WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Oct 9, 2024 – 02:57 pm BST

PDB ID	:	9EXZ
Title	:	Efficient and scalable protein design using a relaxed sequence space
Authors	:	Frank, C.J.; Dietz, H.
Deposited on	:	2024-04-09
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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.
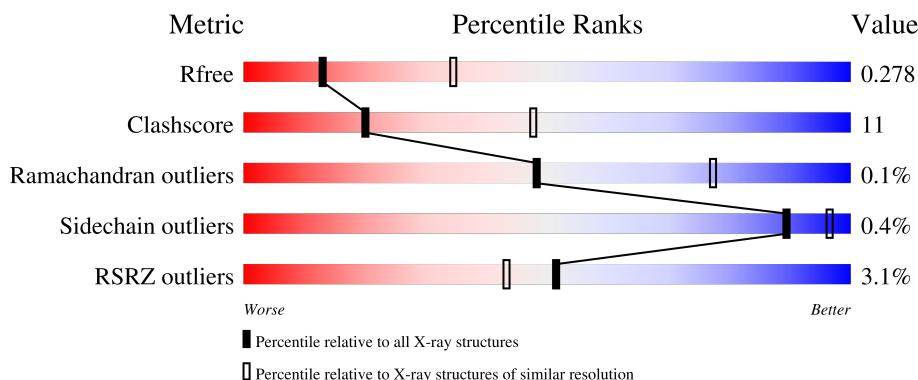
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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 <=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	609	
1	B	609	
1	C	609	
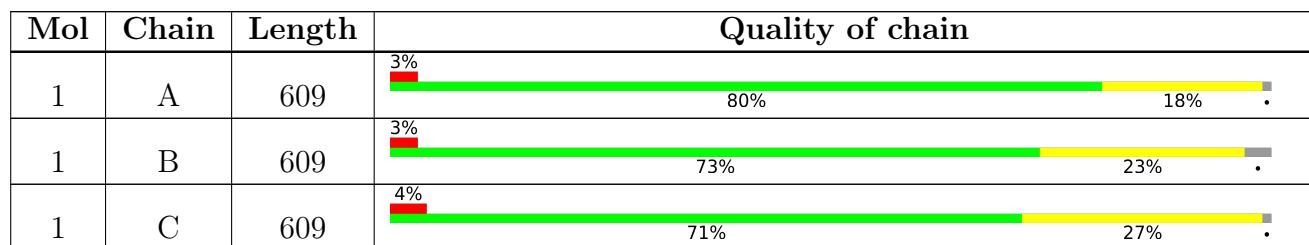
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13929 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 DE NOVO PROTEIN P600.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	602	Total	C	N	O	S	0	0	0
			4680	2983	841	846	10			
1	B	589	Total	C	N	O	S	0	0	0
			4586	2922	828	826	10			
1	C	600	Total	C	N	O	S	0	0	0
			4663	2972	839	842	10			

3 Residue-property plots ⓘ

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: DE NOVO PROTEIN P600

- Molecule 1: DE NOVO PROTEIN P600

• Molecule 1: DE NOVO PROTEIN P600

Chain C:

