



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2017 – 05:25 PM EDT

PDB ID : 3EAN
Title : Crystal structure of recombinant rat selenoprotein thioredoxin reductase 1 with reduced C-terminal tail
Authors : Sandalova, T.; Cheng, Q.; Lindqvist, Y.; Arner, E.
Deposited on : unknown
Resolution : 2.75 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

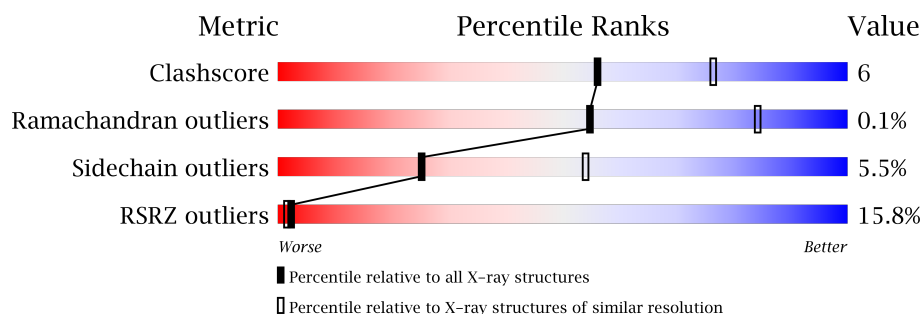
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	112137	4174 (2.80-2.72)
Ramachandran outliers	110173	4103 (2.80-2.72)
Sidechain outliers	110143	4106 (2.80-2.72)
RSRZ outliers	101464	3697 (2.80-2.72)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	499	<div> <div>7%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	B	499	<div> <div>6%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	C	499	<div> <div>24%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>
1	D	499	<div> <div>11%</div> <div>86%</div> <div>10%</div> <div>..</div> </div>
1	E	499	<div> <div>10%</div> <div>83%</div> <div>13%</div> <div>...</div> </div>
1	F	499	<div> <div>33%</div> <div>84%</div> <div>12%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23214 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 Thioredoxin reductase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	B	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	C	486	Total	C	N	O	S	Se	0	0	0
			3731	2368	633	708	21	1			
1	D	491	Total	C	N	O	S	Se	0	0	0
			3777	2399	639	717	21	1			
1	E	490	Total	C	N	O	S	Se	0	0	0
			3768	2393	637	716	21	1			
1	F	489	Total	C	N	O	S	Se	0	0	0
			3762	2390	636	714	21	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ARG	ASN	CONFLICT	UNP O89049
A	53	TRP	GLY	CONFLICT	UNP O89049
B	52	ARG	ASN	CONFLICT	UNP O89049
B	53	TRP	GLY	CONFLICT	UNP O89049
C	52	ARG	ASN	CONFLICT	UNP O89049
C	53	TRP	GLY	CONFLICT	UNP O89049
D	52	ARG	ASN	CONFLICT	UNP O89049
D	53	TRP	GLY	CONFLICT	UNP O89049
E	52	ARG	ASN	CONFLICT	UNP O89049
E	53	TRP	GLY	CONFLICT	UNP O89049
F	52	ARG	ASN	CONFLICT	UNP O89049
F	53	TRP	GLY	CONFLICT	UNP O89049

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	B	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	C	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	D	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	E	1	Total 32	C 11	N 5	O 13	P 3	0	0
3	F	1	Total 32	C 11	N 5	O 13	P 3	0	0

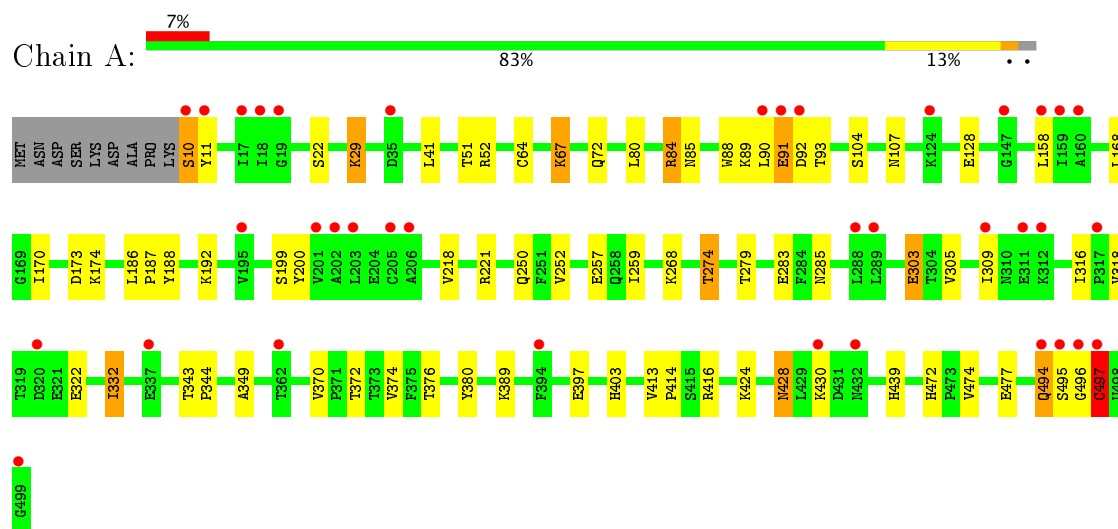
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	23	Total O 23 23	0	0
4	B	20	Total O 20 20	0	0
4	C	14	Total O 14 14	0	0
4	D	35	Total O 35 35	0	0
4	E	26	Total O 26 26	0	0
4	F	12	Total O 12 12	0	0

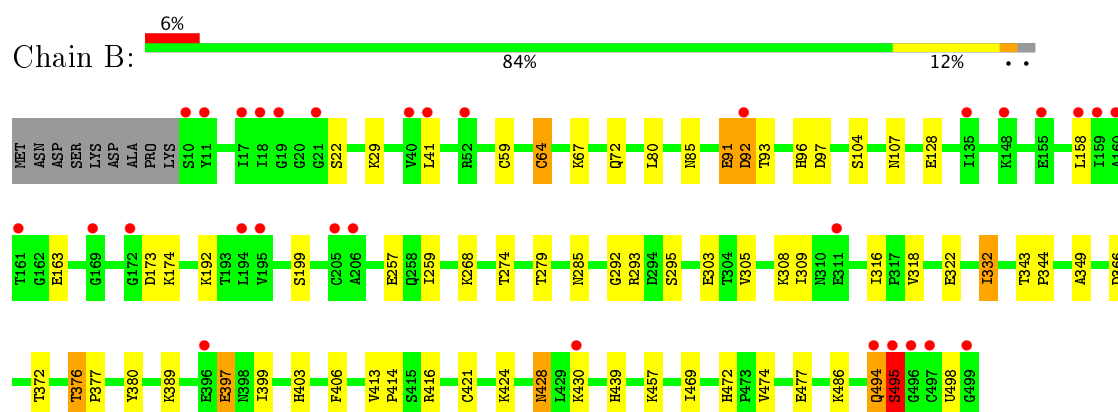
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

