



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:07 PM UTC

PDB ID : 6S62 / pdb_00006s62
Title : Crystal structure of 2-methylcitrate dehydratase (PrpD) from *Pseudomonas aeruginosa* in apo form.
Authors : Wijaya, A.J.; Brear, P.; Dolan, S.K.; Welch, M.
Deposited on : 2019-07-02
Resolution : 2.36 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

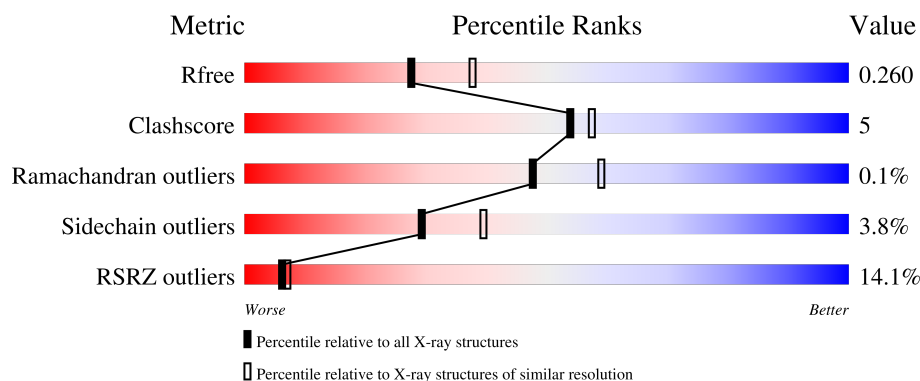
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	494	21% 83% 14% ..
1	B	494	22% 80% 17% ..
1	C	494	0% 86% 11% ..
1	D	494	2% 85% 12% ..
1	E	494	14% 83% 14% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	494	23% 85% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22926 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 Propionate catabolic protein PrpD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3796	2400	685	693	18			
1	B	484	Total	C	N	O	S	0	0	0
			3786	2394	681	693	18			
1	C	483	Total	C	N	O	S	0	0	0
			3777	2388	680	691	18			
1	D	484	Total	C	N	O	S	0	0	0
			3780	2390	684	688	18			
1	E	485	Total	C	N	O	S	0	0	0
			3797	2400	685	694	18			
1	F	485	Total	C	N	O	S	0	0	0
			3797	2400	685	694	18			

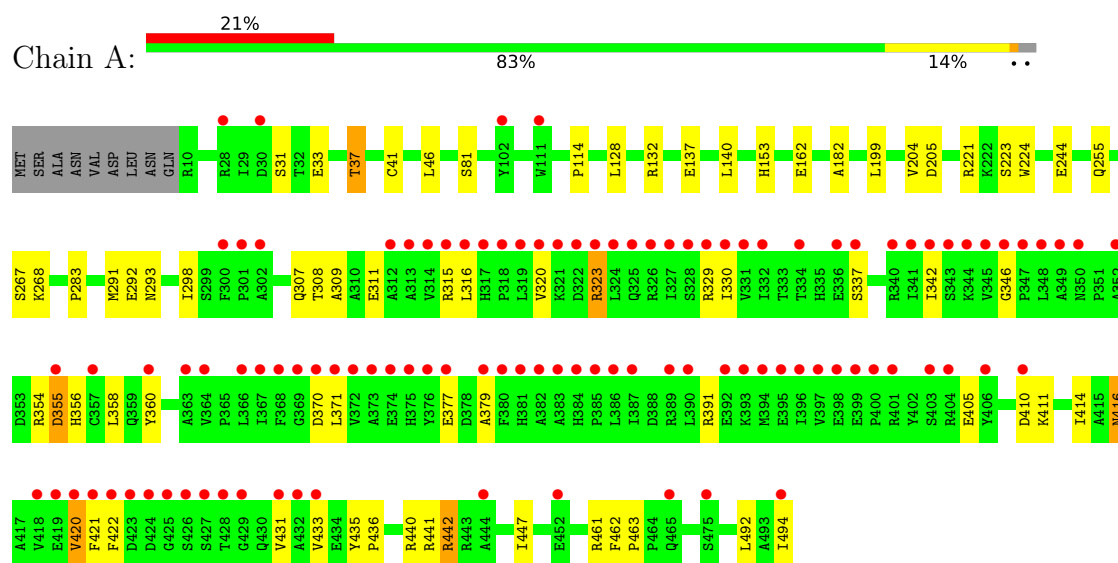
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	22	Total	O	0	0
			22	22		
2	B	41	Total	O	0	0
			41	41		
2	C	50	Total	O	0	0
			50	50		
2	D	33	Total	O	0	0
			33	33		
2	E	24	Total	O	0	0
			24	24		
2	F	23	Total	O	0	0
			23	23		

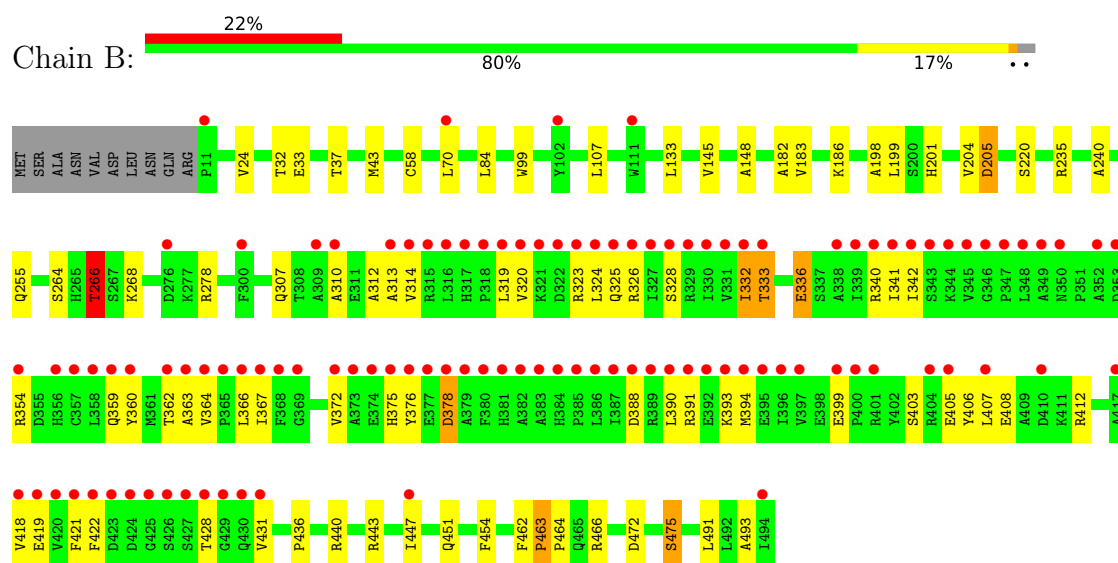
3 Residue-property plots [i](#)

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.