4%

71%　　　　　　　　　　　　　27%
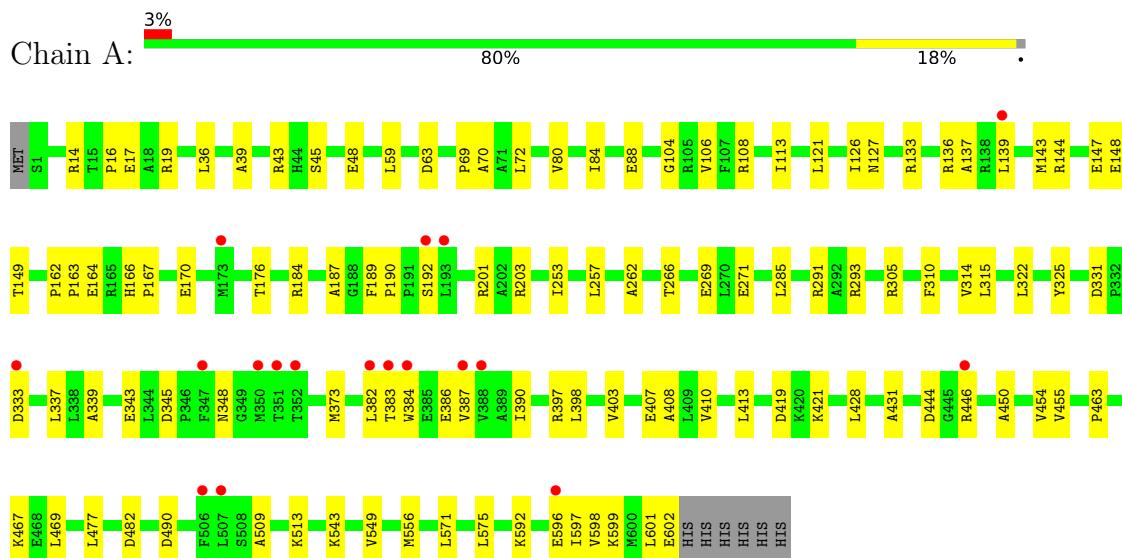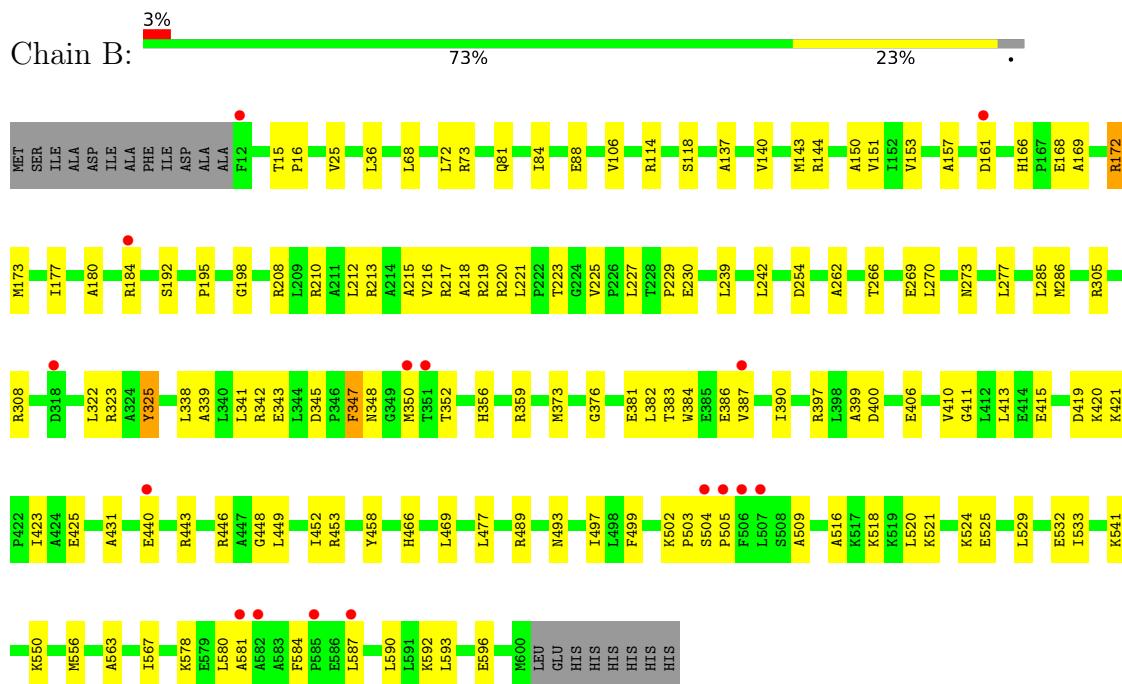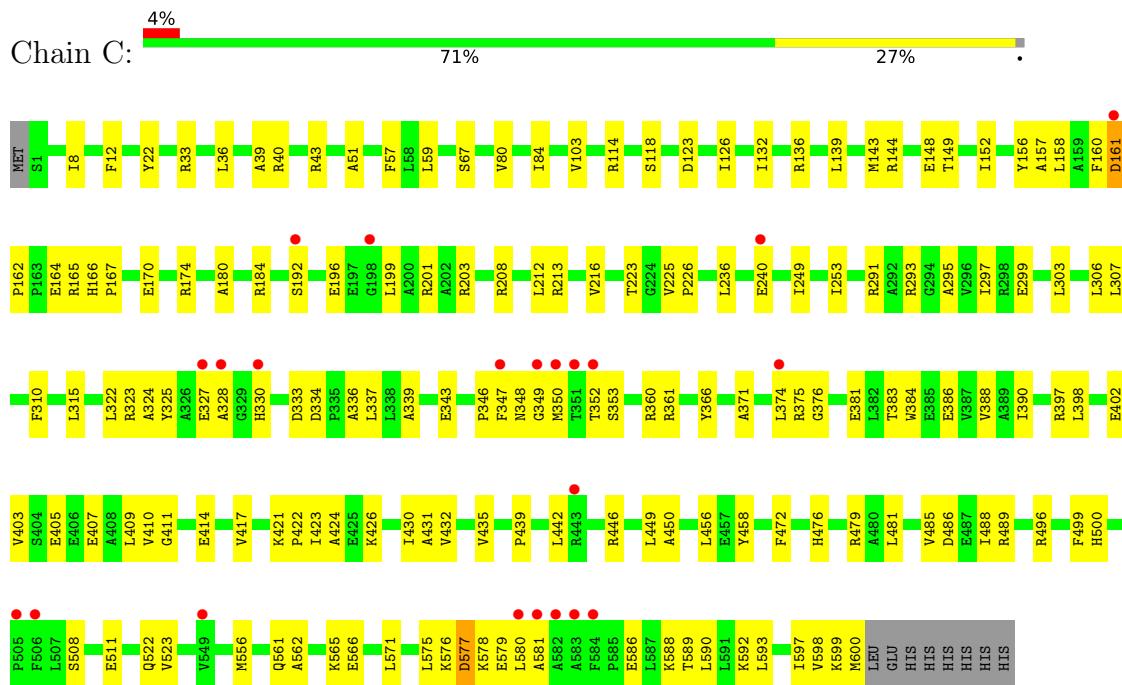
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	163.25Å 67.83Å 173.69Å 90.00° 103.20° 90.00°	Depositor
Resolution (Å)	42.28 – 2.80 42.28 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.28-2.80) 99.6 (42.28-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.1_3865	Depositor
R, R_{free}	0.237 , 0.279 0.237 , 0.278	Depositor DCC
R_{free} test set	2284 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 67.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13929	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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	0.62	0/4749	0.72	0/6428
1	B	0.61	0/4654	0.70	0/6298
1	C	0.61	0/4732	0.71	0/6405
All	All	0.62	0/14135	0.71	0/19131

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ARG	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	4680	0	4896	78	0
1	B	4586	0	4801	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4663	0	4879	135	0
All	All	13929	0	14576	319	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 11.

