



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:42 AM UTC

PDB ID : 4QOY / pdb_00004qoy
Title : Novel binding motif and new flexibility revealed by structural analysis of a pyruvate dehydrogenase-dihydrolipoyl acetyltransferase sub-complex from the escherichia coli pyruvate dehydrogenase multi-enzyme complex
Authors : Furey, W.; Arjunan, P.
Deposited on : 2014-06-20
Resolution : 2.80 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

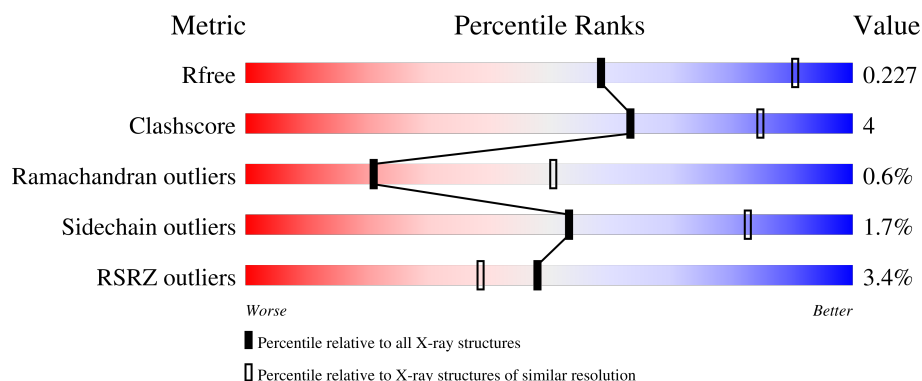
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	886	2% 87% 10% .
1	B	886	3% 87% 9% .
1	C	886	3% 87% 10% ..
1	D	886	3% 87% 8% ...
2	E	46	9% 85% 15%

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Mol	Chain	Length	Quality of chain
2	F	46	17% 80% 20%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 29167 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 Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	862	Total	C	N	O	S	0	0	0
			6824	4318	1181	1298	27			
1	B	854	Total	C	N	O	S	0	0	0
			6772	4287	1170	1288	27			
1	C	864	Total	C	N	O	S	0	0	0
			6826	4317	1183	1299	27			
1	D	849	Total	C	N	O	S	0	0	0
			6722	4254	1163	1278	27			

- Molecule 2 is a protein called Pyruvate dehydrogenase (Dihydrolipoyltransacetylase component).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	46	Total	C	N	O	0	0	0
			365	230	76	59			
2	F	46	Total	C	N	O	0	0	0
			365	230	76	59			

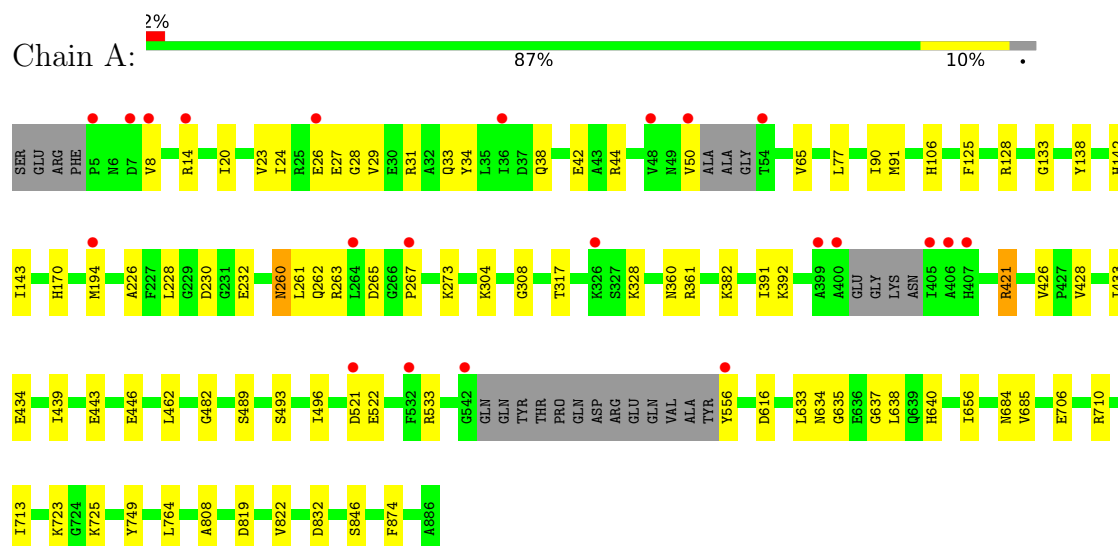
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	401	Total	O	0	0
			401	401		
3	B	436	Total	O	0	0
			436	436		
3	C	224	Total	O	0	0
			224	224		
3	D	224	Total	O	0	0
			224	224		
3	E	5	Total	O	0	0
			5	5		
3	F	3	Total	O	0	0
			3	3		