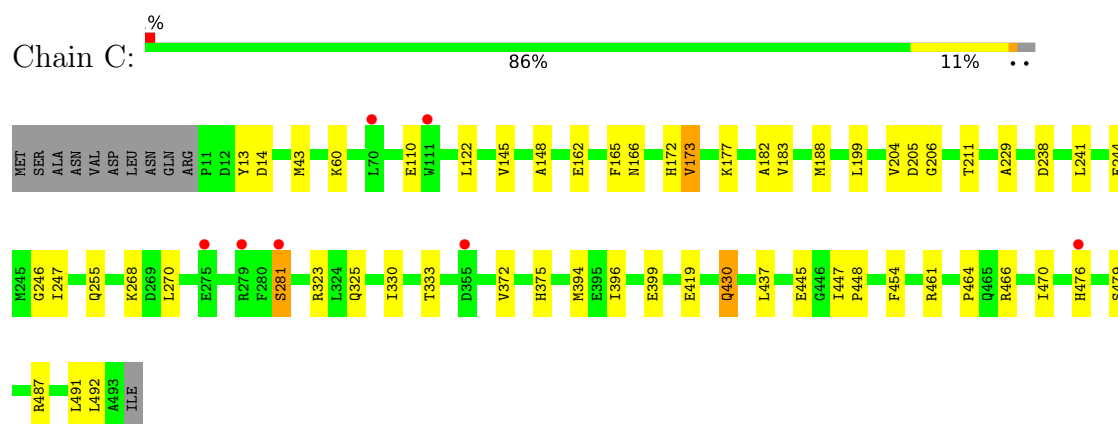
• Molecule 1: Propionate catabolic protein PrpD



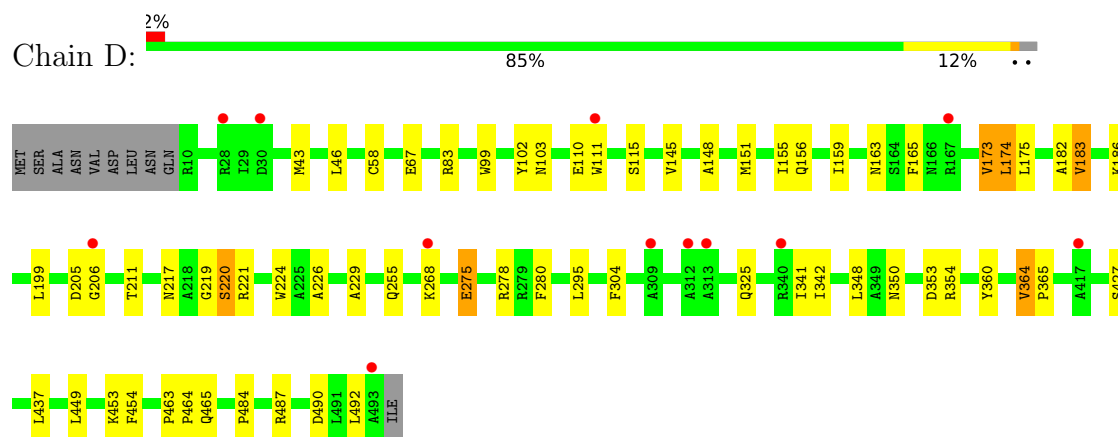
• Molecule 1: Propionate catabolic protein PrpD



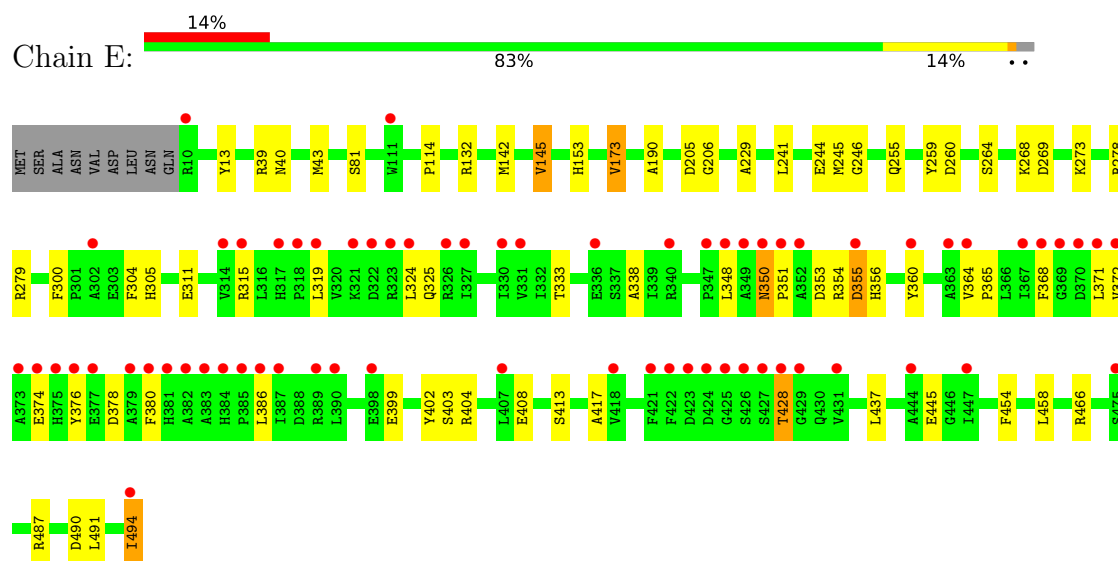
• Molecule 1: Propionate catabolic protein PrpD



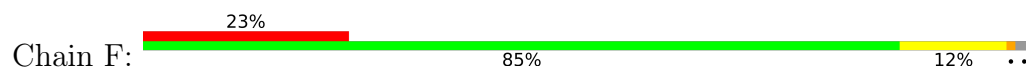
• Molecule 1: Propionate catabolic protein PrpD