All (319) 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:578:LYS:HE3	1:C:580:LEU:HB3	1.54	0.87
1:A:419:ASP:HB2	1:A:421:LYS:HG3	1.62	0.82
1:C:333:ASP:OD1	1:C:371:ALA:HB1	1.81	0.80
1:B:516:ALA:O	1:B:520:LEU:HD12	1.81	0.80
1:A:269:GLU:HG2	1:A:285:LEU:HD21	1.64	0.80
1:A:382:LEU:HD22	1:A:386:GLU:OE1	1.83	0.79
1:C:347:PHE:HA	1:C:350:MET:HG3	1.62	0.79
1:A:382:LEU:CD2	1:A:386:GLU:OE1	2.31	0.78
1:C:578:LYS:HG3	1:C:581:ALA:H	1.47	0.78
1:B:308:ARG:HG2	1:B:359:ARG:HH22	1.50	0.75
1:C:174:ARG:HH22	1:C:196:GLU:HG2	1.52	0.75
1:C:499:PHE:HZ	1:C:580:LEU:HG	1.50	0.75
1:C:157:ALA:O	1:C:161:ASP:HB3	1.87	0.75
1:A:386:GLU:O	1:A:390:ILE:HD12	1.87	0.74
1:A:339:ALA:O	1:A:343:GLU:HG2	1.88	0.74
1:B:524:LYS:HG3	1:B:590:LEU:HD21	1.69	0.73
1:C:208:ARG:HG3	1:C:343:GLU:CG	2.19	0.73
1:B:208:ARG:HD3	1:B:343:GLU:HB3	1.70	0.73
1:C:449:LEU:HD21	1:C:481:LEU:HD23	1.69	0.73
1:B:504:SER:HB2	1:B:505:PRO:HD2	1.72	0.71
1:A:598:VAL:O	1:A:602:GLU:HG3	1.90	0.71
1:A:144:ARG:O	1:A:148:GLU:HG3	1.90	0.71
1:B:322:LEU:HD11	1:B:341:LEU:HD11	1.72	0.71
1:A:170:GLU:OE2	1:A:203:ARG:NH2	2.22	0.71
1:B:592:LYS:O	1:B:596:GLU:HG3	1.91	0.70
1:A:463:PRO:CD	1:A:543:LYS:HD3	2.20	0.70
1:C:575:LEU:HD21	1:C:588:LYS:HG2	1.73	0.69
1:A:428:LEU:HD21	1:A:454:VAL:HG12	1.75	0.68
1:B:269:GLU:HG2	1:B:285:LEU:HD21	1.75	0.68
1:C:208:ARG:HG3	1:C:343:GLU:HG3	1.76	0.68
1:A:184:ARG:HG2	1:A:189:PHE:HB2	1.74	0.68
1:A:322:LEU:HA	1:A:337:LEU:HD21	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:LEU:O	1:C:203:ARG:HG3	1.95	0.67
1:B:36:LEU:CD2	1:B:489:ARG:HE	2.08	0.66
1:B:440:GLU:HB2	1:B:443:ARG:HD3	1.77	0.66
1:B:114:ARG:O	1:B:118:SER:HB2	1.96	0.66
1:C:201:ARG:NH2	1:C:349:GLY:HA3	2.11	0.66
1:C:421:LYS:HB2	1:C:423:ILE:HG12	1.78	0.65
1:B:305:ARG:HA	1:B:308:ARG:CZ	2.26	0.65
1:A:571:LEU:O	1:A:575:LEU:HD23	1.97	0.65
1:B:383:THR:OG1	1:B:386:GLU:HG3	1.96	0.65
1:C:499:PHE:CZ	1:C:580:LEU:HG	2.32	0.64
1:C:496:ARG:O	1:C:500:HIS:HD2	1.80	0.64
1:B:446:ARG:NH1	1:B:525:GLU:OE2	2.31	0.64
1:C:561:GLN:HG2	1:C:565:LYS:HE3	1.80	0.64
1:C:575:LEU:HD11	1:C:588:LYS:HA	1.80	0.64
1:B:524:LYS:CG	1:B:590:LEU:HD21	2.28	0.63
1:B:504:SER:HB2	1:B:505:PRO:CD	2.28	0.63
1:C:439:PRO:HB2	1:C:479:ARG:HH12	1.63	0.63
1:B:157:ALA:O	1:B:161:ASP:CG	2.36	0.63
1:B:347:PHE:HA	1:B:350:MET:SD	2.39	0.63
1:C:22:TYR:OH	1:C:67:SER:HB3	1.99	0.62
1:C:346:PRO:HG2	1:C:347:PHE:CE2	2.35	0.62
1:B:323:ARG:HG3	1:B:384:TRP:HZ3	1.65	0.61
1:B:382:LEU:HD11	1:B:421:LYS:HG3	1.81	0.61
1:B:143:MET:HG3	1:B:184:ARG:HD3	1.82	0.61
1:C:132:ILE:O	1:C:136:ARG:HG2	2.01	0.61
1:B:308:ARG:HG2	1:B:359:ARG:NH2	2.16	0.61
1:B:584:PHE:O	1:B:587:LEU:HG	1.99	0.61
1:A:383:THR:OG1	1:A:386:GLU:HG3	2.01	0.60
1:B:269:GLU:HG2	1:B:285:LEU:CD2	2.32	0.60
1:C:315:LEU:HD12	1:C:398:LEU:HD11	1.83	0.60
1:A:382:LEU:HD23	1:A:386:GLU:OE1	2.01	0.60
1:C:114:ARG:O	1:C:118:SER:HB2	2.02	0.59