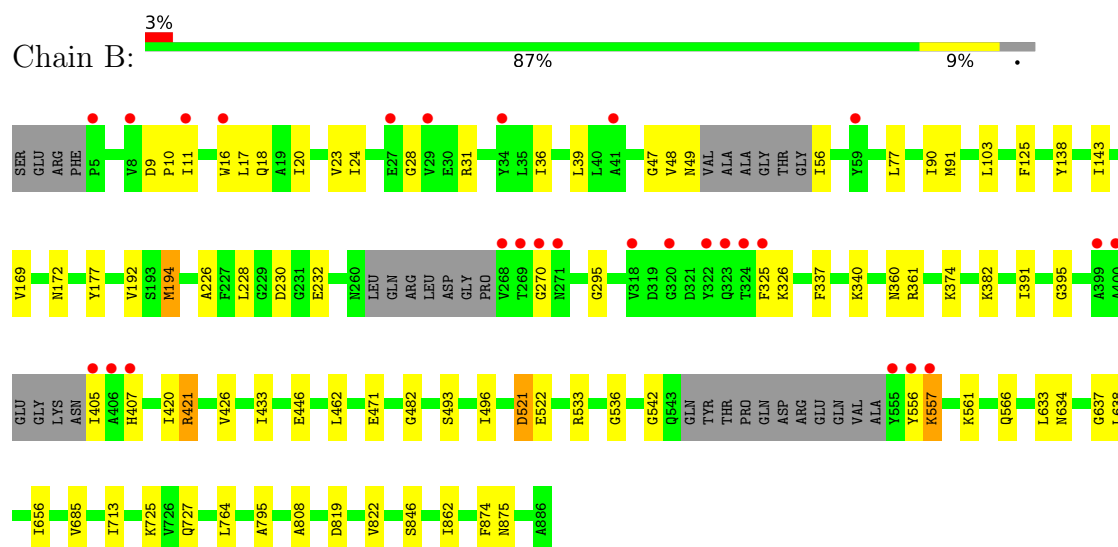
3 Residue-property plots [i](#)

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.

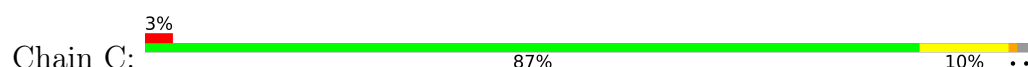
• Molecule 1: Pyruvate dehydrogenase E1 component

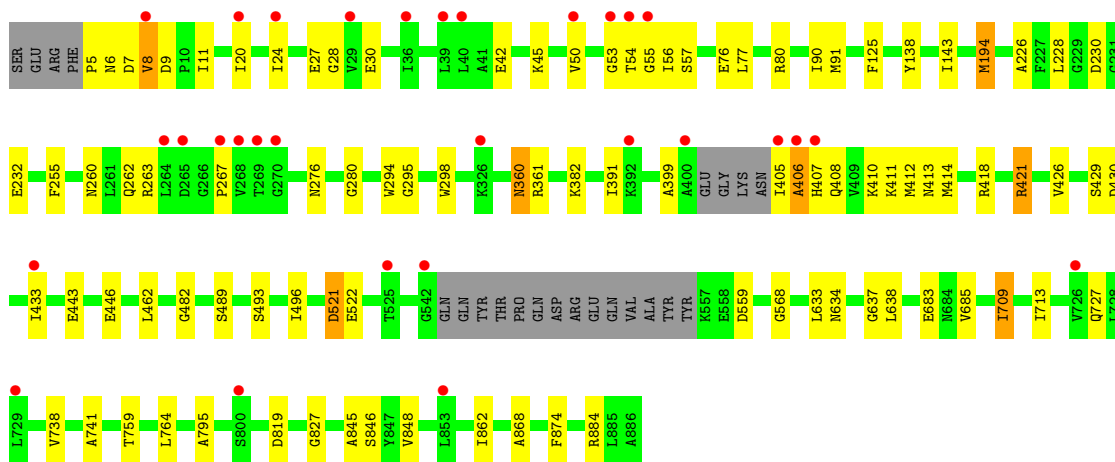


• Molecule 1: Pyruvate dehydrogenase E1 component

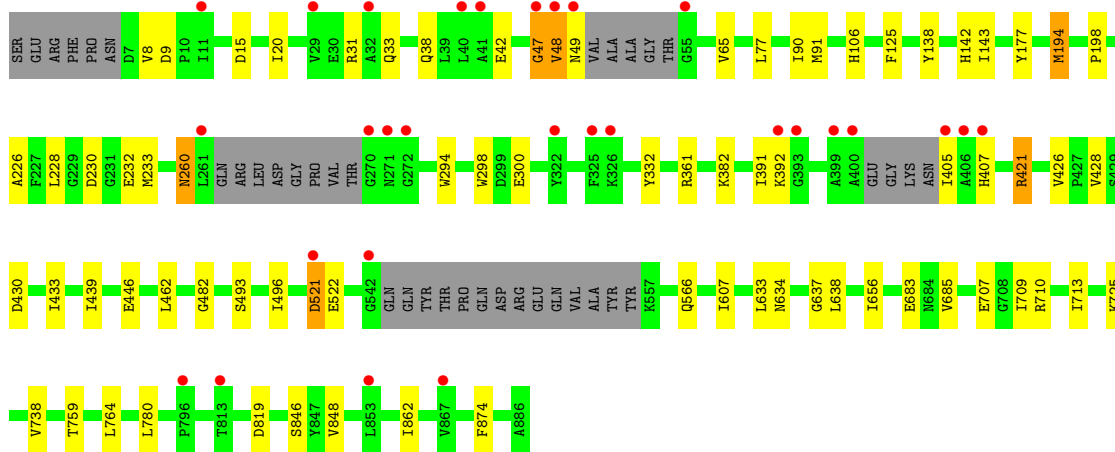
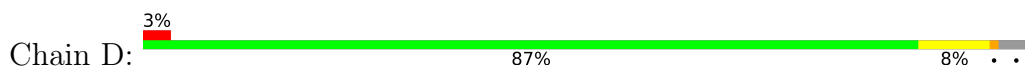


