



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:17 PM UTC

PDB ID : 5GIV / pdb_00005giv
Title : Crystal structure of M32 carboxypeptidase from *Deinococcus radiodurans* R1
Authors : Sharma, B.; Singh, R.; Yadav, P.; Ghosh, B.; Kumar, A.; Jamdar, S.N.;
Makde, R.D.
Deposited on : 2016-06-25
Resolution : 2.40 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

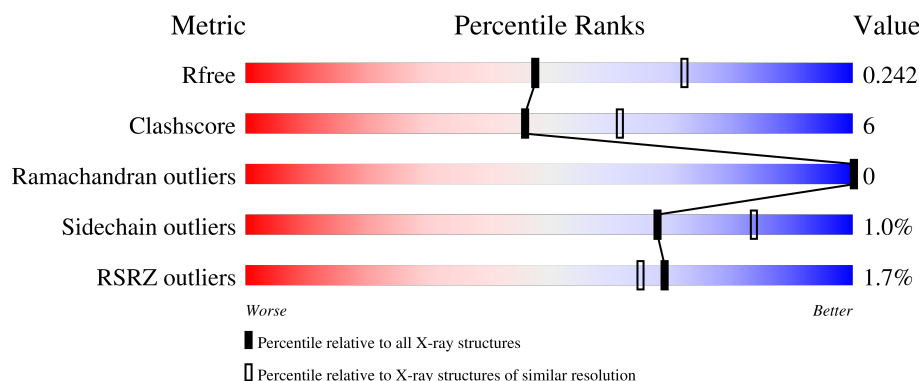
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	503	89% 9% ..
1	B	503	88% 11%
1	C	503	87% 12% .
1	D	503	88% 10% .
1	E	503	3% 83% 16% .

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Mol	Chain	Length	Quality of chain
1	F	503	3% 84% 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24483 atoms, of which 3 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 Carboxypeptidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3908	2464	700	738	6			
1	B	501	Total	C	N	O	S	0	1	0
			3958	2492	709	751	6			
1	C	495	Total	C	N	O	S	0	0	0
			3916	2468	703	739	6			
1	D	497	Total	C	N	O	S	0	0	0
			3922	2471	703	742	6			
1	E	497	Total	C	N	O	S	0	0	0
			3908	2465	698	739	6			
1	F	501	Total	C	N	O	S	0	0	0
			3943	2484	709	744	6			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	H	O	0	0
			7	2	3	2		

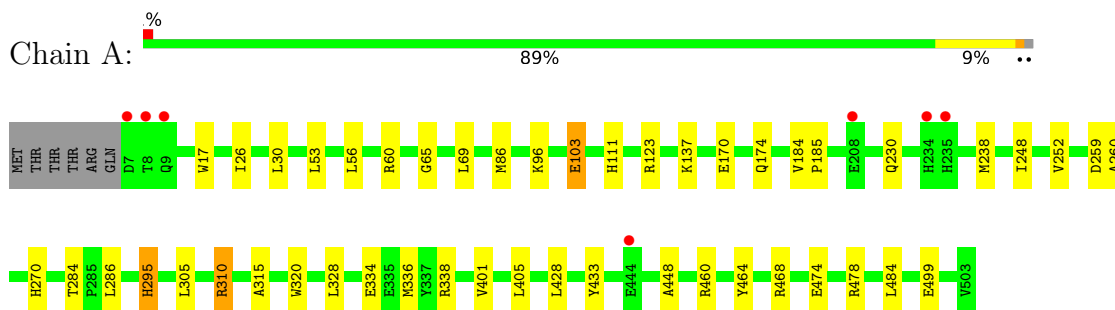
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	175	Total	O	0	1
			176	176		
4	B	196	Total	O	0	1
			197	197		
4	C	158	Total	O	0	0
			158	158		
4	D	192	Total	O	0	5
			197	197		
4	E	93	Total	O	0	1
			94	94		
4	F	93	Total	O	0	0
			93	93		

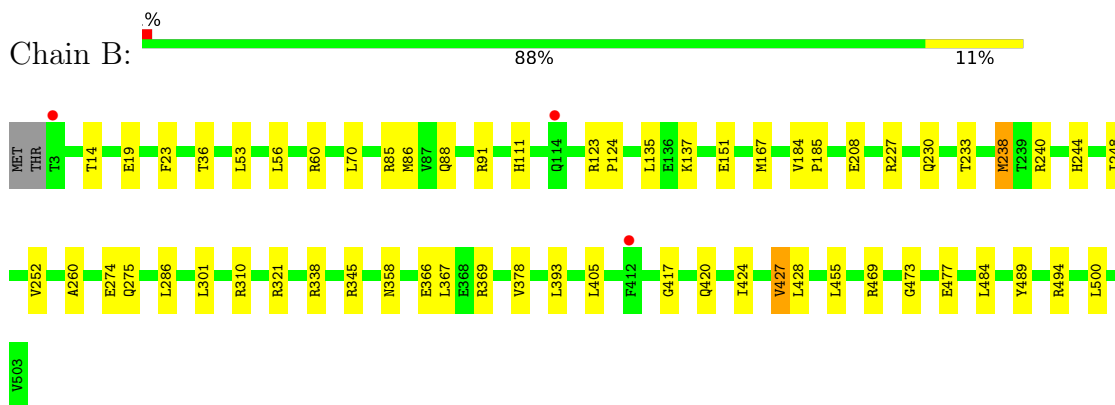
3 Residue-property plots [i](#)

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.