1:C:410:VAL:O	1:C:414:GLU:HG3	2.03	0.59
1:B:503:PRO:HG2	1:B:509:ALA:HB2	1.85	0.58
1:C:386:GLU:O	1:C:390:ILE:HD13	2.04	0.58
1:A:108:ARG:HD2	1:C:51:ALA:CB	2.33	0.58
1:A:162:PRO:HB2	1:A:164:GLU:OE2	2.02	0.58
1:C:208:ARG:HG3	1:C:343:GLU:HG2	1.84	0.58
1:A:106:VAL:CG2	1:A:137:ALA:HB2	2.34	0.58
1:C:325:TYR:O	1:C:330:HIS:N	2.36	0.58
1:B:144:ARG:HG2	1:B:352:THR:HB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:576:LYS:O	1:C:579:GLU:N	2.38	0.57
1:A:69:PRO:HD2	1:A:72:LEU:HD12	1.87	0.57
1:B:466:HIS:HB3	1:B:469:LEU:HD12	1.85	0.57
1:A:184:ARG:HD2	1:A:190:PRO:O	2.04	0.57
1:C:366:TYR:HB2	1:C:409:LEU:HD11	1.87	0.57
1:A:322:LEU:HD23	1:A:337:LEU:CD2	2.35	0.57
1:C:201:ARG:CZ	1:C:349:GLY:HA3	2.34	0.57
1:A:143:MET:O	1:A:147:GLU:HG3	2.05	0.57
1:B:322:LEU:CD1	1:B:341:LEU:HD11	2.33	0.57
1:B:563:ALA:O	1:B:567:ILE:HG13	2.05	0.57
1:C:144:ARG:HD3	1:C:352:THR:HB	1.87	0.57
1:C:442:LEU:HD11	1:C:476:HIS:HD2	1.69	0.56
1:C:589:THR:O	1:C:592:LYS:HG2	2.06	0.56
1:A:467:LYS:HE3	1:A:549:VAL:HG23	1.86	0.56
1:C:439:PRO:HB2	1:C:479:ARG:NH1	2.20	0.56
1:B:161:ASP:OD1	1:B:166:HIS:NE2	2.38	0.56
1:B:305:ARG:HA	1:B:308:ARG:NH2	2.19	0.56
1:B:381:GLU:CD	1:B:423:ILE:HG23	2.25	0.56
1:C:161:ASP:OD2	1:C:165:ARG:HB2	2.06	0.56
1:B:213:ARG:HH21	1:B:217:ARG:HH12	1.54	0.55
1:B:419:ASP:HB3	1:B:421:LYS:HE3	1.88	0.55
1:C:249:ILE:HD13	1:C:307:LEU:HD23	1.88	0.55
1:C:402:GLU:CD	1:C:522:GLN:HE22	2.10	0.55
1:C:576:LYS:O	1:C:577:ASP:C	2.44	0.55
1:B:184:ARG:HH22	1:B:192:SER:HB3	1.71	0.55
1:A:36:LEU:HD11	1:A:490:ASP:OD1	2.06	0.55
1:C:421:LYS:HB3	1:C:422:PRO:HD2	1.88	0.55
1:B:230:GLU:CD	1:B:230:GLU:H	2.10	0.55
1:C:499:PHE:CD2	1:C:581:ALA:HA	2.42	0.55
1:A:419:ASP:HB2	1:A:421:LYS:CG	2.36	0.54
1:B:413:LEU:HD11	1:B:431:ALA:CB	2.37	0.54
1:A:14:ARG:HH21	1:A:291:ARG:HH11	1.56	0.54
1:B:419:ASP:O	1:B:420:LYS:HB2	2.07	0.54
1:C:426:LYS:O	1:C:430:ILE:HG12	2.06	0.54
1:A:322:LEU:HD23	1:A:337:LEU:HD21	1.90	0.53
1:B:520:LEU:HD21	1:B:587:LEU:HD23	1.90	0.53
1:A:455:VAL:HG13	1:A:469:LEU:HB3	1.90	0.53
1:B:347:PHE:CD1	1:B:356:HIS:CD2	2.97	0.53
1:C:59:LEU:HD23	1:C:103:VAL:HG13	1.90	0.53
1:B:68:LEU:HD22	1:B:72:LEU:HD23	1.91	0.53
1:B:218:ALA:HB3	1:B:220:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ALA:HA	1:B:587:LEU:HD12	1.91	0.52
1:A:70:ALA:N	1:A:127:ASN:HD21	2.07	0.52
1:C:162:PRO:HB2	1:C:164:GLU:OE1	2.09	0.52
1:A:310:PHE:O	1:A:314:VAL:HG23	2.10	0.52
1:B:382:LEU:HG	1:B:386:GLU:OE1	2.09	0.52
1:A:147:GLU:OE1	1:A:192:SER:OG	2.26	0.52
1:B:397:ARG:NH2	1:B:411:GLY:HA3	2.25	0.52
1:C:322:LEU:HD23	1:C:337:LEU:HD21	1.92	0.52
1:C:405:GLU:O	1:C:409:LEU:HD23	2.09	0.52
1:C:410:VAL:HG11	1:C:450:ALA:HB3	1.91	0.52
1:A:509:ALA:O	1:A:513:LYS:HD3	2.10	0.51
1:A:121:LEU:HB2	1:A:126:ILE:HD11	1.93	0.51
1:C:325:TYR:CE1	1:C:337:LEU:HD13	2.44	0.51
1:C:12:PHE:HA	1:C:291:ARG:HH12	1.75	0.51