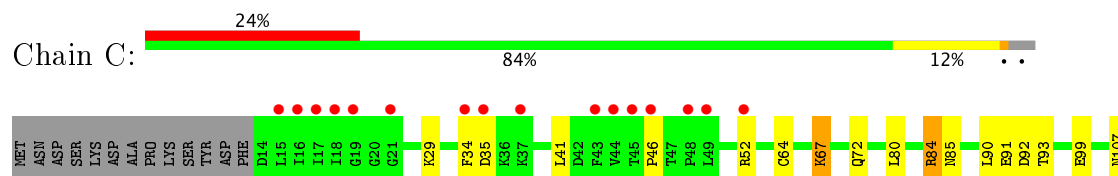
• Molecule 1: Thioredoxin reductase 1

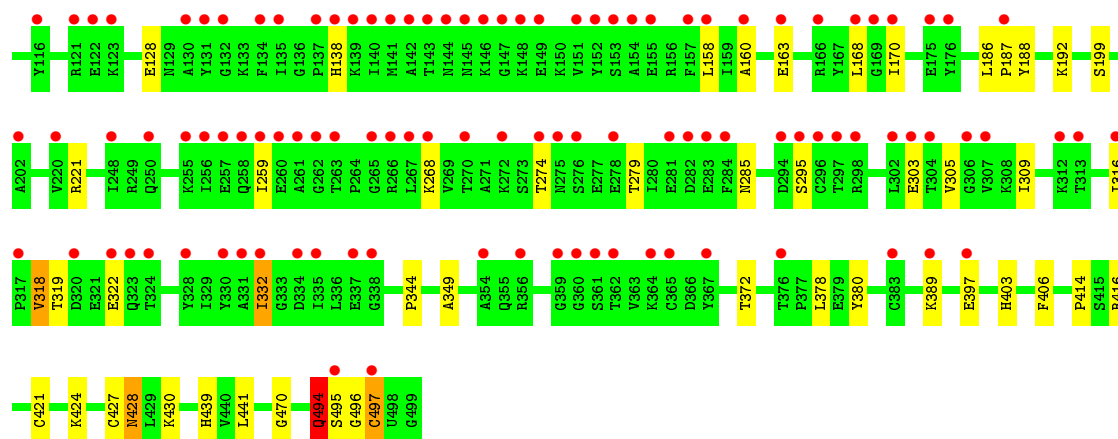


• Molecule 1: Thioredoxin reductase 1

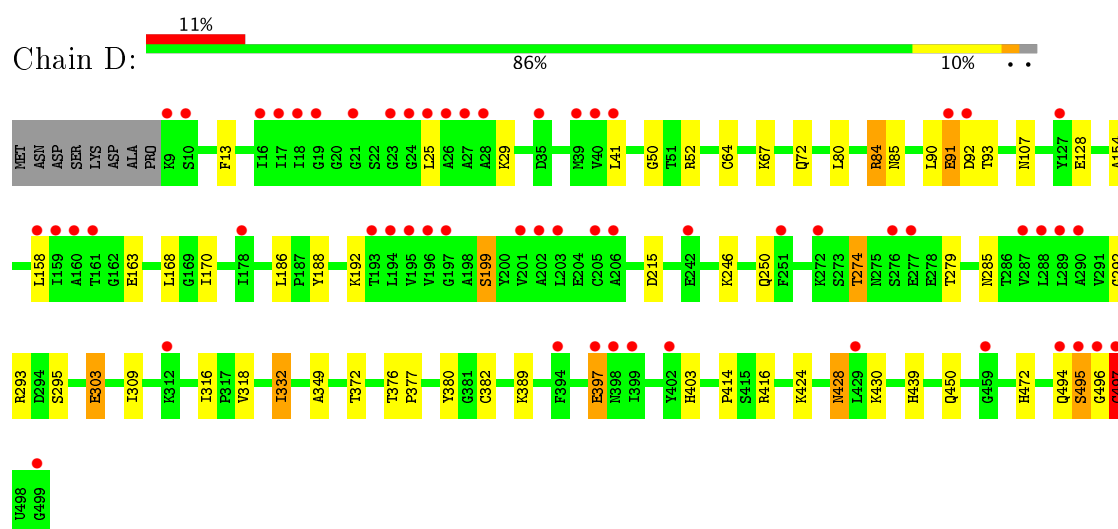


• Molecule 1: Thioredoxin reductase 1

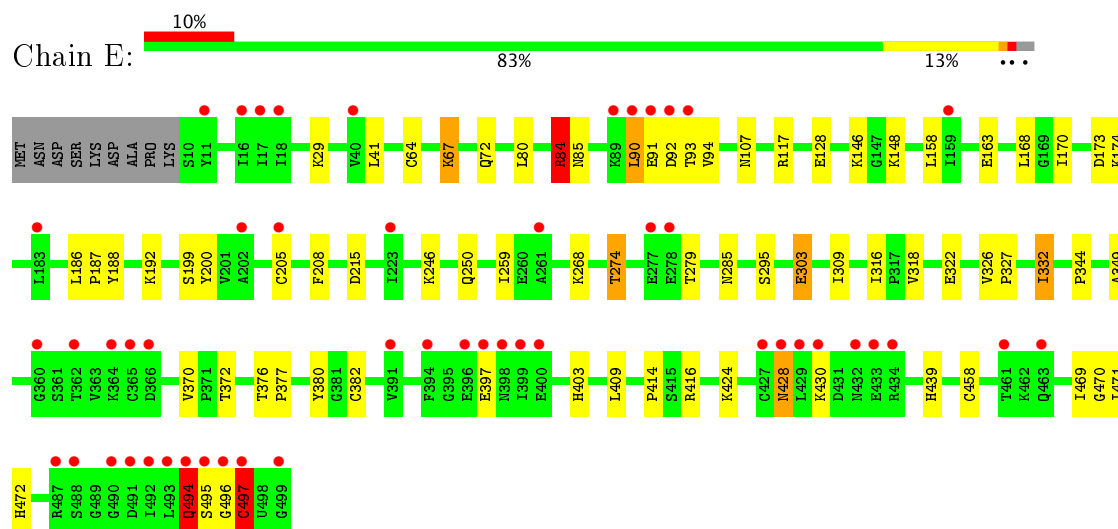




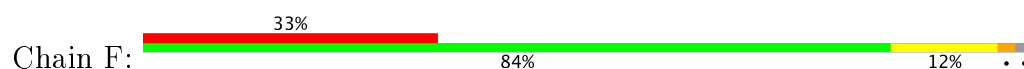
• Molecule 1: Thioredoxin reductase 1



• Molecule 1: Thioredoxin reductase 1



• Molecule 1: Thioredoxin reductase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.57Å 140.67Å 171.17Å 90.00° 94.50° 90.00°	Depositor
Resolution (Å)	29.74 – 2.75 29.74 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.74-2.75) 99.5 (29.74-2.75)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.236 0.272 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	23214	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, SEC, FAD

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	0.77	3/3835 (0.1%)	0.70	0/5185
1	B	0.78	1/3835 (0.0%)	0.71	0/5185
1	C	0.65	1/3796 (0.0%)	0.67	1/5132 (0.0%)
1	D	0.79	2/3844 (0.1%)	0.73	0/5196
1	E	0.75	3/3835 (0.1%)	0.71	2/5185 (0.0%)
1	F	0.63	1/3829 (0.0%)	0.66	1/5177 (0.0%)
All	All	0.73	11/22974 (0.0%)	0.70	4/31060 (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	C	0	2
1	E	0	1
1	F	0	1
All	All	0	4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	495	SER	CB-OG	5.96	1.50	1.42
1	F	11	TYR	N-CA	5.94	1.58	1.46
1	E	200	TYR	CD2-CE2	5.79	1.48	1.39
1	D	495	SER	CB-OG	5.78	1.49	1.42
1	E	382	CYS	CB-SG	-5.63	1.72	1.81
1	E	200	TYR	CD1-CE1	5.54	1.47	1.39
1	A	200	TYR	CE2-CZ	5.36	1.45	1.38
1	A	200	TYR	CD2-CE2	5.34	1.47	1.39
1	C	427	CYS	CB-SG	-5.28	1.73	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	CB-CG2	-5.15	1.42	1.52
1	D	382	CYS	CB-SG	-5.01	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	114	TRP	CA-CB-CG	-7.31	99.81	113.70
1	E	84	ARG	NE-CZ-NH2	5.45	123.02	120.30
1	E	117	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	221	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	494	GLN	Peptide
1	C	496	GLY	Peptide
1	E	494	GLN	Peptide
1	F	11	TYR	Mainchain

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	3768	0	3767	56	0
1	B	3768	0	3769	50	0
1	C	3731	0	3740	53	0
1	D	3777	0	3780	34	0
1	E	3768	0	3767	55	0
1	F	3762	0	3762	46	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	0	0
2	D	53	0	31	0	0
2	E	53	0	31	0	0
2	F	53	0	31	0	0
3	A	32	0	11	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	11	2	0
3	C	32	0	11	1	0
3	D	32	0	11	1	0
3	E	32	0	11	1	0
3	F	32	0	11	1	0
4	A	23	0	0	2	0
4	B	20	0	0	5	0
4	C	14	0	0	7	0
4	D	35	0	0	0	0
4	E	26	0	0	0	0
4	F	12	0	0	1	0
All	All	23214	0	22837	266	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 6.