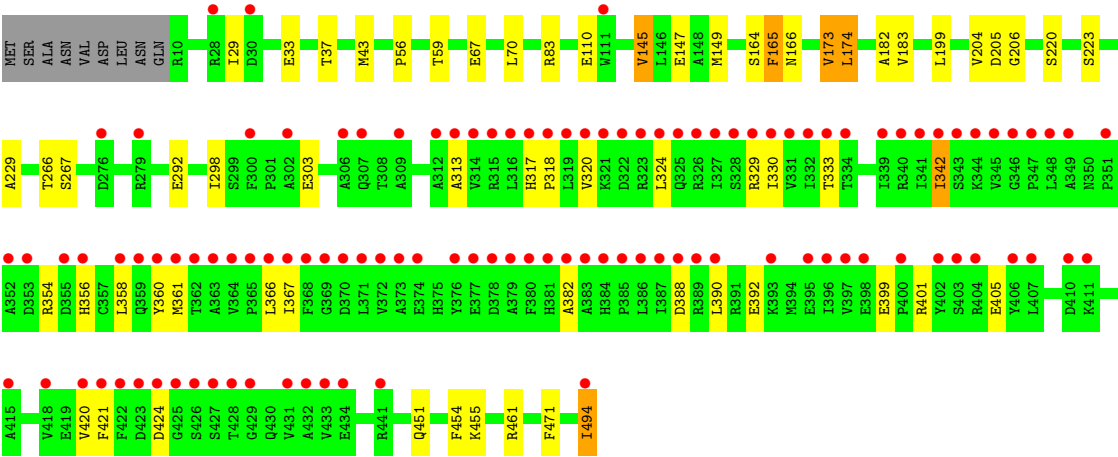


• Molecule 1: Propionate catabolic protein PrpD



• Molecule 1: Propionate catabolic protein PrpD





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	123.48Å 124.54Å 126.85Å 90.00° 116.85° 90.00°	Depositor
Resolution (Å)	113.17 – 2.36 113.17 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.3 (113.17-2.36) 99.5 (113.17-2.36)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.206 , 0.260 0.208 , 0.260	Depositor DCC
R_{free} test set	7175 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22926	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.46	0/3882	0.62	0/5269
1	B	0.50	2/3872 (0.1%)	0.66	6/5254 (0.1%)
1	C	0.56	1/3863 (0.0%)	0.69	0/5243
1	D	0.49	2/3866 (0.1%)	0.65	3/5248 (0.1%)
1	E	0.43	0/3883	0.63	0/5269
1	F	0.41	0/3883	0.60	4/5269 (0.1%)
All	All	0.48	5/23249 (0.0%)	0.64	13/31552 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	464	PRO	C-O	-6.49	1.16	1.24
1	C	464	PRO	C-O	-5.68	1.16	1.24
1	B	463	PRO	C-O	-5.59	1.18	1.24
1	B	464	PRO	C-O	-5.54	1.16	1.24
1	D	463	PRO	C-O	-5.46	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	GLY	CA-C-N	6.95	129.90	120.38
1	D	219	GLY	C-N-CA	6.95	129.90	120.38
1	F	298	ILE	CA-C-N	-6.75	115.90	123.13
1	F	298	ILE	C-N-CA	-6.75	115.90	123.13
1	F	165	PHE	CB-CA-C	6.43	120.50	109.24
1	B	33	GLU	CB-CG-CD	6.27	123.25	112.60
1	F	165	PHE	N-CA-C	-5.97	106.12	113.41
1	B	493	ALA	CA-C-N	5.49	131.59	121.70
1	B	493	ALA	C-N-CA	5.49	131.59	121.70
1	B	37	THR	CA-CB-OG1	-5.45	101.43	109.60
1	D	490	ASP	CA-CB-CG	5.36	117.96	112.60
1	B	266	THR	CA-CB-OG1	-5.21	101.79	109.60
1	B	266	THR	CB-CA-C	5.09	118.16	109.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3796	0	3767	38	0
1	B	3786	0	3755	50	0
1	C	3777	0	3744	34	0
1	D	3780	0	3748	37	0
1	E	3797	0	3767	44	0
1	F	3797	0	3767	37	0
2	A	22	0	0	0	0
2	B	41	0	0	1	0
2	C	50	0	0	1	0
2	D	33	0	0	0	0
2	E	24	0	0	0	0
2	F	23	0	0	0	0
All	All	22926	0	22548	222	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 5.