1:C:123:ASP:HA	1:C:126:ILE:HD12	1.93	0.51
1:A:201:ARG:NH2	1:A:345:ASP:O	2.42	0.51
1:B:221:LEU:CD2	1:B:227:LEU:HD11	2.40	0.51
1:C:442:LEU:HD11	1:C:476:HIS:CD2	2.45	0.51
1:C:592:LYS:HG2	1:C:593:LEU:N	2.25	0.51
1:B:150:ALA:O	1:B:153:VAL:HG12	2.11	0.51
1:B:273:ASN:HB3	1:B:277:LEU:HD21	1.93	0.51
1:B:503:PRO:CG	1:B:509:ALA:HB2	2.40	0.50
1:B:502:LYS:HD2	1:B:502:LYS:N	2.25	0.50
1:C:431:ALA:O	1:C:435:VAL:HG23	2.11	0.50
1:C:561:GLN:HG3	1:C:598:VAL:HG13	1.94	0.50
1:A:113:ILE:HD11	1:A:133:ARG:CZ	2.41	0.50
1:C:348:ASN:C	1:C:350:MET:H	2.15	0.50
1:C:575:LEU:O	1:C:575:LEU:HD23	2.12	0.50
1:B:223:THR:HG1	1:B:325:TYR:HE1	1.57	0.50
1:A:463:PRO:HD3	1:A:543:LYS:HD3	1.92	0.50
1:C:346:PRO:HG2	1:C:347:PHE:CZ	2.47	0.50
1:B:520:LEU:HD21	1:B:587:LEU:CD2	2.41	0.49
1:C:148:GLU:OE2	1:C:352:THR:OG1	2.25	0.49
1:B:270:LEU:HD21	1:B:286:MET:HG2	1.94	0.49
1:A:397:ARG:HH11	1:A:408:ALA:HA	1.76	0.49
1:B:173:MET:HE1	1:B:198:GLY:O	2.11	0.49
1:C:36:LEU:HD11	1:C:486:ASP:CG	2.33	0.49
1:A:14:ARG:NH2	1:A:291:ARG:HH11	2.11	0.49
1:C:226:PRO:HD2	1:C:330:HIS:CE1	2.47	0.49
1:B:413:LEU:HD11	1:B:431:ALA:HB2	1.94	0.49
1:B:143:MET:HG3	1:B:184:ARG:CD	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG21	1:B:325:TYR:CE1	2.48	0.49
1:B:381:GLU:C	1:B:382:LEU:HD12	2.33	0.49
1:C:240:GLU:OE2	1:C:240:GLU:HA	2.12	0.49
1:A:139:LEU:O	1:A:143:MET:HG2	2.13	0.48
1:A:201:ARG:HH21	1:A:348:ASN:HB3	1.78	0.48
1:B:411:GLY:O	1:B:415:GLU:HG2	2.13	0.48
1:C:456:LEU:HD11	1:C:556:MET:HE3	1.95	0.48
1:C:421:LYS:HB3	1:C:422:PRO:CD	2.43	0.48
1:B:347:PHE:CD1	1:B:356:HIS:HD2	2.32	0.48
1:A:428:LEU:HD21	1:A:454:VAL:CG1	2.43	0.48
1:A:592:LYS:O	1:A:596:GLU:HG3	2.13	0.48
1:C:481:LEU:O	1:C:485:VAL:HG23	2.14	0.48
1:B:503:PRO:HB3	1:B:509:ALA:N	2.29	0.48
1:C:381:GLU:OE2	1:C:422:PRO:HD2	2.14	0.48
1:B:383:THR:HG1	1:B:386:GLU:HG3	1.79	0.48
1:A:184:ARG:NH2	1:A:192:SER:OG	2.47	0.47
1:B:593:LEU:HA	1:B:596:GLU:OE2	2.14	0.47
1:A:63:ASP:OD2	1:A:293:ARG:NH2	2.47	0.47
1:A:262:ALA:O	1:A:266:THR:HG23	2.13	0.47
1:A:382:LEU:HD21	1:A:421:LYS:HE3	1.97	0.47
1:B:338:LEU:O	1:B:342:ARG:HG3	2.14	0.47
1:B:493:ASN:O	1:B:497:ILE:HG13	2.14	0.47
1:A:315:LEU:HD12	1:A:398:LEU:HD13	1.96	0.47
1:C:39:ALA:O	1:C:43:ARG:HG3	2.14	0.47
1:C:8:ILE:HG23	1:C:12:PHE:CD2	2.49	0.47
1:C:322:LEU:HA	1:C:337:LEU:HD21	1.95	0.47
1:B:73:ARG:O	1:B:81:GLN:NE2	2.47	0.47
1:C:158:LEU:O	1:C:166:HIS:CE1	2.68	0.47
1:C:323:ARG:O	1:C:324:ALA:C	2.53	0.47
1:C:384:TRP:O	1:C:388:VAL:HG23	2.15	0.47
1:B:215:ALA:HA	1:B:220:ARG:HE	1.80	0.47
1:B:448:GLY:O	1:B:452:ILE:HG12	2.14	0.47
1:C:33:ARG:HD3	1:C:57:PHE:HE1	1.80	0.47
1:A:597:ILE:O	1:A:601:LEU:HG	2.15	0.46
1:B:140:VAL:HG13	1:B:184:ARG:NH1	2.31	0.46
1:B:520:LEU:CD2	1:B:587:LEU:HD23	2.44	0.46
1:C:417:VAL:HG13	1:C:458:TYR:HD2	1.80	0.46
1:A:43:ARG:HD2	1:A:482:ASP:OD2	2.15	0.46
1:C:508:SER:HB3	1:C:511:GLU:HG3	1.98	0.46