All (266) 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:C:192:LYS:H	1:C:285:ASN:HD22	1.24	0.85
1:E:496:GLY:N	1:E:497:CYS:HB2	1.92	0.84
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.62	0.83
1:A:10:SER:O	1:A:11:TYR:CG	2.35	0.80
1:B:192:LYS:H	1:B:285:ASN:HD22	1.28	0.78
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.64	0.78
1:A:192:LYS:H	1:A:285:ASN:HD22	1.28	0.77
1:A:10:SER:O	1:A:11:TYR:CD1	2.38	0.77
1:E:192:LYS:H	1:E:285:ASN:HD22	1.30	0.76
1:C:380:TYR:OH	1:C:439:HIS:HD2	1.70	0.75
1:C:494:GLN:HA	1:C:494:GLN:HE21	1.52	0.74
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.71	0.74
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.70	0.73
1:E:469:ILE:HB	1:F:370:VAL:HG13	1.70	0.72
1:D:192:LYS:H	1:D:285:ASN:HD22	1.38	0.71
1:A:221:ARG:HG3	1:A:252:VAL:CG2	2.21	0.70
1:C:84:ARG:HH22	1:C:90:LEU:HB3	1.57	0.70
1:C:46:PRO:HB3	1:C:52:ARG:NH1	2.06	0.69
1:C:138:HIS:HB3	4:C:613:HOH:O	1.93	0.69
1:C:90:LEU:HD11	1:D:90:LEU:HD11	1.75	0.69
1:C:84:ARG:NH2	1:C:90:LEU:HB3	2.07	0.69
1:A:494:GLN:HB3	1:A:495:SER:HA	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.77	0.68
1:F:192:LYS:H	1:F:285:ASN:HD22	1.42	0.67
1:E:72:GLN:HA	1:E:72:GLN:NE2	2.10	0.67
1:D:84:ARG:NH2	1:D:90:LEU:HB3	2.11	0.66
1:C:494:GLN:HA	1:C:494:GLN:NE2	2.10	0.66
1:E:496:GLY:H	1:E:497:CYS:CB	2.09	0.66
1:C:494:GLN:HE21	1:C:494:GLN:CA	2.09	0.65
1:B:494:GLN:HA	1:B:494:GLN:HE21	1.61	0.65
1:E:72:GLN:HA	1:E:72:GLN:HE21	1.60	0.65
1:D:50:GLY:O	1:D:52:ARG:NH1	2.30	0.64
1:F:494:GLN:HB3	1:F:495:SER:HB2	1.79	0.64
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.80	0.64
1:E:496:GLY:H	1:E:497:CYS:HB2	1.62	0.63
1:E:84:ARG:NH2	1:E:90:LEU:HB3	2.15	0.62
1:F:494:GLN:HA	1:F:494:GLN:HE21	1.65	0.61
1:D:186:LEU:HD11	1:D:188:TYR:CZ	2.35	0.61
1:B:486:LYS:CE	4:B:603:HOH:O	2.47	0.61
1:C:46:PRO:CG	1:C:52:ARG:NH1	2.65	0.60
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.82	0.60
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.85	0.59
1:D:84:ARG:HH22	1:D:90:LEU:HB3	1.67	0.59
1:A:91:GLU:CD	1:A:92:ASP:H	2.07	0.58
1:E:84:ARG:HH22	1:E:90:LEU:HB3	1.68	0.58
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.86	0.58
1:E:332:ILE:HD12	1:E:349:ALA:HB1	1.86	0.58
1:F:85:ASN:HD22	1:F:414:PRO:HA	1.69	0.57
1:E:380:TYR:OH	1:E:439:HIS:CD2	2.54	0.57
1:C:192:LYS:N	1:C:285:ASN:HD22	2.00	0.57
1:A:85:ASN:HD22	1:A:414:PRO:HA	1.70	0.57
1:C:46:PRO:CB	1:C:52:ARG:NH1	2.68	0.56
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.86	0.56
1:B:332:ILE:HD12	1:B:349:ALA:CB	2.35	0.56
1:D:309:ILE:HG22	1:D:316:ILE:HG12	1.87	0.56
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.87	0.56
1:F:158:LEU:HD11	1:F:332:ILE:HG12	1.88	0.56
1:B:332:ILE:HD12	1:B:349:ALA:HB1	1.86	0.56
1:E:309:ILE:HG22	1:E:316:ILE:HG12	1.88	0.55
1:E:496:GLY:N	1:E:497:CYS:CB	2.64	0.55
3:B:601:NAP:H51A	4:B:612:HOH:O	2.05	0.55
1:F:332:ILE:HD12	1:F:349:ALA:HB1	1.89	0.55
1:B:380:TYR:OH	1:B:439:HIS:CD2	2.51	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:PHE:CZ	1:C:421:CYS:HB3	2.42	0.55
1:F:309:ILE:HG22	1:F:316:ILE:HG12	1.89	0.55
3:B:601:NAP:C5B	4:B:612:HOH:O	2.55	0.54
1:D:158:LEU:HD11	1:D:332:ILE:HG12	1.89	0.54
1:A:72:GLN:NE2	1:A:72:GLN:HA	2.23	0.54
1:B:486:LYS:HE3	4:B:603:HOH:O	2.06	0.54
1:A:221:ARG:HG3	1:A:252:VAL:HG22	1.89	0.54
1:B:22:SER:OG	1:B:343:THR:HG23	2.07	0.54
1:A:84:ARG:NH2	1:A:90:LEU:HB3	2.23	0.54
1:D:84:ARG:CZ	1:D:84:ARG:HB2	2.38	0.54
1:E:192:LYS:N	1:E:285:ASN:HD22	2.04	0.54
1:A:259:ILE:HD11	1:A:268:LYS:HB2	1.89	0.54
1:B:332:ILE:CD1	1:B:349:ALA:HB1	2.37	0.54
1:C:72:GLN:NE2	1:C:72:GLN:HA	2.22	0.53
1:C:138:HIS:CB	4:C:613:HOH:O	2.55	0.53
1:D:199:SER:HB3	3:D:601:NAP:O1N	2.09	0.52
1:F:332:ILE:HD12	1:F:349:ALA:CB	2.39	0.52
1:E:332:ILE:HD12	1:E:349:ALA:CB	2.39	0.52
1:E:85:ASN:HD22	1:E:414:PRO:HA	1.74	0.52
1:A:29:LYS:NZ	1:B:498:SEC:SE	2.93	0.52
1:C:72:GLN:HE21	1:C:72:GLN:HA	1.75	0.52
1:C:380:TYR:OH	1:C:439:HIS:CD2	2.57	0.52
1:C:428:ASN:ND2	1:C:430:LYS:H	2.07	0.52
1:B:308:LYS:HD2	4:B:614:HOH:O	2.09	0.51
1:B:259:ILE:HD11	1:B:268:LYS:HB2	1.92	0.51
1:F:72:GLN:HA	1:F:72:GLN:NE2	2.25	0.51
1:A:168:LEU:HB2	1:A:170:ILE:HG12	1.92	0.51
1:C:199:SER:HB3	3:C:601:NAP:O1N	2.10	0.51
1:A:380:TYR:OH	1:A:439:HIS:CD2	2.60	0.51
1:D:496:GLY:N	1:D:497:CYS:HB2	2.25	0.51
1:C:84:ARG:HB2	1:C:84:ARG:CZ	2.40	0.51
1:F:494:GLN:CA	1:F:494:GLN:HE21	2.23	0.51
1:A:374:VAL:HG12	1:A:376:THR:HG23	1.93	0.51
1:E:332:ILE:CD1	1:E:349:ALA:HB1	2.40	0.51
1:A:89:LYS:HE3	1:B:97:ASP:HB2	1.93	0.51
1:C:46:PRO:HG3	1:C:52:ARG:NH1	2.26	0.51
1:B:59:CYS:CB	1:B:64:CYS:HG	2.23	0.50
1:F:494:GLN:HB3	1:F:495:SER:CB	2.41	0.50
1:F:13:PHE:O	1:F:154:ALA:HA	2.11	0.50
1:C:309:ILE:HG22	1:C:316:ILE:HG12	1.94	0.50
1:F:406:PHE:CZ	1:F:421:CYS:HB3	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLN:NE2	1:B:72:GLN:HA	2.26	0.50
1:C:259:ILE:HD11	1:C:268:LYS:HB2	1.93	0.50
1:A:84:ARG:HB2	1:A:84:ARG:CZ	2.41	0.49
1:A:104:SER:HB3	1:B:413:VAL:HG13	1.94	0.49
1:E:163:GLU:HG2	1:E:295:SER:HA	1.94	0.49
1:B:494:GLN:CA	1:B:494:GLN:HE21	2.24	0.49
1:D:91:GLU:CD	1:D:92:ASP:H	2.15	0.49
1:F:374:VAL:HG12	1:F:376:THR:HG23	1.94	0.49
1:F:494:GLN:HA	1:F:494:GLN:NE2	2.26	0.49
1:A:41:LEU:HD23	1:A:128:GLU:HB3	1.95	0.49
1:B:85:ASN:HD22	1:B:414:PRO:HA	1.77	0.49
1:D:303:GLU:CD	1:D:303:GLU:H	2.17	0.48
1:F:72:GLN:HA	1:F:72:GLN:HE21	1.78	0.48
1:B:366:ASP:OD2	1:B:457:LYS:HE3	2.13	0.48
1:D:13:PHE:O	1:D:154:ALA:HA	2.14	0.48
1:D:85:ASN:HD22	1:D:414:PRO:HA	1.78	0.48
1:C:186:LEU:HD11	1:C:188:TYR:CZ	2.48	0.47
1:B:474:VAL:O	1:B:477:GLU:HG2	2.14	0.47
1:F:168:LEU:HB2	1:F:170:ILE:HG12	1.95	0.47
1:A:428:ASN:ND2	1:A:430:LYS:H	2.13	0.47
1:A:67:LYS:HB3	1:A:67:LYS:HE2	1.75	0.47
1:F:41:LEU:HD23	1:F:128:GLU:HB3	1.95	0.47
1:C:168:LEU:HB2	1:C:170:ILE:HG12	1.97	0.47
1:E:471:ILE:HG21	1:F:373:THR:OG1	2.14	0.47
1:A:199:SER:HB3	3:A:601:NAP:O1N	2.15	0.46
1:D:332:ILE:HD12	1:D:349:ALA:HB1	1.97	0.46
1:A:494:GLN:HE21	1:A:494:GLN:N	2.13	0.46
1:C:46:PRO:CG	1:C:52:ARG:HH12	2.28	0.46
1:C:41:LEU:HD23	1:C:128:GLU:HB3	1.98	0.46
1:B:332:ILE:HA	1:B:332:ILE:HD13	1.70	0.46
1:D:84:ARG:HB2	1:D:84:ARG:NH2	2.31	0.46
1:F:474:VAL:O	1:F:477:GLU:HG2	2.16	0.46