All (222) 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:244:GLU:OE1	1:D:220:SER:HB3	1.56	1.03
1:C:476:HIS:HD2	1:C:479:SER:H	1.21	0.88
1:C:476:HIS:CD2	1:C:479:SER:H	1.96	0.83
1:B:332:ILE:HD13	1:B:418:VAL:HG22	1.74	0.70
1:C:244:GLU:OE1	1:D:220:SER:CB	2.38	0.69
1:D:182:ALA:HB2	1:D:199:LEU:HD21	1.76	0.68
1:B:341:ILE:HG22	1:B:342:ILE:HG23	1.74	0.68
1:A:182:ALA:HB2	1:A:199:LEU:HD21	1.78	0.66
1:B:312:ALA:HB1	1:B:431:VAL:HG23	1.78	0.65
1:D:173:VAL:HG13	1:D:229:ALA:HB2	1.78	0.65
1:C:173:VAL:HG13	1:C:229:ALA:HB2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:ARG:HB3	1:F:421:PHE:HB2	1.79	0.65
1:F:342:ILE:HG23	1:F:358:LEU:HB2	1.77	0.64
1:B:319:LEU:HB3	1:B:428:THR:HG21	1.79	0.64
1:E:319:LEU:HD22	1:E:428:THR:HG22	1.78	0.64
1:C:188:MET:HE2	1:C:241:LEU:HG	1.80	0.64
1:C:188:MET:HE1	1:C:238:ASP:HA	1.79	0.64
1:E:273:LYS:O	1:E:278:ARG:NH1	2.31	0.64
1:D:83:ARG:HD2	1:F:67:GLU:OE2	1.98	0.63
1:A:255:GLN:HG3	1:B:268:LYS:HA	1.81	0.62
1:C:268:LYS:HA	1:D:255:GLN:HG3	1.81	0.62
1:D:221:ARG:HD2	1:D:224:TRP:CH2	2.36	0.61
1:E:350:ASN:N	1:E:350:ASN:OD1	2.32	0.60
1:A:316:LEU:HD11	1:A:431:VAL:HB	1.83	0.60
1:C:162:GLU:OE2	1:C:281:SER:HB3	2.02	0.59
1:A:320:VAL:HG11	1:A:420:VAL:HG11	1.84	0.59
1:A:323:ARG:HB2	1:A:422:PHE:CE1	2.38	0.59
1:F:110:GLU:OE1	1:F:165:PHE:N	2.30	0.58
1:E:114:PRO:HB2	1:E:153:HIS:CE1	2.39	0.57
1:E:374:GLU:N	1:E:374:GLU:OE1	2.37	0.57
1:A:377:GLU:OE1	1:A:379:ALA:N	2.35	0.57
1:F:320:VAL:CG1	1:F:420:VAL:HG11	2.34	0.57
1:B:354:ARG:HH12	1:B:378:ASP:HA	1.70	0.56
1:E:255:GLN:O	1:F:267:SER:OG	2.22	0.56
1:E:372:VAL:HG23	1:E:374:GLU:H	1.70	0.56
1:B:388:ASP:HA	1:B:391:ARG:HB2	1.88	0.56
1:D:67:GLU:OE2	1:F:83:ARG:HD2	2.06	0.56
1:A:132:ARG:HD2	1:A:140:LEU:HD12	1.86	0.55
1:E:466:ARG:NH1	1:E:491:LEU:O	2.35	0.55
1:A:33:GLU:O	1:A:37:THR:HG23	2.06	0.55
1:D:58:CYS:HB2	1:D:99:TRP:CD2	2.43	0.54
1:A:405:GLU:HG2	1:A:411:LYS:HD2	1.88	0.54
1:A:342:ILE:HD12	1:A:358:LEU:HB2	1.89	0.54
1:E:365:PRO:HG3	1:E:371:LEU:HB2	1.88	0.54
1:A:309:ALA:HB2	1:A:416:ASN:OD1	2.08	0.54
1:B:354:ARG:HH12	1:B:378:ASP:CA	2.20	0.53
1:C:148:ALA:HB1	1:C:183:VAL:CG1	2.39	0.53
1:E:40:ASN:HA	1:E:43:MET:HE2	1.89	0.53
1:B:320:VAL:HG12	1:B:422:PHE:CZ	2.43	0.53
1:F:320:VAL:HG11	1:F:420:VAL:HG11	1.91	0.53
1:F:173:VAL:HG13	1:F:229:ALA:HB2	1.90	0.53
1:F:33:GLU:HG2	1:F:292:GLU:HG2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ILE:CG2	1:F:358:LEU:HB2	2.38	0.52
1:A:81:SER:HB3	1:A:494:ILE:HG12	1.92	0.52
1:A:414:ILE:HD12	1:A:436:PRO:HG3	1.91	0.52
1:B:463:PRO:HG3	1:C:60:LYS:HB3	1.91	0.52
1:F:330:ILE:HG12	1:F:420:VAL:HG23	1.92	0.52
1:A:81:SER:CB	1:A:494:ILE:HD11	2.40	0.52
1:D:43:MET:HG2	1:D:454:PHE:CE2	2.44	0.52
1:E:494:ILE:O	1:E:494:ILE:HG22	2.08	0.52
1:B:43:MET:HE3	1:B:454:PHE:CD2	2.45	0.52
1:B:43:MET:HE1	1:B:451:GLN:HG2	1.92	0.52
1:E:245:MET:HE3	1:F:220:SER:OG	2.10	0.52
1:B:266:THR:HG23	2:B:530:HOH:O	2.11	0.51
1:C:447:ILE:HB	1:C:448:PRO:HD3	1.91	0.51
1:B:148:ALA:HB1	1:B:183:VAL:HG13	1.92	0.51
1:C:255:GLN:CD	1:D:268:LYS:HG2	2.35	0.51
1:D:341:ILE:HG22	1:D:342:ILE:HG23	1.93	0.51
1:E:355:ASP:HB3	1:E:356:HIS:ND1	2.26	0.51
1:C:13:TYR:OH	1:C:246:GLY:HA3	2.11	0.51
1:D:156:GLN:HG3	1:D:175:LEU:HB3	1.93	0.51
1:B:264:SER:HB2	1:B:278:ARG:HD2	1.92	0.50
1:D:174:LEU:C	1:D:174:LEU:HD23	2.35	0.50
1:E:364:VAL:HB	1:E:365:PRO:HD3	1.94	0.50
1:A:46:LEU:HD13	1:A:492:LEU:HD11	1.93	0.50
1:B:406:TYR:HD1	1:B:407:LEU:HD22	1.76	0.50
1:B:340:ARG:HG3	1:B:341:ILE:HD12	1.93	0.50