1:A:407:GLU:OE2	1:A:446:ARG:NH1	2.48	0.46
1:C:423:ILE:HG13	1:C:424:ALA:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HH22	1:B:192:SER:CB	2.28	0.46
1:A:413:LEU:HD11	1:A:431:ALA:CB	2.46	0.46
1:B:212:LEU:O	1:B:216:VAL:HG23	2.16	0.46
1:C:226:PRO:HD2	1:C:330:HIS:HE1	1.80	0.46
1:C:407:GLU:OE2	1:C:446:ARG:NH1	2.48	0.46
1:A:84:ILE:O	1:A:88:GLU:HG3	2.16	0.45
1:A:397:ARG:HG2	1:A:403:VAL:HG11	1.98	0.45
1:B:390:ILE:HG23	1:B:415:GLU:HG3	1.98	0.45
1:C:336:ALA:O	1:C:339:ALA:HB3	2.15	0.45
1:B:213:ARG:HH21	1:B:217:ARG:NH1	2.14	0.45
1:B:239:LEU:O	1:B:242:LEU:HB2	2.17	0.45
1:B:180:ALA:O	1:B:184:ARG:HG2	2.16	0.45
1:B:399:ALA:O	1:B:400:ASP:C	2.54	0.45
1:B:518:LYS:O	1:B:521:LYS:HB3	2.16	0.45
1:B:221:LEU:HD23	1:B:227:LEU:HD11	1.98	0.45
1:C:485:VAL:O	1:C:489:ARG:HG3	2.16	0.45
1:C:562:ALA:O	1:C:566:GLU:HG3	2.17	0.45
1:A:45:SER:OG	1:A:48:GLU:HG3	2.17	0.45
1:B:177:ILE:HD12	1:B:195:PRO:HA	1.99	0.45
1:C:323:ARG:HG2	1:C:327:GLU:HB2	1.98	0.45
1:B:345:ASP:HB3	1:B:348:ASN:HB2	1.99	0.44
1:B:373:MET:HG2	1:B:387:VAL:HG22	1.99	0.44
1:B:499:PHE:CE2	1:B:580:LEU:HA	2.52	0.44
1:B:529:LEU:O	1:B:533:ILE:HG13	2.17	0.44
1:C:236:LEU:O	1:C:240:GLU:HG2	2.17	0.44
1:A:80:VAL:O	1:A:84:ILE:HG13	2.16	0.44
1:A:373:MET:HG2	1:A:387:VAL:HG22	2.00	0.44
1:C:303:LEU:O	1:C:307:LEU:HG	2.17	0.44
1:B:449:LEU:O	1:B:533:ILE:HD11	2.17	0.44
1:C:184:ARG:CZ	1:C:192:SER:HB3	2.48	0.44
1:C:397:ARG:HG2	1:C:403:VAL:HG11	2.00	0.44
1:A:106:VAL:HG21	1:A:137:ALA:HB2	1.98	0.44
1:B:168:GLU:HG2	1:B:169:ALA:N	2.30	0.44
1:C:383:THR:HG23	1:C:386:GLU:CD	2.38	0.44
1:B:172:ARG:NH2	1:B:254:ASP:OD2	2.51	0.44
1:B:347:PHE:O	1:B:350:MET:HB2	2.17	0.44
1:A:108:ARG:HD2	1:C:51:ALA:HB3	2.00	0.44
1:C:166:HIS:N	1:C:167:PRO:CD	2.81	0.44
1:A:133:ARG:NH1	1:A:271:GLU:OE2	2.49	0.44
1:C:223:THR:HG21	1:C:325:TYR:OH	2.18	0.44
1:C:360:ARG:HE	1:C:361:ARG:HH22	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:ALA:HA	1:B:342:ARG:CZ	2.48	0.44
1:C:589:THR:HA	1:C:592:LYS:HD3	1.99	0.43
1:A:599:LYS:C	1:A:601:LEU:N	2.71	0.43
1:C:12:PHE:HA	1:C:291:ARG:NH1	2.32	0.43
1:C:586:GLU:O	1:C:590:LEU:HG	2.18	0.43
1:A:59:LEU:HD23	1:A:59:LEU:HA	1.87	0.43
1:B:262:ALA:O	1:B:266:THR:HG23	2.19	0.43
1:C:152:ILE:HD11	1:C:346:PRO:O	2.18	0.43
1:C:180:ALA:O	1:C:184:ARG:HG3	2.19	0.43
1:C:417:VAL:CG1	1:C:458:TYR:HD2	2.32	0.43
1:B:15:THR:HB	1:B:16:PRO:HD2	2.01	0.43
1:A:410:VAL:HG11	1:A:450:ALA:HB3	2.01	0.43
1:B:453:ARG:HD3	1:B:532:GLU:OE1	2.18	0.43
1:C:347:PHE:HA	1:C:350:MET:CG	2.41	0.43
1:A:104:GLY:O	1:A:108:ARG:HG3	2.19	0.43
1:A:556:MET:HB3	1:A:556:MET:HE2	1.85	0.43
1:B:151:VAL:HG22	1:B:173:MET:CE	2.49	0.43
1:B:406:GLU:O	1:B:410:VAL:HG23	2.18	0.43
1:C:293:ARG:O	1:C:297:ILE:HG13	2.19	0.43
1:C:333:ASP:O	1:C:334:ASP:C	2.57	0.43
1:C:374:LEU:C	1:C:376:GLY:N	2.70	0.43
1:A:384:TRP:CZ3	1:A:387:VAL:HG11	2.53	0.42
1:C:149:THR:CG2	1:C:253:ILE:HD11	2.49	0.42
