	ILE
1	B	531	THR
1	B	538	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	556	THR
1	B	558	SER
1	B	559	ASN
1	B	563	SER
1	B	572	LYS
1	B	592	ASP
1	C	396	ASN
1	C	397	ASP
1	C	402	TRP
1	C	403	THR
1	C	414	SER
1	C	428	CYS
1	C	438	LEU
1	C	440	VAL
1	C	452	THR
1	C	456	GLU
1	C	466	LEU
1	C	473	LEU
1	C	478	SER
1	C	480	ASP
1	C	490	ASP
1	C	512	LYS
1	C	513	ILE
1	C	523	ASP
1	C	524	LYS
1	C	531	THR
1	C	538	LEU
1	C	556	THR
1	C	571	ASN
1	C	572	LYS
1	C	573	THR
1	C	575	LYS
1	C	594	GLU
1	D	402	TRP
1	D	404	THR
1	D	414	SER
1	D	419	SER
1	D	435	SER
1	D	437	SER
1	D	438	LEU
1	D	440	VAL
1	D	444	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	452	THR
1	D	454	PRO
1	D	473	LEU
1	D	490	ASP
1	D	493	ILE
1	D	516	ASN
1	D	520	ASN
1	D	531	THR
1	D	538	LEU
1	D	572	LYS
1	D	592	ASP
1	E	402	TRP
1	E	413	VAL
1	E	428	CYS
1	E	430	SER
1	E	438	LEU
1	E	440	VAL
1	E	442	LYS
1	E	452	THR
1	E	457	ASP
1	E	460	LYS
1	E	466	LEU
1	E	489	LYS
1	E	506	ASN
1	E	514	ILE
1	E	516	ASN
1	E	531	THR
1	E	538	LEU
1	E	549	THR
1	E	551	SER
1	E	559	ASN
1	E	563	SER
1	E	572	LYS
1	F	398	ARG
1	F	402	TRP
1	F	403	THR
1	F	415	GLU
1	F	416	GLU
1	F	427	LYS
1	F	437	SER
1	F	438	LEU
1	F	466	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	488	ASN
1	F	489	LYS
1	F	491	SER
1	F	492	VAL
1	F	506	ASN
1	F	513	ILE
1	F	516	ASN
1	F	523	ASP
1	F	531	THR
1	F	557	GLU
1	F	561	VAL
1	F	572	LYS
1	F	573	THR
1	F	592	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	431	GLN
1	A	450	ASN
1	A	488	ASN
1	A	506	ASN
1	A	515	ASN
1	A	516	ASN
1	A	559	ASN
1	A	576	ASN
1	B	450	ASN
1	B	488	ASN
1	B	506	ASN
1	B	535	ASN
1	B	576	ASN
1	C	506	ASN
1	C	515	ASN
1	C	516	ASN
1	C	520	ASN
1	C	535	ASN
1	C	559	ASN
1	C	576	ASN
1	D	396	ASN
1	D	431	GLN
1	D	450	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	506	ASN
1	D	515	ASN
1	D	516	ASN
1	D	576	ASN
1	E	431	GLN
1	E	450	ASN
1	E	488	ASN
1	E	506	ASN
1	E	559	ASN
1	E	576	ASN
1	F	431	GLN
1	F	450	ASN
1	F	488	ASN
1	F	506	ASN
1	F	535	ASN
1	F	576	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	SO4	A	601	-	4,4,4	0.37	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	200/223 (89%)	0.07	5 (2%) 57 53	46, 69, 109, 142	0
1	B	200/223 (89%)	0.78	19 (9%) 8 5	44, 78, 176, 248	0
1	C	200/223 (89%)	0.34	8 (4%) 38 35	53, 88, 136, 173	0
1	D	200/223 (89%)	0.43	13 (6%) 18 15	44, 72, 167, 214	0
1	E	200/223 (89%)	0.26	4 (2%) 65 62	54, 83, 126, 160	0
1	F	200/223 (89%)	0.45	10 (5%) 28 26	56, 81, 147, 207	0
All	All	1200/1338 (89%)	0.39	59 (4%) 29 27	44, 78, 143, 248	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	515	ASN	11.6
1	B	521	PRO	11.2
1	F	515	ASN	11.0
1	D	517	GLY	9.9
1	D	515	ASN	9.4
1	D	395	GLU	8.6
1	D	514	ILE	7.8
1	B	494	GLY	7.4
1	B	513	ILE	7.3
1	B	490	ASP	7.3
1	F	517	GLY	6.8
1	B	518	THR	6.7
1	D	518	THR	6.7
1	C	515	ASN	6.3
1	F	516	ASN	6.2
1	B	520	ASN	5.9
1	B	523	ASP	5.8
1	F	520	ASN	5.7
1	C	514	ILE	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	522	GLU	5.2
1	B	517	GLY	5.1
1	C	517	GLY	5.1
1	F	518	THR	5.0
1	B	516	ASN	4.9
1	B	483	TYR	4.8
1	F	521	PRO	4.7
1	C	519	ALA	4.5
1	D	491	SER	4.3
1	B	519	ALA	4.0
1	E	396	ASN	4.0
1	C	518	THR	3.8
1	D	516	ASN	3.8
1	B	491	SER	3.7
1	C	516	ASN	3.6
1	A	594	GLU	3.5
1	D	494	GLY	3.5
1	F	513	ILE	3.4
1	D	519	ALA	3.3
1	A	593	ALA	3.3
1	A	517	GLY	3.2
1	B	495	SER	3.2
1	A	397	ASP	3.0
1	E	518	THR	3.0
1	B	397	ASP	2.9
1	F	519	ALA	2.9
1	D	483	TYR	2.8
1	B	493	ILE	2.8
1	C	398	ARG	2.8
1	B	489	LYS	2.7
1	D	594	GLU	2.7
1	E	524	LYS	2.6
1	F	514	ILE	2.5
1	F	593	ALA	2.5
1	C	397	ASP	2.5
1	D	490	ASP	2.4
1	D	397	ASP	2.3
1	A	451	LYS	2.2
1	E	492	VAL	2.1
1	B	555	GLU	2.1

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	SO4	A	601	5/5	0.84	0.54	125,131,143,160	0

6.5 Other polymers (i)

There are no such residues in this entry.