1:C:43:MET:HE3	1:C:454:PHE:CD2	2.46	0.50
1:D:295:LEU:HB3	1:D:304:PHE:CZ	2.47	0.50
1:E:351:PRO:HB3	1:E:376:TYR:O	2.12	0.50
1:A:346:GLY:O	1:A:391:ARG:NH2	2.36	0.49
1:F:313:ALA:HB1	1:F:366:LEU:HG	1.93	0.49
1:B:24:VAL:O	1:B:186:LYS:HE2	2.12	0.49
1:C:206:GLY:C	1:D:206:GLY:HA3	2.36	0.49
1:F:455:LYS:HE3	1:F:471:PHE:CE2	2.46	0.49
1:B:354:ARG:HB3	1:B:376:TYR:HD1	1.78	0.49
1:E:325:GLN:NE2	1:E:386:LEU:HD21	2.27	0.49
1:B:107:LEU:O	1:B:412:ARG:NH2	2.45	0.49
1:A:81:SER:HB2	1:A:494:ILE:HD11	1.94	0.49
1:A:114:PRO:HB2	1:A:153:HIS:CD2	2.47	0.49
1:C:206:GLY:HA3	1:D:206:GLY:C	2.37	0.49
1:C:476:HIS:HD2	1:C:479:SER:N	2.01	0.49
1:E:173:VAL:HG13	1:E:229:ALA:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ALA:HB2	1:C:199:LEU:HD21	1.95	0.48
1:A:267:SER:OG	1:B:255:GLN:O	2.31	0.48
1:A:355:ASP:HB3	1:A:356:HIS:ND1	2.27	0.48
1:D:151:MET:HE1	1:D:186:LYS:HE2	1.96	0.48
1:E:368:PHE:CE2	1:E:380:PHE:HZ	2.32	0.48
1:E:487:ARG:NH1	1:E:490:ASP:OD2	2.46	0.48
1:A:244:GLU:OE2	1:B:220:SER:OG	2.27	0.48
1:A:435:TYR:O	1:A:442:ARG:HD3	2.14	0.48
1:B:333:THR:HG22	1:B:399:GLU:HB2	1.96	0.48
1:F:29:ILE:HD12	1:F:147:GLU:HG2	1.95	0.48
1:F:401:ARG:O	1:F:405:GLU:HG3	2.14	0.48
1:B:336:GLU:N	1:B:403:SER:OG	2.45	0.48
1:C:14:ASP:HB3	2:C:517:HOH:O	2.13	0.48
1:C:419:GLU:HB2	1:C:430:GLN:HG3	1.96	0.48
1:E:81:SER:HB3	1:E:494:ILE:CG1	2.44	0.48
1:D:360:TYR:O	1:D:364:VAL:HG13	2.14	0.47
1:A:330:ILE:HG12	1:A:420:VAL:HB	1.96	0.47
1:D:484:PRO:HD2	1:D:487:ARG:HD3	1.97	0.47
1:F:354:ARG:HB3	1:F:360:TYR:CD2	2.49	0.47
1:F:303:GLU:H	1:F:361:MET:HE1	1.78	0.47
1:B:405:GLU:HA	1:B:408:GLU:HG3	1.97	0.47
1:C:470:ILE:HD13	1:C:492:LEU:HD23	1.97	0.47
1:D:275:GLU:HA	1:D:278:ARG:HG3	1.97	0.47
1:A:370:ASP:OD1	1:A:371:LEU:N	2.48	0.46
1:B:201:HIS:HA	1:B:204:VAL:HG12	1.96	0.46
1:D:348:LEU:HD22	1:D:353:ASP:HB3	1.96	0.46
1:D:148:ALA:HB1	1:D:183:VAL:HG13	1.96	0.46
1:E:81:SER:HB3	1:E:494:ILE:HG13	1.97	0.46
1:B:324:LEU:HA	1:B:324:LEU:HD12	1.63	0.46
1:B:367:ILE:HD11	1:B:390:LEU:HD12	1.97	0.46
1:D:111:TRP:HH2	1:D:341:ILE:HD13	1.80	0.46
1:E:190:ALA:HB2	1:E:241:LEU:HD21	1.98	0.46
1:E:354:ARG:HD3	1:E:360:TYR:CZ	2.50	0.46
1:E:13:TYR:OH	1:E:246:GLY:HA3	2.16	0.46
1:E:142:MET:HA	1:E:145:VAL:HG13	1.97	0.46
1:E:350:ASN:HB2	1:E:351:PRO:HD2	1.97	0.46
1:B:58:CYS:HB2	1:B:99:TRP:CD2	2.51	0.46
1:A:308:THR:OG1	1:A:416:ASN:HB2	2.16	0.46
1:B:320:VAL:HG12	1:B:422:PHE:HZ	1.80	0.46
1:D:103:ASN:ND2	1:D:115:SER:OG	2.48	0.46
1:B:182:ALA:HB2	1:B:199:LEU:HD21	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HB2	1:A:137:GLU:HB2	1.98	0.45
1:B:364:VAL:HG11	1:B:375:HIS:CG	2.51	0.45
1:C:437:LEU:HD23	1:C:437:LEU:HA	1.84	0.45
1:E:333:THR:HB	1:E:417:ALA:HB3	1.98	0.45
1:E:260:ASP:O	1:E:264:SER:OG	2.26	0.45
1:F:388:ASP:O	1:F:392:GLU:HG2	2.17	0.45
1:C:247:ILE:HG23	1:D:217:ASN:HB3	1.99	0.45
1:F:33:GLU:O	1:F:37:THR:HG23	2.17	0.45
1:F:317:HIS:HB3	1:F:318:PRO:HD3	1.97	0.45
1:B:363:ALA:HB2	1:B:394:MET:HE1	1.99	0.45
1:F:333:THR:HG22	1:F:399:GLU:HB2	1.99	0.45
1:A:162:GLU:HG3	1:A:283:PRO:HD3	1.99	0.45
1:A:293:ASN:ND2	1:A:440:ARG:HD2	2.31	0.45
1:C:372:VAL:HG22	1:C:375:HIS:CE1	2.52	0.45
1:B:354:ARG:NH1	1:B:378:ASP:HA	2.33	0.44
1:D:110:GLU:OE1	1:D:165:PHE:N	2.50	0.44
1:F:494:ILE:O	1:F:494:ILE:HG23	2.18	0.44
1:B:419:GLU:HG2	1:B:421:PHE:CE1	2.52	0.44
1:B:359:GLN:HB2	1:B:391:ARG:HE	1.81	0.44
1:C:333:THR:CG2	1:C:399:GLU:HB2	2.48	0.44
1:E:259:TYR:CE1	1:E:279:ARG:HA	2.53	0.44