1:F:332:ILE:CD1	1:F:349:ALA:HB1	2.45	0.46
1:A:22:SER:OG	1:A:343:THR:HG23	2.16	0.46
1:A:332:ILE:HD12	1:A:349:ALA:HB1	1.97	0.46
1:B:158:LEU:HD11	1:B:332:ILE:HG12	1.98	0.46
1:D:72:GLN:HA	1:D:72:GLN:NE2	2.31	0.46
1:C:332:ILE:HD12	1:C:349:ALA:HB1	1.98	0.46
1:D:72:GLN:HA	1:D:72:GLN:HE21	1.79	0.46
1:C:35:ASP:CB	4:C:614:HOH:O	2.63	0.46
1:A:413:VAL:HG13	1:B:104:SER:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:GLN:HB3	1:D:274:THR:HB	1.97	0.45
1:D:397:GLU:HG2	1:D:397:GLU:O	2.16	0.45
1:E:322:GLU:HG2	1:E:332:ILE:CD1	2.46	0.45
1:E:496:GLY:H	1:E:497:CYS:HB3	1.80	0.45
1:A:370:VAL:HG13	1:B:469:ILE:HB	1.99	0.45
1:B:67:LYS:HE2	1:B:67:LYS:HB3	1.82	0.45
1:E:158:LEU:HD11	1:E:332:ILE:HG12	1.97	0.45
1:E:303:GLU:CD	1:E:303:GLU:H	2.19	0.45
1:F:250:GLN:HB3	1:F:274:THR:HB	1.98	0.45
1:B:322:GLU:HG2	1:B:332:ILE:HD13	1.98	0.45
1:C:160:ALA:HB1	4:C:605:HOH:O	2.16	0.45
1:C:67:LYS:HE2	1:C:67:LYS:HB3	1.67	0.45
1:A:84:ARG:HH22	1:A:90:LEU:HB3	1.79	0.45
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.51	0.45
1:B:91:GLU:CD	1:B:92:ASP:H	2.20	0.45
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.99	0.45
1:B:309:ILE:HG22	1:B:316:ILE:HG12	1.98	0.45
1:E:322:GLU:HG2	1:E:332:ILE:HD13	1.98	0.45
1:A:332:ILE:HD12	1:A:349:ALA:CB	2.46	0.45
1:B:173:ASP:OD1	1:B:174:LYS:N	2.50	0.45
1:B:494:GLN:HB3	1:B:495:SER:HA	1.99	0.45
1:E:84:ARG:CZ	1:E:84:ARG:HB2	2.47	0.44
1:B:163:GLU:HG2	1:B:295:SER:HA	2.00	0.44
1:E:205:CYS:HA	1:E:208:PHE:CE2	2.52	0.44
1:E:332:ILE:HD13	1:E:332:ILE:HA	1.70	0.44
1:A:186:LEU:HD11	1:A:188:TYR:CZ	2.53	0.44
1:A:389:LYS:HA	1:A:389:LYS:HD2	1.82	0.44
1:E:173:ASP:OD1	1:E:174:LYS:N	2.51	0.44
1:E:250:GLN:HB3	1:E:274:THR:HB	1.99	0.44
1:E:494:GLN:HB3	1:E:495:SER:HA	2.00	0.44
1:C:99:GLU:OE1	1:E:148:LYS:HE3	2.18	0.44
1:B:322:GLU:HG2	1:B:332:ILE:CD1	2.47	0.44
1:C:322:GLU:HG2	1:C:332:ILE:CD1	2.48	0.43
1:D:168:LEU:HB2	1:D:170:ILE:HG12	2.00	0.43
1:E:67:LYS:HE2	1:E:67:LYS:HB3	1.67	0.43
1:E:469:ILE:HG21	1:F:345:VAL:HG23	1.99	0.43
1:A:84:ARG:HB2	1:A:84:ARG:NH2	2.33	0.43
1:B:41:LEU:HD23	1:B:128:GLU:HB3	2.00	0.43
1:E:458:CYS:HB2	1:F:458:CYS:HB2	2.01	0.43
1:A:173:ASP:OD1	1:A:174:LYS:N	2.51	0.43
1:C:187:PRO:HB3	1:E:146:LYS:NZ	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:186:LEU:HD11	1:F:188:TYR:CZ	2.52	0.43
1:E:469:ILE:CB	1:F:370:VAL:HG13	2.44	0.43
1:E:370:VAL:HG13	1:F:469:ILE:HB	2.00	0.43
1:A:494:GLN:HB3	1:A:495:SER:CA	2.44	0.43
1:A:72:GLN:HE21	1:A:72:GLN:HA	1.81	0.43
1:B:389:LYS:HD2	1:B:389:LYS:HA	1.78	0.43
1:B:72:GLN:HA	1:B:72:GLN:HE21	1.83	0.43
1:E:428:ASN:ND2	1:E:430:LYS:H	2.16	0.43
1:A:250:GLN:HB3	1:A:274:THR:HB	2.01	0.43
1:C:318:VAL:HG13	1:C:319:THR:O	2.19	0.43
1:C:85:ASN:HD22	1:C:414:PRO:HA	1.83	0.43
1:F:199:SER:HB3	3:F:601:NAP:O1N	2.19	0.43
1:F:397:GLU:O	1:F:397:GLU:HG2	2.17	0.43
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.80	0.43
1:D:41:LEU:HD23	1:D:128:GLU:HB3	1.99	0.43
1:D:428:ASN:ND2	1:D:430:LYS:H	2.16	0.43
1:C:80:LEU:HD23	1:D:80:LEU:HD23	2.00	0.43
1:E:472:HIS:HB2	1:F:344:PRO:HG3	1.99	0.43
1:F:322:GLU:HG2	1:F:332:ILE:HD13	2.00	0.43
1:C:35:ASP:HB2	4:C:614:HOH:O	2.19	0.43
1:F:259:ILE:HD11	1:F:268:LYS:HB2	2.01	0.43
1:A:283:GLU:HG3	4:A:620:HOH:O	2.18	0.43
1:C:138:HIS:CG	4:C:613:HOH:O	2.71	0.43
1:A:309:ILE:HG22	1:A:316:ILE:HG12	2.01	0.43
1:B:292:GLY:C	1:B:293:ARG:HG2	2.39	0.43
1:D:25:LEU:HD23	1:D:25:LEU:HA	1.88	0.43
1:D:163:GLU:HG2	1:D:295:SER:HA	2.01	0.42
1:E:90:LEU:HD11	1:F:90:LEU:HD11	2.01	0.42
1:C:163:GLU:HG2	1:C:295:SER:HA	2.01	0.42
1:A:303:GLU:H	1:A:303:GLU:CD	2.21	0.42
1:E:41:LEU:HD23	1:E:128:GLU:HB3	2.02	0.42
1:F:483:SER:N	4:F:606:HOH:O	2.50	0.42
1:F:496:GLY:N	1:F:497:CYS:HB3	2.34	0.42
1:A:322:GLU:HG2	1:A:332:ILE:CD1	2.50	0.42
1:C:389:LYS:HD2	1:C:389:LYS:HA	1.82	0.42
1:D:292:GLY:C	1:D:293:ARG:HG2	2.40	0.42
1:E:470:GLY:O	1:F:344:PRO:HG2	2.20	0.42
1:B:428:ASN:ND2	1:B:430:LYS:H	2.18	0.42
1:C:322:GLU:HG2	1:C:332:ILE:HD13	2.01	0.42
1:E:215:ASP:OD1	1:E:246:LYS:NZ	2.52	0.42
1:C:332:ILE:HD13	1:C:332:ILE:HA	1.76	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LEU:HA	1:E:187:PRO:HD3	1.73	0.42
1:A:332:ILE:CD1	1:A:349:ALA:HB1	2.50	0.41
1:E:199:SER:HB3	3:E:601:NAP:O1N	2.20	0.41
1:F:366:ASP:OD2	1:F:457:LYS:HE3	2.20	0.41
1:E:259:ILE:HD11	1:E:268:LYS:HB2	2.02	0.41
1:C:378:LEU:CD2	1:C:441:LEU:HG	2.50	0.41
1:E:326:VAL:HA	1:E:327:PRO:HD3	1.93	0.41
1:B:376:THR:O	1:B:377:PRO:C	2.59	0.41
1:E:168:LEU:HB2	1:E:170:ILE:HG12	2.03	0.41
1:A:186:LEU:HA	1:A:187:PRO:HD3	1.81	0.41
1:C:46:PRO:CB	1:C:52:ARG:HH12	2.32	0.41
1:D:376:THR:O	1:D:377:PRO:C	2.57	0.41
1:A:51:THR:HA	4:A:611:HOH:O	2.19	0.41
1:B:397:GLU:O	1:B:397:GLU:HG2	2.20	0.41
1:D:215:ASP:OD1	1:D:246:LYS:NZ	2.53	0.41
1:D:389:LYS:HD2	1:D:389:LYS:HA	1.82	0.41
1:E:409:LEU:HD23	1:F:68:LYS:HG2	2.02	0.41
1:E:186:LEU:HD11	1:E:188:TYR:CZ	2.55	0.41
1:A:29:LYS:HZ3	1:B:498:SEC:SE	2.53	0.41
1:B:91:GLU:CD	1:B:92:ASP:N	2.74	0.41
1:C:332:ILE:HD12	1:C:349:ALA:CB	2.50	0.41
1:E:376:THR:O	1:E:377:PRO:C	2.59	0.41
1:A:496:GLY:H	1:A:497:CYS:HB3	1.85	0.41
1:A:80:LEU:CD2	1:B:80:LEU:HD23	2.51	0.41
1:A:29:LYS:HZ2	1:B:498:SEC:SE	2.54	0.41
1:F:12:ASP:HB3	1:F:13:PHE:CD2	2.56	0.40
1:A:474:VAL:O	1:A:477:GLU:HG2	2.22	0.40
1:A:88:TRP:CZ3	1:B:96:HIS:HB2	2.56	0.40
1:C:46:PRO:HG3	1:C:52:ARG:CZ	2.50	0.40
1:C:470:GLY:HA2	1:D:450:GLN:OE1	2.21	0.40
1:F:322:GLU:HG2	1:F:332:ILE:CD1	2.51	0.40
1:A:259:ILE:CD1	1:A:268:LYS:HB2	2.51	0.40
1:E:344:PRO:HG2	1:F:470:GLY:O	2.21	0.40
1:A:322:GLU:HG2	1:A:332:ILE:HD13	2.02	0.40
1:B:399:ILE:HA	1:B:399:ILE:HD13	1.91	0.40
1:C:34:PHE:C	4:C:614:HOH:O	2.60	0.40
1:E:80:LEU:HD13	1:E:94:VAL:HG21	2.04	0.40
1:F:332:ILE:HD13	1:F:332:ILE:HA	1.81	0.40
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	487/499 (98%)	460 (94%)	26 (5%)	1 (0%)	51	81
1	B	487/499 (98%)	463 (95%)	24 (5%)	0	100	100
1	C	483/499 (97%)	456 (94%)	26 (5%)	1 (0%)	51	81
1	D	488/499 (98%)	461 (94%)	26 (5%)	1 (0%)	51	81
1	E	487/499 (98%)	462 (95%)	24 (5%)	1 (0%)	51	81
1	F	486/499 (97%)	461 (95%)	25 (5%)	0	100	100
All	All	2918/2994 (98%)	2763 (95%)	151 (5%)	4 (0%)	55	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	497	CYS
1	D	497	CYS
1	E	497	CYS
1	A	497	CYS