• Molecule 1: Pyruvate dehydrogenase E1 component

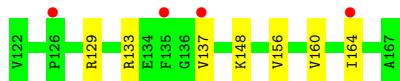
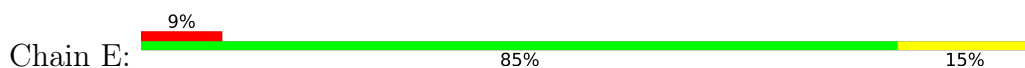




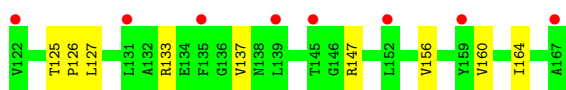
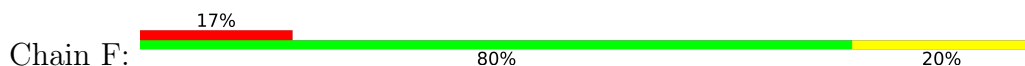
• Molecule 1: Pyruvate dehydrogenase E1 component



• Molecule 2: Pyruvate dehydrogenase (Dihydrolipoyltransacetylase component)



• Molecule 2: Pyruvate dehydrogenase (Dihydrolipoyltransacetylase component)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	210.94Å 326.84Å 77.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.29 – 2.80 32.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.4 (32.29-2.80) 94.3 (32.29-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.81Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.198 , 0.233 0.197 , 0.227	Depositor DCC
R_{free} test set	6292 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	62.9	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 69.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29167	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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	0.81	0/6973	1.28	10/9425 (0.1%)
1	B	0.83	0/6920	1.29	15/9351 (0.2%)
1	C	0.78	0/6975	1.27	11/9429 (0.1%)
1	D	0.79	0/6867	1.28	13/9277 (0.1%)
2	E	0.89	0/368	1.30	0/490
2	F	0.86	0/368	1.35	0/490
All	All	0.80	0/28471	1.28	49/38462 (0.1%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	ASN	CA-CB-CG	8.94	121.54	112.60
1	D	633	LEU	CA-C-N	7.54	130.39	120.28
1	D	633	LEU	C-N-CA	7.54	130.39	120.28
1	C	633	LEU	CA-C-N	7.53	130.37	120.28
1	C	633	LEU	C-N-CA	7.53	130.37	120.28
1	A	633	LEU	CA-C-N	7.42	130.22	120.28
1	A	633	LEU	C-N-CA	7.42	130.22	120.28
1	B	633	LEU	CA-C-N	6.92	129.55	120.28
1	B	633	LEU	C-N-CA	6.92	129.55	120.28
1	A	634	ASN	N-CA-C	6.60	118.47	111.28
1	D	634	ASN	N-CA-C	6.46	118.32	111.28
1	C	634	ASN	N-CA-C	6.41	118.27	111.28
1	B	634	ASN	N-CA-C	6.39	118.25	111.28
1	B	23	VAL	N-CA-C	-5.81	106.81	111.81
1	B	295	GLY	CA-C-N	5.77	128.81	120.38
1	B	295	GLY	C-N-CA	5.77	128.81	120.38
1	B	637	GLY	CA-C-N	5.72	129.40	120.82
1	B	637	GLY	C-N-CA	5.72	129.40	120.82
1	A	637	GLY	CA-C-N	5.58	129.20	120.82
1	A	637	GLY	C-N-CA	5.58	129.20	120.82
1	C	637	GLY	CA-C-N	5.55	129.15	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	637	GLY	C-N-CA	5.55	129.15	120.82
1	B	561	LYS	CA-C-N	5.48	125.18	119.92
1	B	561	LYS	C-N-CA	5.48	125.18	119.92
1	D	637	GLY	CA-C-N	5.46	129.01	120.82
1	D	637	GLY	C-N-CA	5.46	129.01	120.82
1	C	559	ASP	CA-CB-CG	5.41	118.01	112.60
1	D	230	ASP	CA-CB-CG	5.40	118.00	112.60
1	C	709	ILE	CA-C-N	5.34	127.43	120.28
1	C	709	ILE	C-N-CA	5.34	127.43	120.28
1	C	360	ASN	CA-CB-CG	5.24	117.84	112.60
1	D	260	ASN	CA-CB-CG	5.24	117.84	112.60
1	D	607	ILE	CA-C-N	5.23	125.90	119.99
1	D	607	ILE	C-N-CA	5.23	125.90	119.99
1	B	325	PHE	CA-CB-CG	5.22	119.02	113.80
1	B	230	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	360	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	230	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	260	ASN	CA-C-N	5.11	131.07	123.05
1	A	260	ASN	C-N-CA	5.11	131.07	123.05
1	D	332	TYR	CA-C-N	5.10	127.73	120.53
1	D	332	TYR	C-N-CA	5.10	127.73	120.53
1	B	542	GLY	CA-C-N	5.09	130.86	121.70
1	B	542	GLY	C-N-CA	5.09	130.86	121.70
1	C	230	ASP	CA-CB-CG	5.08	117.68	112.60
1	D	65	VAL	CA-C-N	5.05	127.30	120.38
1	D	65	VAL	C-N-CA	5.05	127.30	120.38
1	A	328	LYS	CB-CA-C	-5.03	109.82	117.07
1	C	255	PHE	CA-CB-CG	5.03	118.83	113.80

There are no chirality outliers.

There are no planarity outliers.

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	6824	0	6661	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6772	0	6601	58	0
1	C	6826	0	6666	70	0
1	D	6722	0	6559	50	0
2	E	365	0	401	5	0
2	F	365	0	401	13	0
3	A	401	0	0	2	0
3	B	436	0	0	3	0
3	C	224	0	0	0	0
3	D	224	0	0	2	0
3	E	5	0	0	0	0
3	F	3	0	0	0	0
All	All	29167	0	27289	218	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 4.