1:E:311:GLU:OE1	1:E:315:ARG:NH2	2.50	0.44
1:D:354:ARG:HD3	1:D:360:TYR:CZ	2.53	0.44
1:A:31:SER:OG	1:A:292:GLU:OE2	2.35	0.44
1:E:350:ASN:O	1:E:354:ARG:HG3	2.17	0.44
1:B:462:PHE:CD1	1:B:466:ARG:HD2	2.54	0.43
1:B:372:VAL:HG22	1:B:375:HIS:CE1	2.53	0.43
1:C:476:HIS:CD2	1:C:479:SER:OG	2.72	0.43
1:E:348:LEU:HD22	1:E:353:ASP:HB3	2.00	0.43
1:D:364:VAL:HG22	1:D:365:PRO:HD3	1.99	0.43
1:B:332:ILE:HD11	1:B:362:THR:HG21	2.01	0.43
1:F:56:PRO:HA	1:F:59:THR:OG1	2.18	0.43
1:F:145:VAL:O	1:F:149:MET:HG3	2.19	0.43
1:A:132:ARG:HE	1:A:132:ARG:HB3	1.52	0.43
1:C:110:GLU:OE1	1:C:165:PHE:N	2.51	0.43
1:E:39:ARG:O	1:E:43:MET:HG3	2.19	0.43
1:B:472:ASP:O	1:B:475:SER:HB2	2.19	0.43
1:C:148:ALA:HB1	1:C:183:VAL:HG11	2.00	0.43
1:E:325:GLN:HE22	1:E:386:LEU:HD21	1.83	0.43
1:C:445:GLU:O	1:C:448:PRO:HD2	2.19	0.43
1:F:367:ILE:HD11	1:F:390:LEU:HD13	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:O	1:A:315:ARG:HG2	2.19	0.42
1:D:174:LEU:HD23	1:D:175:LEU:HD23	2.01	0.42
1:F:182:ALA:HB2	1:F:199:LEU:HD21	2.01	0.42
1:C:466:ARG:NH1	1:C:491:LEU:O	2.44	0.42
1:F:354:ARG:HD3	1:F:360:TYR:CZ	2.54	0.42
1:A:221:ARG:HD2	1:A:224:TRP:CH2	2.55	0.42
1:A:329:ARG:O	1:A:421:PHE:N	2.45	0.42
1:C:330:ILE:O	1:C:394:MET:HA	2.19	0.42
1:E:324:LEU:N	1:E:324:LEU:HD12	2.34	0.42
1:B:148:ALA:HB1	1:B:183:VAL:CG1	2.50	0.42
1:D:102:TYR:CZ	1:D:453:LYS:HE3	2.54	0.42
1:C:110:GLU:OE2	1:C:172:HIS:HB3	2.20	0.42
1:F:342:ILE:HD11	1:F:356:HIS:HA	2.00	0.42
1:B:323:ARG:HG2	1:B:326:ARG:HE	1.84	0.42
1:E:300:PHE:HB3	1:E:371:LEU:HD22	2.01	0.42
1:E:305:HIS:HB3	1:E:338:ALA:HB2	2.02	0.42
1:F:43:MET:HE3	1:F:454:PHE:CD2	2.55	0.42
1:A:41:CYS:HB2	1:A:291:MET:HE1	2.01	0.42
1:B:313:ALA:HB1	1:B:366:LEU:HG	2.02	0.42
1:D:437:LEU:HD21	1:D:449:LEU:HD12	2.02	0.42
1:E:404:ARG:HG2	1:E:408:GLU:OE2	2.19	0.42
1:F:165:PHE:CD1	1:F:174:LEU:HD21	2.55	0.42
1:D:46:LEU:HD13	1:D:492:LEU:HD11	2.03	0.41
1:B:354:ARG:HG2	1:B:360:TYR:CD2	2.55	0.41
1:A:435:TYR:CE2	1:A:441:ARG:HD3	2.56	0.41
1:D:163:ASN:OD1	1:D:280:PHE:HA	2.20	0.41
1:F:43:MET:HE1	1:F:451:GLN:HG2	2.03	0.41
1:B:198:ALA:HB2	1:B:240:ALA:CB	2.51	0.41
1:B:324:LEU:HB3	1:B:325:GLN:HE21	1.86	0.41
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.86	0.41
1:B:440:ARG:HA	1:B:443:ARG:HG2	2.02	0.41
1:C:487:ARG:HA	1:C:487:ARG:HD2	1.96	0.41
1:D:155:ILE:O	1:D:159:ILE:HG13	2.21	0.41
1:E:206:GLY:C	1:F:206:GLY:HA3	2.46	0.41
1:E:399:GLU:HG3	1:E:402:TYR:H	1.86	0.41
1:F:354:ARG:HB3	1:F:360:TYR:CE2	2.56	0.41
1:A:354:ARG:HB3	1:A:360:TYR:CD2	2.55	0.40
1:D:58:CYS:HB2	1:D:99:TRP:CE2	2.56	0.40
1:D:173:VAL:HG22	1:D:226:ALA:HA	2.03	0.40
1:E:206:GLY:HA3	1:F:206:GLY:C	2.46	0.40
1:B:328:SER:O	1:B:393:LYS:HG2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:HH11	1:E:132:ARG:HG2	1.86	0.40
1:A:462:PHE:HA	1:A:463:PRO:HD3	1.90	0.40
1:B:310:ALA:O	1:B:314:VAL:HG23	2.20	0.40
1:E:454:PHE:CZ	1:E:458:LEU:HD11	2.56	0.40
1:B:307:GLN:HB3	1:B:436:PRO:HB3	2.04	0.40
1:E:244:GLU:OE2	1:F:220:SER:OG	2.33	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	483/494 (98%)	465 (96%)	18 (4%)	0	100	100
1	B	482/494 (98%)	469 (97%)	12 (2%)	1 (0%)	43	52
1	C	481/494 (97%)	467 (97%)	14 (3%)	0	100	100
1	D	482/494 (98%)	470 (98%)	12 (2%)	0	100	100
1	E	483/494 (98%)	467 (97%)	15 (3%)	1 (0%)	43	52
1	F	483/494 (98%)	467 (97%)	15 (3%)	1 (0%)	43	52
All	All	2894/2964 (98%)	2805 (97%)	86 (3%)	3 (0%)	48	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	ASP
1	E	428	THR
1	F	382	ALA