1:C:374:LEU:O	1:C:375:ARG:C	2.57	0.42
1:A:149:THR:CG2	1:A:253:ILE:HD11	2.49	0.42
1:A:331:ASP:HB3	1:A:333:ASP:OD1	2.19	0.42
1:C:225:VAL:HG22	1:C:330:HIS:CD2	2.54	0.42
1:C:160:PHE:CE1	1:C:213:ARG:HD3	2.54	0.42
1:A:39:ALA:O	1:A:43:ARG:HG3	2.18	0.42
1:C:33:ARG:HD3	1:C:57:PHE:CE1	2.55	0.42
1:A:477:LEU:HD23	1:A:556:MET:HG2	2.01	0.42
1:B:541:LYS:HG3	1:B:550:LYS:HA	2.02	0.42
1:C:432:VAL:HG13	1:C:472:PHE:CD2	2.54	0.42
1:A:108:ARG:HD2	1:C:51:ALA:HB1	2.02	0.42
1:B:477:LEU:HD22	1:B:556:MET:HE2	2.01	0.42
1:C:295:ALA:O	1:C:299:GLU:HG2	2.19	0.42
1:C:347:PHE:O	1:C:360:ARG:HD2	2.20	0.42
1:A:16:PRO:HD2	1:A:17:GLU:OE1	2.20	0.42
1:B:223:THR:OG1	1:B:225:VAL:HG23	2.20	0.42
1:C:496:ARG:O	1:C:499:PHE:HB3	2.20	0.42
1:C:571:LEU:O	1:C:575:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:161:ASP:CG	1:C:162:PRO:HD2	2.40	0.42
1:C:166:HIS:O	1:C:170:GLU:HG3	2.20	0.42
1:B:376:GLY:HA3	1:B:423:ILE:HG21	2.01	0.41
1:C:139:LEU:O	1:C:143:MET:HG2	2.20	0.41
1:C:383:THR:O	1:C:386:GLU:HB2	2.19	0.41
1:B:210:ARG:HE	1:B:210:ARG:HB2	1.61	0.41
1:C:322:LEU:HD23	1:C:337:LEU:CD2	2.49	0.41
1:A:444:ASP:OD1	1:A:446:ARG:HG3	2.21	0.41
1:A:162:PRO:HA	1:A:163:PRO:HD3	1.98	0.41
1:A:176:THR:HG23	1:A:257:LEU:HD11	2.02	0.41
1:B:443:ARG:HB2	1:B:443:ARG:CZ	2.50	0.41
1:C:80:VAL:O	1:C:84:ILE:HG13	2.21	0.41
1:C:397:ARG:NH2	1:C:411:GLY:HA3	2.35	0.41
1:B:161:ASP:OD1	1:B:161:ASP:O	2.38	0.41
1:C:599:LYS:O	1:C:600:MET:O	2.38	0.41
1:B:219:ARG:HD2	1:B:229:PRO:HG3	2.02	0.41
1:C:148:GLU:OE1	1:C:353:SER:HB3	2.20	0.41
1:C:488:ILE:HG23	1:C:523:VAL:HG13	2.02	0.41
1:A:166:HIS:N	1:A:167:PRO:CD	2.84	0.41
1:B:25:VAL:HG13	1:B:497:ILE:HG21	2.02	0.41
1:B:84:ILE:O	1:B:88:GLU:HG3	2.21	0.41
1:C:36:LEU:O	1:C:40:ARG:HG3	2.21	0.41
1:C:39:ALA:HB2	1:C:489:ARG:NH2	2.35	0.41
1:C:156:TYR:CE1	1:C:310:PHE:HZ	2.39	0.41
1:C:225:VAL:HG22	1:C:330:HIS:CG	2.56	0.41
1:C:324:ALA:O	1:C:328:ALA:N	2.51	0.41
1:C:381:GLU:OE2	1:C:423:ILE:HG23	2.21	0.41
1:C:556:MET:HB3	1:C:556:MET:HE2	1.88	0.41
1:C:575:LEU:HD11	1:C:588:LYS:CA	2.47	0.41
1:C:578:LYS:O	1:C:579:GLU:HB3	2.21	0.41
1:B:578:LYS:HA	1:B:581:ALA:HB3	2.02	0.40
1:C:306:LEU:HD23	1:C:306:LEU:HA	1.96	0.40
1:C:593:LEU:O	1:C:597:ILE:HG13	2.21	0.40
1:A:70:ALA:N	1:A:127:ASN:ND2	2.69	0.40
1:B:425:GLU:HG3	1:B:458:TYR:OH	2.19	0.40
1:A:136:ARG:HB3	1:A:187:ALA:HB1	2.03	0.40
1:B:342:ARG:O	1:B:345:ASP:CB	2.70	0.40
1:B:106:VAL:HG21	1:B:137:ALA:HB2	2.03	0.40
1:B:157:ALA:O	1:B:161:ASP:OD1	2.39	0.40
1:C:149:THR:HG22	1:C:253:ILE:HD11	2.03	0.40
1:C:212:LEU:O	1:C:216:VAL:HG23	2.22	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	600/609 (98%)	588 (98%)	12 (2%)	0	100	100
1	B	587/609 (96%)	566 (96%)	21 (4%)	0	100	100
1	C	598/609 (98%)	579 (97%)	18 (3%)	1 (0%)	44	73
All	All	1785/1827 (98%)	1733 (97%)	51 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	577	ASP