All (218) 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:A:640:HIS:HE1	1:B:192:VAL:HG11	1.14	1.12
1:C:408:GLN:HB2	1:C:413:ASN:HB3	1.26	1.10
1:D:15:ASP:HB3	2:F:125:THR:HG21	1.31	1.10
1:C:295:GLY:HA3	1:C:360:ASN:OD1	1.52	1.07
1:A:640:HIS:HE1	1:B:192:VAL:CG1	1.71	1.03
1:A:640:HIS:CE1	1:B:192:VAL:HG11	1.95	0.99
1:D:430:ASP:O	1:D:433:ILE:HG22	1.64	0.95
1:B:48:VAL:HG12	1:B:49:ASN:H	1.29	0.93
1:D:260:ASN:ND2	1:D:392:LYS:HD2	1.86	0.91
1:C:30:GLU:HA	1:D:49:ASN:ND2	1.87	0.88
1:A:640:HIS:CE1	1:B:192:VAL:CG1	2.55	0.86
1:A:38:GLN:HG3	1:B:17:LEU:HD11	1.56	0.85
1:D:15:ASP:CB	2:F:125:THR:HG21	2.07	0.85
1:C:407:HIS:CE1	1:C:410:LYS:HD3	2.16	0.81
1:C:11:ILE:HG22	2:F:133:ARG:NH1	1.96	0.80
1:C:429:SER:O	1:C:433:ILE:HG23	1.81	0.79
1:D:198:PRO:HD3	1:D:228:LEU:HD21	1.65	0.78
1:B:405:ILE:O	1:B:405:ILE:HG22	1.81	0.78
1:C:407:HIS:NE2	1:C:410:LYS:HD3	1.99	0.78
1:A:24:ILE:HA	1:A:28:GLY:HA3	1.67	0.76
1:D:725:LYS:HE2	3:D:944:HOH:O	1.85	0.76
1:A:106:HIS:NE2	1:A:142:HIS:HD2	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:HIS:NE2	1:A:142:HIS:CD2	2.54	0.74
1:A:656:ILE:HG12	1:A:685:VAL:CG1	2.17	0.74
1:A:20:ILE:HD13	1:B:39:LEU:HG	1.70	0.74
1:B:48:VAL:HG12	1:B:49:ASN:N	2.03	0.73
1:B:24:ILE:HA	1:B:28:GLY:HA3	1.69	0.73
1:B:177:TYR:CB	1:B:192:VAL:CG2	2.67	0.71
1:A:106:HIS:CD2	1:A:142:HIS:HD2	2.08	0.71
1:B:177:TYR:HB3	1:B:192:VAL:CG2	2.22	0.70
1:D:15:ASP:HB3	2:F:125:THR:CG2	2.17	0.70
1:D:198:PRO:HB3	1:D:228:LEU:HD11	1.73	0.70
1:C:30:GLU:HA	1:D:49:ASN:HD22	1.56	0.69
1:C:399:ALA:HA	1:C:405:ILE:HG21	1.76	0.68
1:D:260:ASN:HD21	1:D:392:LYS:HD2	1.56	0.68
1:A:106:HIS:CD2	1:A:142:HIS:CD2	2.82	0.67
1:C:56:ILE:HD12	1:C:276:ASN:O	1.95	0.67
1:C:24:ILE:HA	1:C:28:GLY:HA3	1.77	0.67
1:B:177:TYR:CB	1:B:192:VAL:HG21	2.25	0.66
1:A:26:GLU:HG2	2:E:148:LYS:HB2	1.78	0.66
1:C:411:LYS:O	1:C:412:MET:HB2	1.97	0.64
1:D:656:ILE:HG12	1:D:685:VAL:CG2	2.29	0.63
1:C:11:ILE:HG21	2:F:133:ARG:CZ	2.30	0.62
1:C:263:ARG:HH12	1:D:566:GLN:NE2	1.97	0.62
1:D:228:LEU:HD22	1:D:232:GLU:CD	2.24	0.62
1:A:846:SER:HB2	1:A:874:PHE:HB3	1.80	0.62
1:C:408:GLN:HB2	1:C:413:ASN:CB	2.18	0.62
1:C:57:SER:HB3	1:D:49:ASN:O	1.99	0.62
1:A:29:VAL:HG13	1:B:47:GLY:O	1.99	0.61
1:D:656:ILE:HG12	1:D:685:VAL:HG22	1.82	0.61
1:B:405:ILE:O	1:B:405:ILE:CG2	2.48	0.61
1:B:533:ARG:HG2	1:B:556:TYR:HB3	1.81	0.61
1:A:50:VAL:HG22	1:B:56:ILE:HA	1.81	0.61
1:C:399:ALA:O	1:C:405:ILE:HG13	2.01	0.61
1:A:106:HIS:CE1	1:A:142:HIS:HD2	2.18	0.60
1:B:656:ILE:HG12	1:B:685:VAL:HG22	1.83	0.60
1:D:106:HIS:CE1	1:D:142:HIS:CD2	2.90	0.60
1:B:713:ILE:HB	1:B:764:LEU:HD11	1.84	0.60
1:C:414:MET:HB2	1:C:418:ARG:HH21	1.67	0.59
1:C:11:ILE:CG2	2:F:133:ARG:NH1	2.64	0.59
1:C:7:ASP:O	1:C:8:VAL:HB	2.03	0.59
1:B:656:ILE:HG12	1:B:685:VAL:CG2	2.32	0.59
1:C:55:GLY:C	1:C:56:ILE:HG12	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:ILE:HD11	1:C:280:GLY:CA	2.33	0.58
1:A:26:GLU:O	1:A:26:GLU:OE1	2.22	0.58
1:B:846:SER:HB2	1:B:874:PHE:HB3	1.84	0.58
1:B:395:GLY:O	1:B:420:ILE:HG22	2.03	0.58
1:C:30:GLU:HA	1:D:49:ASN:HD21	1.69	0.58
1:C:713:ILE:HB	1:C:764:LEU:HD11	1.86	0.58
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.86	0.57
1:D:846:SER:HB2	1:D:874:PHE:HB3	1.86	0.57
2:F:125:THR:HG23	2:F:126:PRO:HD2	1.86	0.57
1:D:683:GLU:HB3	1:D:685:VAL:HG12	1.87	0.56
1:D:294:TRP:HB3	1:D:298:TRP:CD1	2.41	0.56