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	397/405 (98%)	380 (96%)	17 (4%)	26	34
1	B	396/405 (98%)	381 (96%)	15 (4%)	29	39
1	C	395/405 (98%)	380 (96%)	15 (4%)	29	39
1	D	394/405 (97%)	381 (97%)	13 (3%)	33	44
1	E	397/405 (98%)	383 (96%)	14 (4%)	32	42
1	F	397/405 (98%)	381 (96%)	16 (4%)	28	37
All	All	2376/2430 (98%)	2286 (96%)	90 (4%)	29	39

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	204	VAL
1	A	205	ASP
1	A	223	SER
1	A	268	LYS
1	A	298	ILE
1	A	307	GLN
1	A	323	ARG
1	A	337	SER
1	A	355	ASP
1	A	410	ASP
1	A	416	ASN
1	A	420	VAL
1	A	433	VAL
1	A	442	ARG
1	A	447	ILE
1	A	461	ARG
1	B	32	THR
1	B	70	LEU
1	B	84	LEU
1	B	133	LEU
1	B	145	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	205	ASP
1	B	235	ARG
1	B	266	THR
1	B	332	ILE
1	B	333	THR
1	B	336	GLU
1	B	378	ASP
1	B	447	ILE
1	B	475	SER
1	B	491	LEU
1	C	122	LEU
1	C	145	VAL
1	C	166	ASN
1	C	173	VAL
1	C	177	LYS
1	C	204	VAL
1	C	205	ASP
1	C	211	THR
1	C	270	LEU
1	C	281	SER
1	C	323	ARG
1	C	325	GLN
1	C	396	ILE
1	C	430	GLN
1	C	461	ARG
1	D	145	VAL
1	D	173	VAL
1	D	174	LEU
1	D	183	VAL
1	D	205	ASP
1	D	211	THR
1	D	220	SER
1	D	275	GLU
1	D	325	GLN
1	D	350	ASN
1	D	364	VAL
1	D	427	SER
1	D	465	GLN
1	E	145	VAL
1	E	173	VAL
1	E	205	ASP
1	E	268	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	269	ASP
1	E	304	PHE
1	E	350	ASN
1	E	355	ASP
1	E	378	ASP
1	E	403	SER
1	E	413	SER
1	E	437	LEU
1	E	445	GLU
1	E	494	ILE
1	F	70	LEU
1	F	145	VAL
1	F	164	SER
1	F	166	ASN
1	F	173	VAL
1	F	174	LEU
1	F	183	VAL
1	F	204	VAL
1	F	205	ASP
1	F	223	SER
1	F	266	THR
1	F	324	LEU
1	F	342	ILE
1	F	424	ASP
1	F	461	ARG
1	F	494	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	HIS
1	A	293	ASN
1	A	384	HIS
1	B	144	GLN
1	B	305	HIS
1	C	40	ASN
1	C	476	HIS
1	D	384	HIS
1	D	486	ASN
1	E	486	ASN
1	F	113	HIS
1	F	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	135	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	485/494 (98%)	0.98	105 (21%) 2 2	16, 33, 77, 94	0
1	B	484/494 (97%)	0.82	108 (22%) 2 2	14, 26, 70, 78	0
1	C	483/494 (97%)	0.07	7 (1%) 73 78	13, 23, 35, 53	0
1	D	484/494 (97%)	0.33	12 (2%) 58 64	16, 28, 45, 164	0
1	E	485/494 (98%)	0.68	67 (13%) 6 7	17, 30, 65, 77	0
1	F	485/494 (98%)	0.97	112 (23%) 2 1	17, 32, 75, 89	0
All	All	2906/2964 (98%)	0.64	411 (14%) 6 7	13, 28, 70, 164	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	312	ALA	11.5
1	D	417	ALA	9.0
1	A	494	ILE	6.6
1	B	494	ILE	6.6
1	B	386	LEU	6.5
1	E	386	LEU	6.4
1	B	324	LEU	6.3
1	A	319	LEU	6.1
1	A	385	PRO	6.0
1	B	421	PHE	5.9
1	A	111	TRP	5.7
1	F	323	ARG	5.6
1	A	345	VAL	5.6
1	B	345	VAL	5.4
1	E	385	PRO	5.3
1	F	494	ILE	5.2
1	E	368	PHE	5.2
1	E	380	PHE	5.2
1	B	420	VAL	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	320	VAL	5.1
1	A	429	GLY	5.1
1	B	383	ALA	5.1
1	F	382	ALA	5.1
1	A	421	PHE	5.1
1	E	383	ALA	5.1
1	F	352	ALA	5.1
1	A	368	PHE	5.0
1	A	324	LEU	5.0
1	B	428	THR	4.8
1	B	331	VAL	4.8
1	F	386	LEU	4.7
1	F	347	PRO	4.7
1	B	418	VAL	4.7
1	A	424	ASP	4.7
1	F	385	PRO	4.7
1	B	380	PHE	4.6
1	A	366	LEU	4.6
1	B	319	LEU	4.5
1	E	494	ILE	4.5
1	E	319	LEU	4.5
1	B	318	PRO	4.5
1	B	327	ILE	4.5
1	E	367	ILE	4.5
1	A	386	LEU	4.4
1	E	318	PRO	4.4
1	A	423	ASP	4.4
1	B	423	ASP	4.4
1	F	322	ASP	4.4
1	A	320	VAL	4.4
1	B	329	ARG	4.3
1	E	372	VAL	4.3
1	F	345	VAL	4.3
1	B	426	SER	4.3
1	B	422	PHE	4.3
1	F	425	GLY	4.3
1	B	366	LEU	4.3
1	B	389	ARG	4.2
1	F	422	PHE	4.2
1	F	279	ARG	4.2
1	A	395	GLU	4.2
1	B	397	VAL	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	383	ALA	4.2
1	F	421	PHE	4.2
1	A	367	ILE	4.1
1	A	331	VAL	4.1
1	F	327	ILE	4.1
1	E	379	ALA	4.1
1	B	111	TRP	4.1
1	A	316	LEU	4.0
1	F	389	ARG	4.0
1	A	330	ILE	4.0
1	A	329	ARG	4.0
1	E	374	GLU	4.0
1	F	367	ILE	4.0
1	B	330	ILE	4.0
1	F	111	TRP	4.0
1	F	321	LYS	4.0
1	F	326	ARG	4.0
1	B	427	SER	4.0
1	F	324	LEU	3.9
1	B	377	GLU	3.9
1	E	373	ALA	3.9
1	B	373	ALA	3.9
1	D	309	ALA	3.9
1	F	330	ILE	3.9
1	F	318	PRO	3.8
1	A	347	PRO	3.8
1	B	367	ILE	3.8
1	F	340	ARG	3.8
1	F	348	LEU	3.8
1	F	428	THR	3.8
1	A	327	ILE	3.8
1	A	431	VAL	3.8
1	B	349	ALA	3.8
1	B	352	ALA	3.8
1	F	373	ALA	3.8
1	B	328	SER	3.8
1	F	341	ILE	3.8
1	B	323	ARG	3.8
1	B	382	ALA	3.7
1	D	493	ALA	3.7
1	B	333	THR	3.7
1	B	362	THR	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	394	MET	3.7
1	A	313	ALA	3.7
1	A	380	PHE	3.7
1	A	425	GLY	3.7
1	B	348	LEU	3.7
1	B	360	TYR	3.7
1	F	349	ALA	3.7
1	A	400	PRO	3.7
1	F	381	HIS	3.6
1	F	407	LEU	3.6
1	B	347	PRO	3.6
1	B	363	ALA	3.6
1	A	387	ILE	3.6
1	E	111	TRP	3.6
1	A	422	PHE	3.6
1	E	429	GLY	3.6
1	F	366	LEU	3.6
1	F	390	LEU	3.6
1	A	418	VAL	3.6
1	F	314	VAL	3.6
1	E	349	ALA	3.6
1	A	340	ARG	3.5
1	B	384	HIS	3.5
1	B	309	ALA	3.5
1	B	417	ALA	3.5
1	F	406	TYR	3.5
1	F	344	LYS	3.5
1	A	326	ARG	3.5
1	F	331	VAL	3.5
1	F	397	VAL	3.5
1	B	322	ASP	3.5
1	F	363	ALA	3.5
1	E	384	HIS	3.5
1	B	316	LEU	3.5
1	B	400	PRO	3.4
1	E	447	ILE	3.4
1	A	382	ALA	3.4