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	405/413 (98%)	381 (94%)	24 (6%)	23	51
1	B	405/413 (98%)	382 (94%)	23 (6%)	24	53
1	C	401/413 (97%)	378 (94%)	23 (6%)	24	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	406/413 (98%)	384 (95%)	22 (5%)	26	55
1	E	405/413 (98%)	383 (95%)	22 (5%)	26	55
1	F	404/413 (98%)	384 (95%)	20 (5%)	28	59
All	All	2426/2478 (98%)	2292 (94%)	134 (6%)	25	54

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

Mol	Chain	Res	Type
1	A	10	SER
1	A	29	LYS
1	A	52	ARG
1	A	64	CYS
1	A	67	LYS
1	A	84	ARG
1	A	91	GLU
1	A	93	THR
1	A	107	ASN
1	A	257	GLU
1	A	274	THR
1	A	279	THR
1	A	303	GLU
1	A	305	VAL
1	A	318	VAL
1	A	332	ILE
1	A	372	THR
1	A	397	GLU
1	A	403	HIS
1	A	416	ARG
1	A	424	LYS
1	A	428	ASN
1	A	494	GLN
1	A	497	CYS
1	B	29	LYS
1	B	64	CYS
1	B	91	GLU
1	B	92	ASP
1	B	93	THR
1	B	107	ASN
1	B	199	SER
1	B	257	GLU
1	B	274	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	279	THR
1	B	303	GLU
1	B	305	VAL
1	B	318	VAL
1	B	332	ILE
1	B	372	THR
1	B	376	THR
1	B	397	GLU
1	B	403	HIS
1	B	416	ARG
1	B	424	LYS
1	B	428	ASN
1	B	494	GLN
1	B	495	SER
1	C	29	LYS
1	C	64	CYS
1	C	67	LYS
1	C	84	ARG
1	C	91	GLU
1	C	92	ASP
1	C	93	THR
1	C	107	ASN
1	C	274	THR
1	C	279	THR
1	C	303	GLU
1	C	305	VAL
1	C	318	VAL
1	C	332	ILE
1	C	372	THR
1	C	397	GLU
1	C	403	HIS
1	C	416	ARG
1	C	424	LYS
1	C	428	ASN
1	C	494	GLN
1	C	495	SER
1	C	497	CYS
1	D	29	LYS
1	D	64	CYS
1	D	67	LYS
1	D	84	ARG
1	D	91	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	93	THR
1	D	107	ASN
1	D	199	SER
1	D	274	THR
1	D	279	THR
1	D	303	GLU
1	D	318	VAL
1	D	332	ILE
1	D	372	THR
1	D	397	GLU
1	D	403	HIS
1	D	416	ARG
1	D	424	LYS
1	D	428	ASN
1	D	494	GLN
1	D	495	SER
1	D	497	CYS
1	E	29	LYS
1	E	64	CYS
1	E	67	LYS
1	E	84	ARG
1	E	90	LEU
1	E	91	GLU
1	E	92	ASP
1	E	93	THR
1	E	107	ASN
1	E	274	THR
1	E	279	THR
1	E	303	GLU
1	E	318	VAL
1	E	332	ILE
1	E	372	THR
1	E	397	GLU
1	E	403	HIS
1	E	416	ARG
1	E	424	LYS
1	E	428	ASN
1	E	494	GLN
1	E	497	CYS
1	F	12	ASP
1	F	29	LYS
1	F	64	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	91	GLU
1	F	92	ASP
1	F	93	THR
1	F	107	ASN
1	F	274	THR
1	F	279	THR
1	F	303	GLU
1	F	318	VAL
1	F	332	ILE
1	F	372	THR
1	F	397	GLU
1	F	403	HIS
1	F	416	ARG
1	F	424	LYS
1	F	428	ASN
1	F	494	GLN
1	F	495	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	285	ASN
1	A	428	ASN
1	A	439	HIS
1	A	494	GLN
1	B	72	GLN
1	B	285	ASN
1	B	428	ASN
1	B	439	HIS
1	B	494	GLN
1	C	72	GLN
1	C	285	ASN
1	C	428	ASN
1	C	439	HIS
1	C	494	GLN
1	D	72	GLN
1	D	285	ASN
1	D	428	ASN
1	D	439	HIS
1	E	72	GLN
1	E	285	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	428	ASN
1	E	439	HIS
1	E	494	GLN
1	F	72	GLN
1	F	285	ASN
1	F	428	ASN
1	F	439	HIS
1	F	494	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	FAD	A	600	-	51,58,58	1.53	5 (9%)	54,89,89	2.00	7 (12%)
3	NAP	A	601	-	28,34,52	1.25	3 (10%)	33,53,80	1.95	2 (6%)
2	FAD	B	600	-	51,58,58	1.83	7 (13%)	54,89,89	2.00	10 (18%)
3	NAP	B	601	-	28,34,52	1.16	3 (10%)	33,53,80	2.09	2 (6%)
2	FAD	C	600	-	51,58,58	1.70	6 (11%)	54,89,89	1.85	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAP	C	601	-	28,34,52	1.15	3 (10%)	33,53,80	1.81	1 (3%)
2	FAD	D	600	-	51,58,58	1.71	7 (13%)	54,89,89	1.94	9 (16%)
3	NAP	D	601	-	28,34,52	1.27	4 (14%)	33,53,80	2.09	4 (12%)
2	FAD	E	600	-	51,58,58	1.74	8 (15%)	54,89,89	1.86	12 (22%)
3	NAP	E	601	-	28,34,52	1.30	3 (10%)	33,53,80	1.90	2 (6%)
2	FAD	F	600	-	51,58,58	1.70	7 (13%)	54,89,89	1.91	7 (12%)
3	NAP	F	601	-	28,34,52	1.14	2 (7%)	33,53,80	1.86	1 (3%)

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	FAD	A	600	-	-	0/28/50/50	0/6/6/6
3	NAP	A	601	-	-	0/20/40/67	0/3/3/5
2	FAD	B	600	-	-	0/28/50/50	0/6/6/6
3	NAP	B	601	-	-	0/20/40/67	0/3/3/5
2	FAD	C	600	-	-	0/28/50/50	0/6/6/6
3	NAP	C	601	-	-	0/20/40/67	0/3/3/5
2	FAD	D	600	-	-	0/28/50/50	0/6/6/6
3	NAP	D	601	-	-	0/20/40/67	0/3/3/5
2	FAD	E	600	-	-	0/28/50/50	0/6/6/6
3	NAP	E	601	-	-	0/20/40/67	0/3/3/5
2	FAD	F	600	-	-	0/28/50/50	0/6/6/6
3	NAP	F	601	-	-	0/20/40/67	0/3/3/5