1:A:27:GLU:HG2	2:E:148:LYS:HE2	1.86	0.56
1:D:106:HIS:HE1	1:D:177:TYR:HE1	1.52	0.56
1:C:295:GLY:CA	1:C:360:ASN:OD1	2.41	0.56
1:D:713:ILE:HB	1:D:764:LEU:HD11	1.87	0.55
1:A:656:ILE:CG1	1:A:685:VAL:CG1	2.84	0.55
2:F:125:THR:CG2	2:F:126:PRO:HD2	2.35	0.55
1:C:407:HIS:CE1	1:C:410:LYS:NZ	2.75	0.55
1:C:405:ILE:C	1:C:407:HIS:H	2.13	0.54
1:C:430:ASP:O	1:C:433:ILE:HG13	2.08	0.54
1:C:430:ASP:O	1:C:433:ILE:CG1	2.55	0.54
1:C:53:GLY:O	1:C:54:THR:HG22	2.06	0.54
1:C:407:HIS:CE1	1:C:410:LYS:CD	2.89	0.54
1:B:48:VAL:CG1	1:B:49:ASN:H	2.10	0.54
1:C:683:GLU:HB3	1:C:685:VAL:HG22	1.88	0.54
1:B:177:TYR:CG	1:B:192:VAL:HG21	2.42	0.54
1:C:421:ARG:HG2	1:C:426:VAL:HB	1.90	0.54
1:D:421:ARG:HG2	1:D:426:VAL:HB	1.90	0.54
1:D:430:ASP:O	1:D:433:ILE:CG2	2.49	0.54
1:B:90:ILE:HD13	1:B:420:ILE:HD12	1.89	0.53
1:D:738:VAL:HG12	1:D:848:VAL:HG21	1.91	0.53
1:C:846:SER:HB2	1:C:874:PHE:HB3	1.90	0.53
1:C:11:ILE:CG2	2:F:133:ARG:CZ	2.87	0.53
1:B:177:TYR:CG	1:B:192:VAL:CG2	2.91	0.53
1:A:421:ARG:HG2	1:A:426:VAL:HB	1.90	0.53
1:A:616:ASP:OD1	1:B:638:LEU:HD13	2.09	0.53
1:C:406:ALA:C	1:C:408:GLN:H	2.17	0.53
1:B:421:ARG:HG2	1:B:426:VAL:HB	1.90	0.52
1:C:868:ALA:HB2	1:D:780:LEU:HD23	1.90	0.52
2:E:137:VAL:HG11	2:E:156:VAL:HG13	1.91	0.52
1:B:194:MET:HB3	1:B:232:GLU:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD21	1:D:446:GLU:HB3	1.92	0.52
1:C:56:ILE:HD11	1:C:280:GLY:HA3	1.91	0.52
1:C:55:GLY:O	1:C:56:ILE:HD13	2.11	0.51
1:C:521:ASP:HB2	1:C:568:GLY:HA2	1.93	0.51
1:A:31:ARG:NH1	1:A:34:TYR:CE2	2.79	0.51
1:B:77:LEU:HD21	1:B:446:GLU:HB3	1.93	0.51
1:B:177:TYR:HB2	1:B:192:VAL:HG21	1.92	0.50
1:C:77:LEU:HD21	1:C:446:GLU:HB3	1.93	0.50
1:C:727:GLN:HG3	1:C:795:ALA:HB3	1.93	0.50
1:D:194:MET:HB3	1:D:232:GLU:HG3	1.94	0.50
2:F:137:VAL:HG11	2:F:156:VAL:HG13	1.92	0.50
1:C:194:MET:HB3	1:C:232:GLU:HG3	1.92	0.50
1:C:54:THR:HG23	1:C:54:THR:O	2.10	0.49
1:C:56:ILE:CD1	1:C:276:ASN:O	2.60	0.49
1:D:106:HIS:HE1	1:D:177:TYR:CE1	2.30	0.49
1:A:8:VAL:HB	1:B:31:ARG:HH11	1.78	0.49
1:C:8:VAL:HG12	1:C:9:ASP:N	2.28	0.48
1:B:192:VAL:HG23	3:B:903:HOH:O	2.14	0.48
1:B:125:PHE:HB3	1:B:462:LEU:HD13	1.95	0.48
1:C:407:HIS:CE1	1:C:410:LYS:CE	2.96	0.48
1:A:635:GLY:HA3	1:B:103:LEU:O	2.14	0.47
1:C:20:ILE:HD11	1:D:42:GLU:HB3	1.96	0.47
1:A:125:PHE:HB3	1:A:462:LEU:HD13	1.96	0.47
1:D:493:SER:H	1:D:496:ILE:HD12	1.79	0.47
1:A:194:MET:HB3	1:A:232:GLU:HG3	1.96	0.47
1:C:125:PHE:HB3	1:C:462:LEU:HD13	1.96	0.47
1:C:407:HIS:CE1	1:C:410:LYS:HZ2	2.31	0.47
1:A:77:LEU:HD21	1:A:446:GLU:HB3	1.95	0.47
1:A:656:ILE:CG1	1:A:685:VAL:HG11	2.44	0.47
1:D:707:GLU:HA	1:D:710:ARG:HH21	1.80	0.47
1:D:47:GLY:O	1:D:48:VAL:HB	2.15	0.47
1:D:125:PHE:HB3	1:D:462:LEU:HD13	1.96	0.47
1:A:493:SER:H	1:A:496:ILE:HD12	1.80	0.47
2:E:129:ARG:O	2:E:133:ARG:HG2	2.15	0.47
1:B:177:TYR:CD2	1:B:192:VAL:HG21	2.51	0.46
1:C:493:SER:H	1:C:496:ILE:HD12	1.80	0.46
1:A:50:VAL:HA	1:B:56:ILE:N	2.30	0.46
1:D:709:ILE:HG23	1:D:759:THR:HG21	1.96	0.46
1:A:273:LYS:HE3	1:A:317:THR:O	2.15	0.46
1:B:20:ILE:HD11	1:B:36:ILE:HD11	1.98	0.46
1:B:493:SER:H	1:B:496:ILE:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:ILE:HG23	1:C:759:THR:HG21	1.98	0.46
1:A:26:GLU:O	1:A:26:GLU:CD	2.58	0.46
1:D:656:ILE:CG1	1:D:685:VAL:CG2	2.94	0.46
1:A:262:GLN:HA	1:A:267:PRO:HA	1.98	0.46
1:A:20:ILE:HG21	1:B:39:LEU:HD21	1.97	0.45