1	B	419	GLU	3.4
1	A	315	ARG	3.4
1	B	339	ILE	3.4
1	B	388	ASP	3.4
1	F	396	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	321	LYS	3.4
1	A	318	PRO	3.4
1	E	364	VAL	3.4
1	C	281	SER	3.4
1	A	322	ASP	3.4
1	B	387	ILE	3.4
1	B	390	LEU	3.3
1	B	385	PRO	3.3
1	B	368	PHE	3.3
1	A	420	VAL	3.3
1	A	369	GLY	3.3
1	B	341	ILE	3.3
1	B	391	ARG	3.3
1	F	300	PHE	3.3
1	B	424	ASP	3.3
1	E	351	PRO	3.3
1	A	336	GLU	3.3
1	F	320	VAL	3.3
1	F	420	VAL	3.3
1	B	396	ILE	3.3
1	F	400	PRO	3.3
1	A	426	SER	3.3
1	F	426	SER	3.3
1	A	432	ALA	3.2
1	B	431	VAL	3.3
1	D	313	ALA	3.2
1	B	410	ASP	3.2
1	A	428	THR	3.2
1	A	377	GLU	3.2
1	A	348	LEU	3.2
1	F	387	ILE	3.2
1	A	392	GLU	3.2
1	E	370	ASP	3.2
1	F	302	ALA	3.2
1	F	432	ALA	3.2
1	B	353	ASP	3.2
1	E	407	LEU	3.2
1	A	28	ARG	3.1
1	B	313	ALA	3.1
1	E	324	LEU	3.1
1	A	332	ILE	3.1
1	B	393	LYS	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	346	GLY	3.1
1	A	390	LEU	3.1
1	B	326	ARG	3.1
1	A	384	HIS	3.1
1	E	426	SER	3.1
1	E	369	GLY	3.1
1	F	370	ASP	3.1
1	F	379	ALA	3.1
1	E	321	LYS	3.1
1	F	332	ILE	3.1
1	B	317	HIS	3.1
1	E	322	ASP	3.1
1	F	429	GLY	3.1
1	E	382	ALA	3.1
1	A	389	ARG	3.1
1	E	390	LEU	3.1
1	F	358	LEU	3.1
1	F	361	MET	3.1
1	A	317	HIS	3.0
1	A	314	VAL	3.0
1	E	376	TYR	3.0
1	A	396	ILE	3.0
1	B	429	GLY	3.0
1	F	346	GLY	3.0
1	F	423	ASP	3.0
1	B	11	PRO	3.0
1	F	319	LEU	3.0
1	A	334	THR	3.0
1	A	30	ASP	3.0
1	B	346	GLY	3.0
1	A	379	ALA	3.0
1	E	352	ALA	3.0
1	F	313	ALA	3.0
1	F	377	GLU	3.0
1	A	393	LYS	3.0
1	B	332	ILE	2.9
1	E	424	ASP	2.9
1	F	384	HIS	2.9
1	F	360	TYR	2.9
1	D	268	LYS	2.9
1	A	383	ALA	2.9
1	E	371	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	364	VAL	2.9
1	B	357	CYS	2.9
1	A	427	SER	2.9
1	B	276	ASP	2.9
1	A	344	LYS	2.8
1	B	343	SER	2.8
1	A	323	ARG	2.8
1	F	325	GLN	2.8
1	B	70	LEU	2.8
1	A	352	ALA	2.8
1	B	425	GLY	2.8
1	F	380	PHE	2.8
1	B	392	GLU	2.8
1	A	397	VAL	2.8
1	A	341	ILE	2.8
1	F	333	THR	2.8
1	F	404	ARG	2.8
1	E	381	HIS	2.8
1	B	359	GLN	2.8
1	B	379	ALA	2.8
1	F	355	ASP	2.8
1	A	357	CYS	2.8
1	D	206	GLY	2.8
1	B	342	ILE	2.7
1	E	428	THR	2.7
1	E	423	ASP	2.7
1	A	301	PRO	2.7
1	A	312	ALA	2.7
1	F	368	PHE	2.7
1	E	427	SER	2.7
1	F	343	SER	2.7
1	B	376	TYR	2.7
1	E	363	ALA	2.7
1	B	372	VAL	2.7
1	E	431	VAL	2.7
1	C	476	HIS	2.7
1	F	372	VAL	2.7
1	E	315	ARG	2.7
1	F	371	LEU	2.7
1	B	381	HIS	2.6
1	B	310	ALA	2.6
1	A	360	TYR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	2.6
1	A	410	ASP	2.6
1	E	350	ASN	2.6
1	F	364	VAL	2.6
1	E	330	ILE	2.6
1	F	329	ARG	2.6
1	F	351	PRO	2.6
1	B	395	GLU	2.6
1	B	405	GLU	2.6
1	F	402	TYR	2.6
1	F	424	ASP	2.6
1	B	354	ARG	2.6
1	F	315	ARG	2.6
1	B	365	PRO	2.6
1	F	365	PRO	2.6
1	A	328	SER	2.6
1	B	430	GLN	2.6
1	E	425	GLY	2.6
1	F	369	GLY	2.6
1	F	376	TYR	2.6
1	F	427	SER	2.6
1	F	393	LYS	2.6
1	B	358	LEU	2.6
1	A	399	GLU	2.6
1	F	398	GLU	2.6
1	B	315	ARG	2.6
1	B	401	ARG	2.6
1	E	355	ASP	2.6
1	A	337	SER	2.6
1	F	317	HIS	2.6
1	B	399	GLU	2.5
1	E	348	LEU	2.5
1	E	323	ARG	2.5
1	A	343	SER	2.5
1	E	375	HIS	2.5
1	A	325	GLN	2.5
1	B	102	TYR	2.5
1	B	404	ARG	2.5
1	E	389	ARG	2.5
1	F	316	LEU	2.5
1	F	334	THR	2.5
1	A	364	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	325	GLN	2.5
1	E	418	VAL	2.5
1	F	339	ILE	2.5
1	B	338	ALA	2.5
1	B	344	LYS	2.5
1	B	350	ASN	2.5
1	F	378	ASP	2.5
1	A	372	VAL	2.5
1	C	111	TRP	2.5
1	D	111	TRP	2.5
1	F	309	ALA	2.5
1	A	404	ARG	2.4
1	B	340	ARG	2.4
1	A	302	ALA	2.4
1	E	475	SER	2.4
1	A	433	VAL	2.4
1	F	433	VAL	2.4
1	A	394	MET	2.4
1	F	359	GLN	2.4
1	B	374	GLU	2.4
1	E	377	GLU	2.4
1	B	407	LEU	2.4
1	E	326	ARG	2.4
1	A	355	ASP	2.4
1	F	353	ASP	2.4
1	B	321	LYS	2.4
1	F	362	THR	2.4
1	E	422	PHE	2.4
1	F	342	ILE	2.4
1	D	340	ARG	2.4
1	C	275	GLU	2.4
1	F	418	VAL	2.3
1	B	369	GLY	2.3
1	A	363	ALA	2.3
1	E	444	ALA	2.3
1	F	328	SER	2.3
1	A	374	GLU	2.3
1	A	371	LEU	2.3
1	A	370	ASP	2.3
1	A	102	TYR	2.3
1	F	415	ALA	2.3
1	E	10	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	381	HIS	2.3
1	F	307	GLN	2.3
1	F	388	ASP	2.3
1	A	406	TYR	2.3
1	A	465	GLN	2.3
1	A	342	ILE	2.3
1	F	411	LYS	2.3
1	B	314	VAL	2.3
1	D	30	ASP	2.2
1	B	375	HIS	2.2
1	E	317	HIS	2.2
1	E	398	GLU	2.2
1	F	306	ALA	2.2
1	F	403	SER	2.2
1	E	387	ILE	2.2
1	E	314	VAL	2.2
1	C	355	ASP	2.2
1	E	340	ARG	2.2
1	A	403	SER	2.2
1	A	475	SER	2.2
1	B	447	ILE	2.2
1	A	401	ARG	2.2
1	E	421	PHE	2.2
1	B	378	ASP	2.1
1	F	410	ASP	2.1
1	A	398	GLU	2.1
1	A	419	GLU	2.1
1	B	356	HIS	2.1
1	A	349	ALA	2.1
1	F	28	ARG	2.1
1	C	279	ARG	2.1
1	D	28	ARG	2.1
1	D	167	ARG	2.1
1	A	373	ALA	2.1
1	F	30	ASP	2.1
1	F	356	HIS	2.1
1	F	431	VAL	2.1
1	A	300	PHE	2.1
1	A	452	GLU	2.1
1	F	395	GLU	2.1
1	A	376	TYR	2.1
1	E	360	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	331	VAL	2.1
1	A	444	ALA	2.0
1	E	336	GLU	2.0
1	A	375	HIS	2.0
1	A	350	ASN	2.0
1	E	327	ILE	2.0
1	E	347	PRO	2.0
1	F	441	ARG	2.0
1	F	374	GLU	2.0
1	F	434	GLU	2.0
1	E	302	ALA	2.0
1	F	312	ALA	2.0
1	C	70	LEU	2.0
1	F	276	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.