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	600	FAD	C2B-C1B	-2.69	1.49	1.53
2	B	600	FAD	C2B-C1B	-2.12	1.50	1.53
2	D	600	FAD	C4A-N3A	-2.10	1.32	1.35
2	E	600	FAD	C5A-N7A	-2.03	1.32	1.39
3	D	601	NAP	P2B-O3X	-2.02	1.46	1.54
3	B	601	NAP	O4B-C1B	2.07	1.44	1.41
3	A	601	NAP	P2B-O1X	2.11	1.57	1.50
3	C	601	NAP	PN-O5D	2.11	1.67	1.59
3	E	601	NAP	O4B-C1B	2.15	1.44	1.41
2	A	600	FAD	O4B-C1B	2.23	1.44	1.41
2	E	600	FAD	C9A-N10	2.25	1.41	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NAP	O4B-C1B	2.26	1.44	1.41
2	D	600	FAD	C4-N3	2.37	1.37	1.33
3	F	601	NAP	O4B-C1B	2.51	1.44	1.41
3	B	601	NAP	PN-O5D	2.54	1.68	1.59
2	C	600	FAD	O4B-C1B	2.59	1.44	1.41
2	F	600	FAD	C2-N1	2.61	1.43	1.38
2	F	600	FAD	O4B-C1B	2.62	1.44	1.41
2	F	600	FAD	C9A-N10	2.62	1.42	1.38
3	D	601	NAP	P2B-O1X	2.80	1.60	1.50
3	D	601	NAP	PN-O5D	2.80	1.69	1.59
2	E	600	FAD	C5X-N5	2.90	1.39	1.35
3	E	601	NAP	P2B-O1X	2.94	1.60	1.50
2	C	600	FAD	C9A-N10	2.96	1.42	1.38
2	A	600	FAD	C4-N3	2.98	1.38	1.33
2	D	600	FAD	C9A-N10	3.22	1.43	1.38
3	A	601	NAP	O4B-C1B	3.23	1.45	1.41
3	C	601	NAP	P2B-O1X	3.26	1.61	1.50
2	E	600	FAD	C4-N3	3.27	1.39	1.33
2	B	600	FAD	C9A-N10	3.33	1.43	1.38
3	B	601	NAP	P2B-O1X	3.47	1.62	1.50
3	A	601	NAP	PN-O5D	3.50	1.72	1.59
2	F	600	FAD	C5X-N5	3.52	1.40	1.35
3	D	601	NAP	O4B-C1B	3.54	1.46	1.41
3	F	601	NAP	P2B-O1X	3.54	1.62	1.50
2	B	600	FAD	C4-N3	3.70	1.39	1.33
2	F	600	FAD	C4-N3	3.72	1.39	1.33
3	E	601	NAP	PN-O5D	4.16	1.74	1.59
2	E	600	FAD	O4B-C1B	4.17	1.47	1.41
2	C	600	FAD	C5X-N5	4.19	1.41	1.35
2	D	600	FAD	O4B-C1B	4.24	1.47	1.41
2	B	600	FAD	C5X-N5	4.41	1.42	1.35
2	D	600	FAD	C10-N1	4.42	1.39	1.33
2	A	600	FAD	C5X-N5	4.44	1.42	1.35
2	C	600	FAD	C4-N3	4.45	1.41	1.33
2	B	600	FAD	C10-N1	4.50	1.39	1.33
2	D	600	FAD	C5X-N5	4.52	1.42	1.35
2	E	600	FAD	C10-N1	4.90	1.40	1.33
2	A	600	FAD	C4X-N5	4.90	1.40	1.33
2	F	600	FAD	C4X-N5	5.43	1.41	1.33
2	A	600	FAD	C10-N1	5.46	1.40	1.33
2	C	600	FAD	C10-N1	5.62	1.41	1.33
2	C	600	FAD	C4X-N5	5.63	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C4X-N5	5.80	1.41	1.33
2	B	600	FAD	O4B-C1B	6.01	1.49	1.41
2	D	600	FAD	C4X-N5	6.04	1.42	1.33
2	E	600	FAD	C4X-N5	6.50	1.42	1.33
2	F	600	FAD	C10-N1	6.61	1.42	1.33

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	601	NAP	N3A-C2A-N1A	-10.25	119.93	128.86
3	D	601	NAP	N3A-C2A-N1A	-9.87	120.27	128.86
2	A	600	FAD	N3A-C2A-N1A	-9.15	120.89	128.86
3	A	601	NAP	N3A-C2A-N1A	-8.97	121.04	128.86
3	F	601	NAP	N3A-C2A-N1A	-8.97	121.05	128.86
2	D	600	FAD	N3A-C2A-N1A	-8.91	121.10	128.86
3	E	601	NAP	N3A-C2A-N1A	-8.89	121.11	128.86
3	C	601	NAP	N3A-C2A-N1A	-8.64	121.33	128.86
2	F	600	FAD	N3A-C2A-N1A	-8.50	121.46	128.86
2	C	600	FAD	N3A-C2A-N1A	-8.29	121.64	128.86
2	B	600	FAD	N3A-C2A-N1A	-8.11	121.80	128.86
2	E	600	FAD	N3A-C2A-N1A	-7.05	122.72	128.86
2	B	600	FAD	C5B-C4B-C3B	-3.38	102.41	115.29
2	B	600	FAD	C4X-C4-N3	-2.94	119.29	123.48
2	A	600	FAD	C4X-C4-N3	-2.71	119.62	123.48
2	B	600	FAD	O3B-C3B-C4B	-2.63	103.40	111.09
2	E	600	FAD	O3'-C3'-C2'	-2.61	102.36	108.82
2	C	600	FAD	C4X-C4-N3	-2.54	119.86	123.48
3	D	601	NAP	C4B-O4B-C1B	-2.50	107.11	109.77
3	A	601	NAP	C4B-O4B-C1B	-2.43	107.18	109.77
2	B	600	FAD	C4B-O4B-C1B	-2.39	107.23	109.77
3	D	601	NAP	O5B-PA-O1A	-2.37	99.69	109.25
2	F	600	FAD	C5B-C4B-C3B	-2.29	106.56	115.29
2	D	600	FAD	C5B-C4B-C3B	-2.21	106.88	115.29
2	A	600	FAD	C5B-C4B-C3B	-2.18	106.99	115.29
2	C	600	FAD	C5B-C4B-C3B	-2.17	107.02	115.29
2	F	600	FAD	C4X-C4-N3	-2.15	120.42	123.48
2	E	600	FAD	C4A-C5A-N7A	-2.15	107.33	109.41
2	E	600	FAD	O3B-C3B-C4B	-2.10	104.95	111.09
2	D	600	FAD	O3'-C3'-C2'	-2.07	103.68	108.82
2	D	600	FAD	C9A-C5X-N5	-2.05	119.19	122.24
3	E	601	NAP	O3X-P2B-O2X	2.01	115.71	107.61
2	D	600	FAD	O2P-P-O1P	2.01	122.68	112.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O2P-P-O1P	2.04	122.86	112.28
3	D	601	NAP	O3X-P2B-O2B	2.10	115.56	106.00
2	E	600	FAD	O2'-C2'-C3'	2.12	114.36	109.09
2	E	600	FAD	O2P-P-O1P	2.13	123.28	112.28
2	C	600	FAD	C4-C4X-N5	2.13	121.02	118.68
2	E	600	FAD	O4'-C4'-C3'	2.19	114.54	109.09
2	E	600	FAD	C4-C4X-N5	2.20	121.09	118.68
2	C	600	FAD	C5X-C9A-N10	2.20	119.29	117.66
2	F	600	FAD	C5X-C9A-N10	2.29	119.36	117.66
2	A	600	FAD	C5X-C9A-N10	2.31	119.37	117.66
2	B	600	FAD	N6A-C6A-N1A	2.37	123.47	118.77
2	D	600	FAD	C1'-N10-C9A	2.44	120.58	118.35
3	B	601	NAP	O3X-P2B-O2X	2.49	117.67	107.61
2	B	600	FAD	C5X-C9A-N10	2.59	119.58	117.66
2	A	600	FAD	C1'-N10-C9A	2.70	120.82	118.35
2	D	600	FAD	C5X-C9A-N10	2.76	119.70	117.66
2	E	600	FAD	C5X-C9A-N10	2.80	119.74	117.66
2	B	600	FAD	C1'-N10-C9A	2.88	120.98	118.35
2	E	600	FAD	C1'-N10-C9A	2.97	121.07	118.35
2	F	600	FAD	C1'-N10-C9A	2.99	121.08	118.35
2	B	600	FAD	C4X-N5-C5X	2.99	119.92	116.76
2	E	600	FAD	C4X-N5-C5X	3.19	120.12	116.76
2	D	600	FAD	C4X-N5-C5X	3.30	120.24	116.76
2	C	600	FAD	C4X-N5-C5X	3.57	120.53	116.76
2	F	600	FAD	C4X-N5-C5X	3.64	120.60	116.76
2	C	600	FAD	C1'-N10-C9A	3.75	121.78	118.35
2	E	600	FAD	C4-N3-C2	6.34	120.70	115.16
2	C	600	FAD	C4-N3-C2	6.36	120.72	115.16
2	D	600	FAD	C4-N3-C2	6.42	120.77	115.16
2	F	600	FAD	C4-N3-C2	7.02	121.30	115.16
2	B	600	FAD	C4-N3-C2	7.41	121.64	115.16
2	A	600	FAD	C4-N3-C2	7.85	122.02	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	NAP	1	0
3	B	601	NAP	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	NAP	1	0
3	D	601	NAP	1	0
3	E	601	NAP	1	0
3	F	601	NAP	1	0