1:A:361:ARG:HD2	1:A:391:ILE:HG13	1.98	0.45
1:D:405:ILE:C	1:D:407:HIS:H	2.22	0.45
1:D:428:VAL:HG23	1:D:439:ILE:HD11	1.97	0.45
1:B:90:ILE:HG21	1:B:420:ILE:HD11	1.97	0.45
1:A:428:VAL:HG23	1:A:439:ILE:HD11	1.98	0.45
1:A:533:ARG:NH2	1:A:556:TYR:CD1	2.84	0.45
1:C:76:GLU:CD	1:C:80:ARG:HH21	2.24	0.45
1:B:405:ILE:C	1:B:407:HIS:H	2.24	0.45
1:C:262:GLN:HA	1:C:267:PRO:HA	1.99	0.45
1:C:406:ALA:C	1:C:408:GLN:N	2.74	0.45
1:A:42:GLU:C	1:A:44:ARG:H	2.26	0.44
1:B:337:PHE:O	1:B:340:LYS:HB2	2.17	0.44
1:C:138:TYR:HB2	1:C:226:ALA:HA	2.00	0.44
1:D:9:ASP:HB2	2:F:147:ARG:HD2	2.00	0.44
1:A:434:GLU:HG3	3:A:1000:HOH:O	2.17	0.44
1:D:228:LEU:HD13	1:D:233:MET:SD	2.58	0.44
1:A:261:LEU:HD11	3:A:919:HOH:O	2.18	0.44
1:D:90:ILE:HG22	1:D:91:MET:HE2	1.99	0.44
1:A:723:LYS:HD2	1:A:749:TYR:O	2.18	0.43
1:C:430:ASP:O	1:C:433:ILE:HG12	2.17	0.43
1:A:31:ARG:HH12	1:A:34:TYR:HE2	1.67	0.43
1:A:90:ILE:HG22	1:A:91:MET:HE2	2.00	0.43
1:A:14:ARG:HD2	1:A:308:GLY:HA3	2.00	0.43
1:A:138:TYR:HB2	1:A:226:ALA:HA	2.00	0.43
1:B:638:LEU:HD23	1:B:638:LEU:C	2.44	0.43
2:F:160:VAL:O	2:F:164:ILE:HG12	2.19	0.43
1:B:656:ILE:CG1	1:B:685:VAL:CG2	2.95	0.43
1:C:90:ILE:HG22	1:C:91:MET:HE2	2.00	0.43
1:C:405:ILE:C	1:C:407:HIS:N	2.77	0.43
1:B:90:ILE:HD13	1:B:420:ILE:CD1	2.49	0.43
1:C:42:GLU:HA	1:C:45:LYS:HD2	1.99	0.43
1:B:138:TYR:HB2	1:B:226:ALA:HA	2.01	0.43
1:C:741:ALA:HB2	1:C:845:ALA:HA	2.00	0.43
2:E:160:VAL:O	2:E:164:ILE:HG12	2.19	0.43
1:B:90:ILE:HG22	1:B:91:MET:HE2	2.00	0.42
1:D:361:ARG:HD2	1:D:391:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:OE1	1:B:49:ASN:N	2.53	0.42
1:A:638:LEU:C	1:A:638:LEU:HD23	2.44	0.42
1:D:15:ASP:CG	2:F:127:LEU:HD23	2.43	0.42
1:D:300:GLU:HB2	3:D:978:HOH:O	2.19	0.42
1:A:706:GLU:O	1:A:710:ARG:HG3	2.19	0.42
1:C:5:PRO:HA	1:C:6:ASN:HA	1.58	0.42
1:A:31:ARG:NH1	1:A:34:TYR:CD2	2.88	0.42
1:A:684:ASN:C	1:A:685:VAL:HG23	2.45	0.42
1:B:536:GLY:CA	1:B:557:LYS:HB2	2.49	0.42
1:C:361:ARG:HD2	1:C:391:ILE:HG13	2.01	0.42
1:C:738:VAL:HG13	1:C:848:VAL:HG11	2.01	0.41
1:D:138:TYR:HB2	1:D:226:ALA:HA	2.01	0.41
1:A:20:ILE:HG23	1:B:16:TRP:HH2	1.85	0.41
1:C:8:VAL:HG11	1:D:31:ARG:HD3	2.01	0.41
1:B:361:ARG:HD2	1:B:391:ILE:HG13	2.02	0.41
1:B:521:ASP:HA	1:B:566:GLN:OE1	2.21	0.41
1:A:106:HIS:CE1	1:A:142:HIS:CD2	3.01	0.41
1:C:56:ILE:CD1	1:C:280:GLY:CA	2.97	0.41
1:C:294:TRP:HB3	1:C:298:TRP:CD1	2.55	0.41
1:C:827:GLY:CA	1:C:884:ARG:HA	2.51	0.41
1:C:50:VAL:HG21	1:D:33:GLN:OE1	2.21	0.41
1:A:128:ARG:HG3	1:A:133:GLY:HA2	2.02	0.41
1:A:170:HIS:HD2	3:B:985:HOH:O	2.04	0.41
1:B:536:GLY:HA3	1:B:557:LYS:HB2	2.02	0.41
1:B:471:GLU:HG2	3:B:1224:HOH:O	2.21	0.41
1:D:656:ILE:CG1	1:D:685:VAL:HG21	2.51	0.41
1:C:263:ARG:HD2	1:D:521:ASP:OD1	2.21	0.40
1:B:727:GLN:HG3	1:B:795:ALA:HB3	2.03	0.40
1:A:808:ALA:HB3	1:A:822:VAL:HG13	2.04	0.40
1:A:260:ASN:ND2	1:A:392:LYS:HD2	2.36	0.40
1:A:832:ASP:OD2	1:B:169:VAL:HB	2.22	0.40
1:B:808:ALA:HB3	1:B:822:VAL:HG13	2.04	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	854/886 (96%)	814 (95%)	37 (4%)	3 (0%)	30	60
1	B	844/886 (95%)	798 (94%)	40 (5%)	6 (1%)	18	47
1	C	858/886 (97%)	811 (94%)	41 (5%)	6 (1%)	18	47
1	D	839/886 (95%)	798 (95%)	35 (4%)	6 (1%)	18	47
2	E	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
2	F	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
All	All	3483/3636 (96%)	3307 (95%)	155 (4%)	21 (1%)	21	51