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	463/470 (98%)	461 (100%)	2 (0%)	89	96
1	B	454/470 (97%)	451 (99%)	3 (1%)	81	94
1	C	461/470 (98%)	460 (100%)	1 (0%)	92	97
All	All	1378/1410 (98%)	1372 (100%)	6 (0%)	89	96

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	325	TYR
1	B	172	ARG
1	B	325	TYR
1	B	347	PHE
1	C	161	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	B	356	HIS
1	B	512	GLN
1	C	356	HIS
1	C	500	HIS
1	C	522	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	602/609 (98%)	0.12	18 (2%)	52	44	26, 59, 99, 142	0
1	B	589/609 (96%)	0.26	16 (2%)	56	47	28, 69, 110, 147	0
1	C	600/609 (98%)	0.24	22 (3%)	45	37	26, 66, 108, 145	0
All	All	1791/1827 (98%)	0.21	56 (3%)	51	43	26, 65, 107, 147	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	5.1
1	C	583	ALA	4.8
1	A	384	TRP	4.6
1	C	584	PHE	4.1
1	A	192	SER	4.0
1	C	330	HIS	3.8
1	C	582	ALA	3.4
1	C	240	GLU	3.3
1	C	506	PHE	3.3
1	C	549	VAL	3.2
1	B	318	ASP	3.2
1	C	161	ASP	3.1
1	C	350	MET	3.1
1	C	374	LEU	3.1
1	B	507	LEU	2.9
1	B	585	PRO	2.8
1	B	504	SER	2.8
1	A	350	MET	2.8
1	C	352	THR	2.7
1	C	327	GLU	2.6
1	B	350	MET	2.6
1	C	443	ARG	2.6
1	A	193	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	506	PHE	2.5
1	A	139	LEU	2.5
1	C	505	PRO	2.5
1	B	184	ARG	2.4
1	B	440	GLU	2.4
1	B	12	PHE	2.4
1	C	347	PHE	2.4
1	A	352	THR	2.4
1	C	580	LEU	2.4
1	B	581	ALA	2.4
1	A	446	ARG	2.4
1	A	347	PHE	2.3
1	C	328	ALA	2.3
1	C	581	ALA	2.3
1	B	351	THR	2.3
1	A	388	VAL	2.3
1	A	507	LEU	2.2
1	A	333	ASP	2.2
1	B	505	PRO	2.2
1	B	587	LEU	2.2
1	B	582	ALA	2.2
1	C	198	GLY	2.1
1	A	506	PHE	2.1
1	A	173	MET	2.1
1	A	351	THR	2.1
1	C	351	THR	2.1
1	A	382	LEU	2.1
1	A	387	VAL	2.1
1	B	387	VAL	2.1
1	C	192	SER	2.1
1	A	383	THR	2.0
1	A	596	GLU	2.0
1	C	349	GLY	2.0

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

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

6.3   Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.