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	489/499 (97%)	0.67	37 (7%) 15 10	24, 63, 74, 102	0
1	B	489/499 (97%)	0.58	31 (6%) 21 16	24, 63, 74, 102	0
1	C	485/499 (97%)	1.32	122 (25%) 1 0	24, 63, 74, 103	0
1	D	490/499 (98%)	0.89	57 (11%) 5 4	24, 63, 75, 102	0
1	E	489/499 (97%)	0.78	50 (10%) 7 5	24, 63, 74, 101	0
1	F	488/499 (97%)	1.60	167 (34%) 0 0	24, 63, 74, 101	0
All	All	2930/2994 (97%)	0.97	464 (15%) 2 1	24, 63, 74, 103	0

All (464) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	495	SER	8.8
1	D	497	CYS	8.5
1	D	499	GLY	8.5
1	D	496	GLY	7.5
1	F	297	THR	7.3
1	F	272	LYS	6.3
1	A	10	SER	6.1
1	F	394	PHE	6.1
1	F	399	ILE	6.1
1	F	294	ASP	6.0
1	F	137	PRO	5.9
1	C	151	VAL	5.9
1	F	135	ILE	5.7
1	F	358	TYR	5.7
1	B	10	SER	5.7
1	F	141	MET	5.6
1	C	169	GLY	5.3
1	F	143	THR	5.3
1	C	320	ASP	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	275	ASN	5.1
1	F	311	GLU	5.1
1	F	279	THR	5.1
1	D	394	PHE	5.0
1	F	283	GLU	5.0
1	E	92	ASP	4.9
1	F	134	PHE	4.9
1	F	223	ILE	4.8
1	C	296	CYS	4.8
1	B	499	GLY	4.8
1	E	497	CYS	4.8
1	B	160	ALA	4.7
1	F	92	ASP	4.7
1	F	306	GLY	4.7
1	F	278	GLU	4.7
1	F	268	LYS	4.7
1	C	154	ALA	4.7
1	F	261	ALA	4.7
1	F	11	TYR	4.7
1	B	496	GLY	4.7
1	F	37	LYS	4.7
1	C	312	LYS	4.7
1	F	142	ALA	4.6
1	F	34	PHE	4.6
1	F	359	GLY	4.6
1	C	281	GLU	4.6
1	F	298	ARG	4.6
1	E	496	GLY	4.6
1	C	365	CYS	4.5
1	E	494	GLN	4.5
1	F	487	ARG	4.5
1	C	282	ASP	4.5
1	F	295	SER	4.5
1	F	52	ARG	4.5
1	C	495	SER	4.4
1	F	247	PHE	4.4
1	F	269	VAL	4.4
1	E	499	GLY	4.4
1	F	35	ASP	4.3
1	F	320	ASP	4.3
1	F	277	GLU	4.3
1	C	35	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	338	GLY	4.3
1	F	361	SER	4.3
1	B	497	CYS	4.3
1	C	255	LYS	4.3
1	A	311	GLU	4.3
1	D	288	LEU	4.2
1	E	396	GLU	4.2
1	E	429	LEU	4.2
1	F	131	TYR	4.2
1	F	151	VAL	4.2
1	F	281	GLU	4.2
1	F	397	GLU	4.2
1	F	313	THR	4.1
1	E	490	GLY	4.1
1	C	361	SER	4.1
1	D	429	LEU	4.1
1	F	132	GLY	4.1
1	A	92	ASP	4.0
1	C	145	ASN	4.0
1	D	495	SER	4.0
1	C	337	GLU	4.0
1	C	153	SER	4.0
1	F	360	GLY	4.0
1	D	397	GLU	4.0
1	A	496	GLY	4.0
1	E	430	LYS	4.0
1	F	319	THR	4.0
1	F	146	LYS	4.0
1	F	144	ASN	3.9
1	C	146	LYS	3.9
1	A	309	ILE	3.9
1	C	268	LYS	3.9
1	C	335	ILE	3.9
1	F	492	ILE	3.9
1	F	262	GLY	3.9
1	C	37	LYS	3.9
1	E	398	ASN	3.9
1	F	36	LYS	3.9
1	F	284	PHE	3.9
1	F	307	VAL	3.9
1	E	491	ASP	3.9
1	F	495	SER	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	364	LYS	3.8
1	A	499	GLY	3.8
1	D	494	GLN	3.8
1	C	157	PHE	3.8
1	A	495	SER	3.8
1	C	137	PRO	3.8
1	F	139	LYS	3.8
1	A	205	CYS	3.8
1	E	277	GLU	3.7
1	C	295	SER	3.7
1	D	17	ILE	3.7
1	F	309	ILE	3.7
1	C	141	MET	3.7
1	D	272	LYS	3.7
1	E	463	GLN	3.6
1	E	159	ILE	3.6
1	F	274	THR	3.6
1	C	297	THR	3.6
1	C	256	ILE	3.6
1	F	305	VAL	3.6
1	C	250	GLN	3.6
1	C	175	GLU	3.6
1	E	397	GLU	3.6
1	C	135	ILE	3.5
1	D	287	VAL	3.5
1	C	139	LYS	3.5
1	C	302	LEU	3.5
1	E	91	GLU	3.5
1	B	17	ILE	3.5
1	C	122	GLU	3.5
1	F	316	ILE	3.5
1	F	419	ASN	3.5
1	B	18	ILE	3.5
1	A	158	LEU	3.5
1	D	9	LYS	3.5
1	C	306	GLY	3.5
1	B	195	VAL	3.5
1	C	313	THR	3.5
1	F	282	ASP	3.5
1	C	266	ARG	3.5
1	F	12	ASP	3.4
1	C	270	THR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	131	TYR	3.4
1	C	152	TYR	3.4
1	E	432	ASN	3.4
1	F	152	TYR	3.4
1	F	331	ALA	3.4
1	F	263	THR	3.4
1	A	91	GLU	3.4
1	E	487	ARG	3.4
1	A	312	LYS	3.4
1	C	48	PRO	3.4
1	F	328	TYR	3.4
1	C	149	GLU	3.4
1	F	494	GLN	3.4
1	F	398	ASN	3.3
1	F	400	GLU	3.3
1	F	150	LYS	3.3
1	C	16	ILE	3.3
1	C	275	ASN	3.3
1	F	251	PHE	3.3
1	D	312	LYS	3.3
1	F	340	LEU	3.3
1	C	18	ILE	3.3
1	F	265	GLY	3.3
1	C	497	CYS	3.3
1	A	494	GLN	3.3
1	E	428	ASN	3.3
1	C	360	GLY	3.3
1	F	431	ASP	3.3
1	C	148	LYS	3.2
1	C	283	GLU	3.2
1	A	288	LEU	3.2
1	C	147	GLY	3.2
1	D	40	VAL	3.2
1	F	496	GLY	3.2
1	F	248	ILE	3.2
1	E	433	GLU	3.2
1	D	276	SER	3.2
1	C	324	THR	3.2
1	F	18	ILE	3.2
1	B	495	SER	3.1
1	B	205	CYS	3.1
1	C	143	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	17	ILE	3.1
1	E	493	LEU	3.1
1	F	387	GLU	3.1
1	B	430	LYS	3.1
1	C	257	GLU	3.1
1	C	274	THR	3.1
1	F	260	GLU	3.1
1	F	324	THR	3.1
1	F	148	LYS	3.1
1	D	195	VAL	3.1
1	F	334	ASP	3.0
1	F	497	CYS	3.0
1	B	92	ASP	3.0
1	F	276	SER	3.0
1	C	265	GLY	3.0
1	C	359	GLY	3.0
1	C	168	LEU	3.0
1	C	307	VAL	3.0
1	C	140	ILE	3.0
1	C	170	ILE	3.0
1	F	155	GLU	3.0
1	C	261	ALA	3.0
1	F	249	ARG	2.9
1	F	280	ILE	2.9
1	C	397	GLU	2.9
1	B	169	GLY	2.9
1	D	289	LEU	2.9
1	F	266	ARG	2.9
1	E	362	THR	2.9
1	F	254	THR	2.9
1	E	391	VAL	2.9
1	F	436	VAL	2.9
1	C	202	ALA	2.9
1	D	18	ILE	2.9
1	C	267	LEU	2.9
1	B	11	TYR	2.9
1	F	499	GLY	2.9
1	C	356	ARG	2.9
1	E	488	SER	2.9
1	D	196	VAL	2.9
1	D	35	ASP	2.9
1	F	335	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	202	ALA	2.9
1	B	52	ARG	2.9
1	A	317	PRO	2.9
1	D	459	GLY	2.8
1	F	169	GLY	2.8
1	D	160	ALA	2.8