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	482	GLY
1	A	522	GLU
1	B	482	GLY
1	C	482	GLY
1	C	522	GLU
1	D	482	GLY
1	B	522	GLU
1	C	8	VAL
1	D	48	VAL
1	D	522	GLU
1	A	521	ASP
1	B	270	GLY
1	B	521	ASP
1	C	521	ASP
1	D	521	ASP
1	B	9	ASP
1	C	27	GLU
1	D	47	GLY
1	B	10	PRO
1	C	406	ALA
1	D	8	VAL

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	716/735 (97%)	702 (98%)	14 (2%)	48	80
1	B	710/735 (97%)	694 (98%)	16 (2%)	44	78
1	C	715/735 (97%)	704 (98%)	11 (2%)	57	84
1	D	704/735 (96%)	695 (99%)	9 (1%)	61	86
2	E	36/36 (100%)	36 (100%)	0	100	100
2	F	36/36 (100%)	36 (100%)	0	100	100
All	All	2917/3012 (97%)	2867 (98%)	50 (2%)	53	83

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	65	VAL
1	A	143	ILE
1	A	228	LEU
1	A	263	ARG
1	A	265	ASP
1	A	304	LYS
1	A	382	LYS
1	A	421	ARG
1	A	433	ILE
1	A	443	GLU
1	A	489	SER
1	A	725	LYS
1	A	819	ASP
1	B	11	ILE
1	B	18	GLN
1	B	143	ILE
1	B	172	ASN
1	B	194	MET
1	B	228	LEU
1	B	326	LYS
1	B	374	LYS

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Mol	Chain	Res	Type
1	B	382	LYS
1	B	421	ARG
1	B	433	ILE
1	B	557	LYS
1	B	725	LYS
1	B	819	ASP
1	B	862	ILE
1	B	875	ASN
1	C	143	ILE
1	C	194	MET
1	C	228	LEU
1	C	260	ASN
1	C	382	LYS
1	C	421	ARG
1	C	443	GLU
1	C	489	SER
1	C	638	LEU
1	C	819	ASP
1	C	862	ILE
1	D	20	ILE
1	D	38	GLN
1	D	143	ILE
1	D	194	MET
1	D	382	LYS
1	D	421	ARG
1	D	638	LEU
1	D	819	ASP
1	D	862	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	38	GLN
1	A	142	HIS
1	A	260	ASN
1	A	262	GLN
1	A	276	ASN
1	A	407	HIS
1	A	408	GLN
1	A	454	GLN
1	A	618	GLN

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Mol	Chain	Res	Type
1	A	639	GLN
1	A	640	HIS
1	A	695	ASN
1	A	737	HIS
1	B	33	GLN
1	B	122	ASN
1	B	213	HIS
1	B	222	GLN
1	B	454	GLN
1	B	588	ASN
1	B	618	GLN
1	B	737	HIS
1	C	262	GLN
1	C	288	ASN
1	C	323	GLN
1	C	448	HIS
1	C	454	GLN
1	C	534	GLN
1	C	541	ASN
1	C	618	GLN
1	C	695	ASN
1	C	810	GLN
1	D	49	ASN
1	D	106	HIS
1	D	142	HIS
1	D	288	ASN
1	D	407	HIS
1	D	419	HIS
1	D	448	HIS
1	D	454	GLN
1	D	534	GLN
1	D	566	GLN
1	D	618	GLN
1	D	695	ASN
1	D	810	GLN

5.3.3 RNA ⓘ

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	862/886 (97%)	-0.27	22 (2%) 57 47	41, 61, 116, 158	0
1	B	854/886 (96%)	-0.31	27 (3%) 50 40	38, 55, 127, 170	0
1	C	864/886 (97%)	0.17	30 (3%) 47 38	51, 88, 144, 186	0
1	D	849/886 (95%)	0.23	29 (3%) 48 39	48, 89, 143, 185	0
2	E	46/46 (100%)	0.75	4 (8%) 16 11	108, 124, 143, 152	0
2	F	46/46 (100%)	1.18	8 (17%) 4 3	119, 142, 155, 167	0
All	All	3521/3636 (96%)	-0.02	120 (3%) 48 39	38, 73, 140, 186	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	407	HIS	5.3
1	C	264	LEU	4.7
1	A	48	VAL	4.6
1	B	406	ALA	4.6
1	D	48	VAL	4.5
2	F	167	ALA	4.3
1	A	50	VAL	4.2
1	D	261	LEU	4.1
1	B	11	ILE	4.1
1	B	269	THR	4.1
1	C	400	ALA	4.0
1	A	400	ALA	4.0
1	B	322	TYR	4.0
1	A	326	LYS	3.9
1	D	406	ALA	3.7
1	B	8	VAL	3.6
1	C	40	LEU	3.6
1	D	40	LEU	3.6
1	B	400	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	49	ASN	3.5
1	C	24	ILE	3.5
1	C	406	ALA	3.4
1	A	264	LEU	3.2
1	D	407	HIS	3.2
1	B	29	VAL	3.2
1	C	8	VAL	3.2
1	B	318	VAL	3.2
1	A	8	VAL	3.1
1	C	269	THR	3.1
1	B	320	GLY	3.0
1	B	268	VAL	3.0
1	B	16	TRP	3.0
1	A	405	ILE	3.0
1	C	392	LYS	3.0
1	D	393	GLY	3.0
1	B	34	TYR	2.9
1	B	555	TYR	2.9
1	D	322	TYR	2.9
1	A	521	ASP	2.9
1	D	326	LYS	2.9
1	C	267	PRO	2.9
1	D	542	GLY	2.9
2	F	122	VAL	2.9
1	C	36	ILE	2.9
1	C	55	GLY	2.8
1	B	324	THR	2.8
1	B	557	LYS	2.8
1	C	53	GLY	2.8
1	D	867	VAL	2.8
1	B	59	TYR	2.8
1	D	853	LEU	2.8
1	D	271	ASN	2.8
1	A	7	ASP	2.7
2	E	126	PRO	2.7
1	A	532	PHE	2.7
1	C	542	GLY	2.7
1	D	405	ILE	2.6
1	A	54	THR	2.6
1	C	268	VAL	2.6
1	B	399	ALA	2.6
1	B	325	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	139	LEU	2.6
1	D	325	PHE	2.6
2	E	164	ILE	2.6
1	C	29	VAL	2.5
1	B	323	GLN	2.5
1	C	54	THR	2.5
1	C	729	LEU	2.5
1	B	405	ILE	2.5
1	C	39	LEU	2.5
1	B	5	PRO	2.5
1	C	20	ILE	2.5
1	D	47	GLY	2.5
1	A	556	TYR	2.5
1	D	400	ALA	2.5
1	D	11	ILE	2.4
1	D	270	GLY	2.4
2	F	135	PHE	2.4
1	A	406	ALA	2.4
1	B	270	GLY	2.4
1	A	14	ARG	2.4
1	B	556	TYR	2.4
1	A	36	ILE	2.4
1	A	5	PRO	2.4
1	D	29	VAL	2.4
2	F	131	LEU	2.4
1	A	399	ALA	2.3
1	A	267	PRO	2.3
1	D	521	ASP	2.3
1	B	407	HIS	2.3
1	C	405	ILE	2.3
1	D	399	ALA	2.3
1	C	433	ILE	2.2
1	C	407	HIS	2.2
1	A	542	GLY	2.2
1	D	32	ALA	2.2
1	C	853	LEU	2.2
1	A	26	GLU	2.2
1	C	50	VAL	2.2
1	C	265	ASP	2.2
1	C	800	SER	2.2
2	F	152	LEU	2.2
1	C	726	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	145	THR	2.1
1	B	271	ASN	2.1
1	A	194	MET	2.1
1	C	270	GLY	2.1
1	D	272	GLY	2.1
1	D	41	ALA	2.1
1	C	525	THR	2.1
1	D	813	THR	2.1
1	B	41	ALA	2.1
1	D	55	GLY	2.0
2	E	135	PHE	2.0
1	D	392	LYS	2.0
2	F	159	TYR	2.0
1	D	796	PRO	2.0
1	B	27	GLU	2.0
1	C	326	LYS	2.0
2	E	137	VAL	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.