1	D	205	CYS	2.8
1	C	322	GLU	2.8
1	F	140	ILE	2.8
1	C	284	PHE	2.8
1	B	158	LEU	2.8
1	E	394	PHE	2.8
1	E	261	ALA	2.8
1	F	267	LEU	2.8
1	F	308	LYS	2.8
1	D	28	ALA	2.8
1	F	486	LYS	2.8
1	E	427	CYS	2.8
1	C	46	PRO	2.8
1	C	354	ALA	2.8
1	D	203	LEU	2.8
1	D	27	ALA	2.7
1	F	250	GLN	2.7
1	F	395	GLY	2.7
1	C	278	GLU	2.7
1	D	161	THR	2.7
1	F	149	GLU	2.7
1	F	171	PRO	2.7
1	A	195	VAL	2.7
1	C	144	ASN	2.7
1	F	13	PHE	2.7
1	F	176	TYR	2.7
1	F	175	GLU	2.7
1	D	251	PHE	2.7
1	F	167	TYR	2.7
1	F	93	THR	2.7
1	C	317	PRO	2.7
1	C	272	LYS	2.7
1	E	492	ILE	2.7
1	A	147	GLY	2.6
1	C	132	GLY	2.6
1	C	260	GLU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	19	GLY	2.6
1	F	130	ALA	2.6
1	C	163	GLU	2.6
1	F	339	LYS	2.6
1	E	399	ILE	2.6
1	F	459	GLY	2.6
1	F	337	GLU	2.6
1	F	293	ARG	2.6
1	F	314	GLY	2.6
1	D	202	ALA	2.6
1	D	41	LEU	2.6
1	F	270	THR	2.6
1	F	45	THR	2.6
1	D	91	GLU	2.6
1	D	194	LEU	2.6
1	C	330	TYR	2.5
1	A	203	LEU	2.5
1	B	19	GLY	2.5
1	F	219	MET	2.5
1	C	259	ILE	2.5
1	F	362	THR	2.5
1	F	390	ALA	2.5
1	E	365	CYS	2.5
1	A	17	ILE	2.5
1	C	328	TYR	2.5
1	D	25	LEU	2.5
1	C	34	PHE	2.5
1	D	92	ASP	2.5
1	A	160	ALA	2.5
1	C	142	ALA	2.5
1	E	223	ILE	2.5
1	F	389	LYS	2.5
1	D	201	VAL	2.5
1	E	400	GLU	2.5
1	F	428	ASN	2.5
1	D	24	GLY	2.5
1	C	323	GLN	2.5
1	C	276	SER	2.5
1	D	178	ILE	2.5
1	C	303	GLU	2.5
1	A	11	TYR	2.5
1	C	134	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	277	GLU	2.5
1	F	491	ASP	2.5
1	F	252	VAL	2.4
1	F	145	ASN	2.4
1	F	256	ILE	2.4
1	F	302	LEU	2.4
1	C	155	GLU	2.4
1	C	331	ALA	2.4
1	C	15	LEU	2.4
1	E	90	LEU	2.4
1	E	278	GLU	2.4
1	D	39	MET	2.4
1	B	194	LEU	2.4
1	A	430	LYS	2.4
1	F	259	ILE	2.4
1	F	114	TRP	2.4
1	C	176	TYR	2.4
1	C	166	ARG	2.4
1	E	434	ARG	2.4
1	C	45	THR	2.4
1	D	290	ALA	2.4
1	C	332	ILE	2.4
1	E	18	ILE	2.4
1	C	262	GLY	2.4
1	F	323	GLN	2.4
1	F	172	GLY	2.4
1	C	44	VAL	2.4
1	B	206	ALA	2.3
1	F	22	SER	2.3
1	A	432	ASN	2.3
1	F	241	GLU	2.3
1	F	392	GLU	2.3
1	D	242	GLU	2.3
1	C	17	ILE	2.3
1	B	40	VAL	2.3
1	E	205	CYS	2.3
1	C	334	ASP	2.3
1	F	327	PRO	2.3
1	D	23	GLY	2.3
1	F	352	LEU	2.3
1	C	43	PHE	2.3
1	E	364	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	383	CYS	2.3
1	A	90	LEU	2.3
1	E	360	GLY	2.3
1	C	304	THR	2.3
1	D	206	ALA	2.3
1	F	322	GLU	2.3
1	F	228	PHE	2.3
1	C	294	ASP	2.3
1	B	21	GLY	2.3
1	C	376	THR	2.3
1	F	354	ALA	2.3
1	B	159	ILE	2.3
1	C	298	ARG	2.3
1	F	438	PHE	2.3
1	E	183	LEU	2.3
1	C	160	ALA	2.3
1	C	263	THR	2.3
1	A	497	CYS	2.3
1	E	11	TYR	2.3
1	F	296	CYS	2.3
1	C	123	LYS	2.3
1	C	248	ILE	2.3
1	F	157	PHE	2.3
1	F	14	ASP	2.3
1	F	355	GLN	2.2
1	C	52	ARG	2.2
1	A	206	ALA	2.2
1	E	93	THR	2.2
1	D	16	ILE	2.2
1	F	432	ASN	2.2
1	C	158	LEU	2.2
1	D	158	LEU	2.2
1	A	362	THR	2.2
1	F	147	GLY	2.2
1	B	135	ILE	2.2
1	F	15	LEU	2.2
1	F	341	GLU	2.2
1	C	121	ARG	2.2
1	F	41	LEU	2.2
1	D	197	GLY	2.2
1	F	226	ARG	2.2
1	D	10	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	366	ASP	2.2
1	D	193	THR	2.2
1	F	372	THR	2.2
1	B	494	GLN	2.2
1	A	320	ASP	2.2
1	C	362	THR	2.2
1	C	116	TYR	2.1
1	A	19	GLY	2.1
1	F	136	GLY	2.1
1	B	161	THR	2.1
1	A	201	VAL	2.1
1	A	35	ASP	2.1
1	E	202	ALA	2.1
1	A	394	PHE	2.1
1	D	398	ASN	2.1
1	F	365	CYS	2.1
1	E	40	VAL	2.1
1	F	196	VAL	2.1
1	B	41	LEU	2.1
1	C	19	GLY	2.1
1	F	264	PRO	2.1
1	F	403	HIS	2.1
1	A	289	LEU	2.1
1	C	367	TYR	2.1
1	D	21	GLY	2.1
1	D	399	ILE	2.1
1	F	257	GLU	2.1
1	D	26	ALA	2.1
1	C	21	GLY	2.1
1	C	187	PRO	2.1
1	F	273	SER	2.1
1	F	338	GLY	2.1
1	A	18	ILE	2.1
1	E	16	ILE	2.1
1	F	348	GLN	2.1
1	F	463	GLN	2.1
1	F	315	LYS	2.1
1	F	166	ARG	2.1
1	F	405	PHE	2.1
1	B	155	GLU	2.1
1	F	21	GLY	2.1
1	F	42	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	49	LEU	2.1
1	F	493	LEU	2.1
1	A	159	ILE	2.1
1	A	124	LYS	2.1
1	B	396	GLU	2.1
1	E	461	THR	2.1
1	F	231	ASP	2.1
1	C	138	HIS	2.0
1	C	389	LYS	2.0
1	F	17	ILE	2.0
1	F	253	PRO	2.0
1	D	127	TYR	2.0
1	F	227	GLY	2.0
1	B	148	LYS	2.0
1	C	220	VAL	2.0
1	D	402	TYR	2.0
1	C	130	ALA	2.0
1	B	172	GLY	2.0
1	E	89	LYS	2.0
1	A	337	GLU	2.0
1	B	311	GLU	2.0
1	C	316	ILE	2.0
1	D	159	ILE	2.0
1	C	258	GLN	2.0
1	F	48	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NAP	F	601	32/48	0.82	0.31	0.19	64,74,99,100	0
2	FAD	F	600	53/53	0.81	0.27	-0.11	60,64,70,71	0
3	NAP	C	601	32/48	0.82	0.26	-0.23	64,74,99,100	0
2	FAD	E	600	53/53	0.95	0.22	-0.30	60,64,70,71	0
2	FAD	C	600	53/53	0.84	0.25	-0.48	60,64,70,71	0
2	FAD	D	600	53/53	0.96	0.24	-0.56	60,64,70,72	0
2	FAD	B	600	53/53	0.95	0.18	-0.82	60,64,70,72	0
3	NAP	E	601	32/48	0.88	0.19	-0.87	64,74,99,100	0
3	NAP	D	601	32/48	0.90	0.20	-0.96	64,74,99,100	0
2	FAD	A	600	53/53	0.95	0.17	-1.12	60,64,70,71	0
3	NAP	B	601	32/48	0.91	0.19	-1.15	64,74,99,100	0
3	NAP	A	601	32/48	0.93	0.16	-1.63	64,74,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.