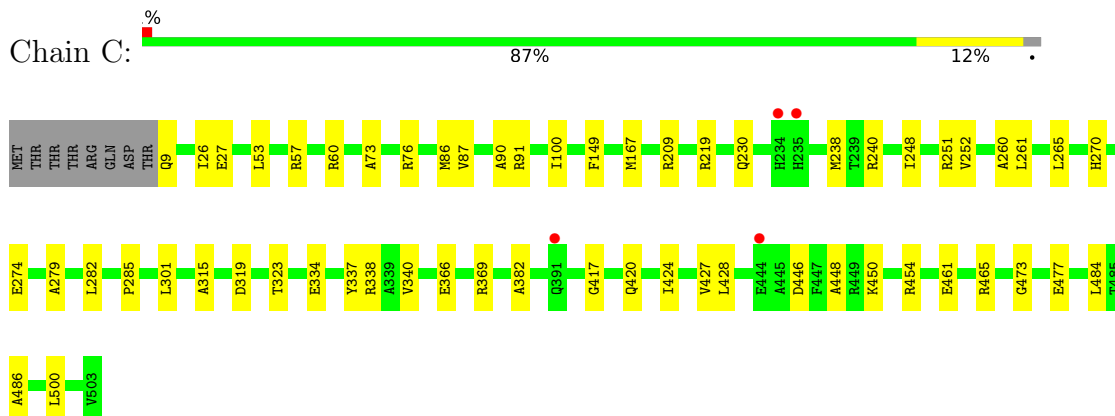
- Molecule 1: Carboxypeptidase 1



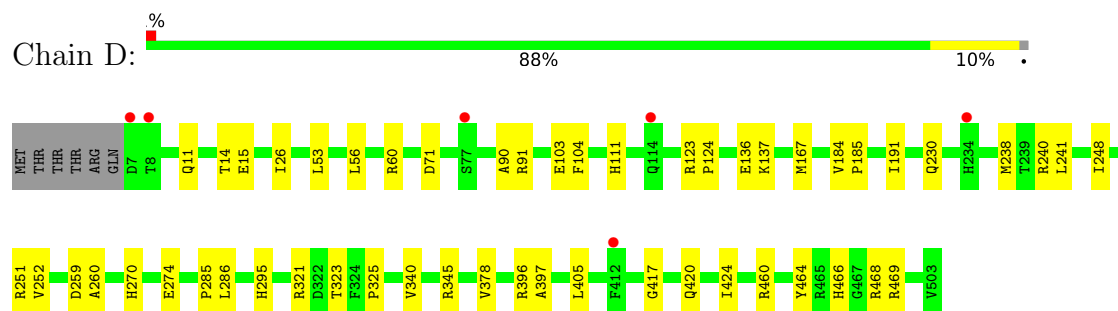
- Molecule 1: Carboxypeptidase 1



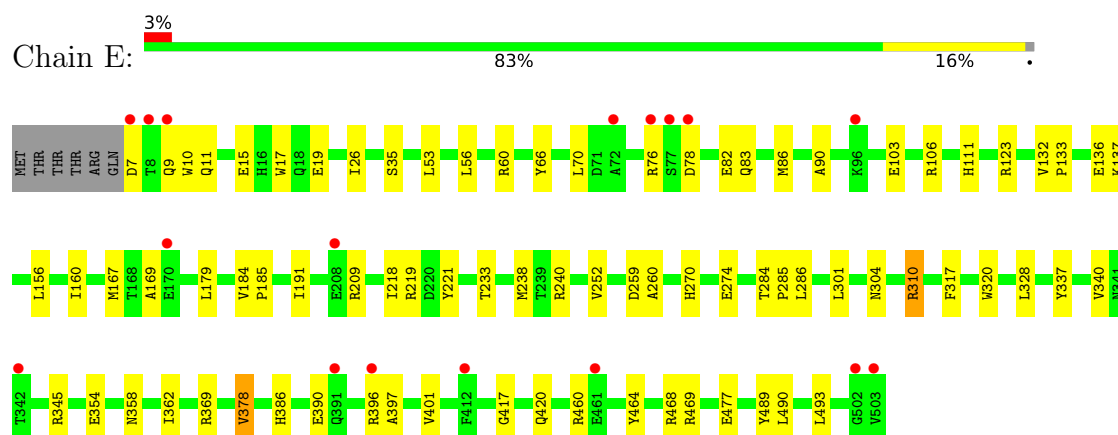
- Molecule 1: Carboxypeptidase 1



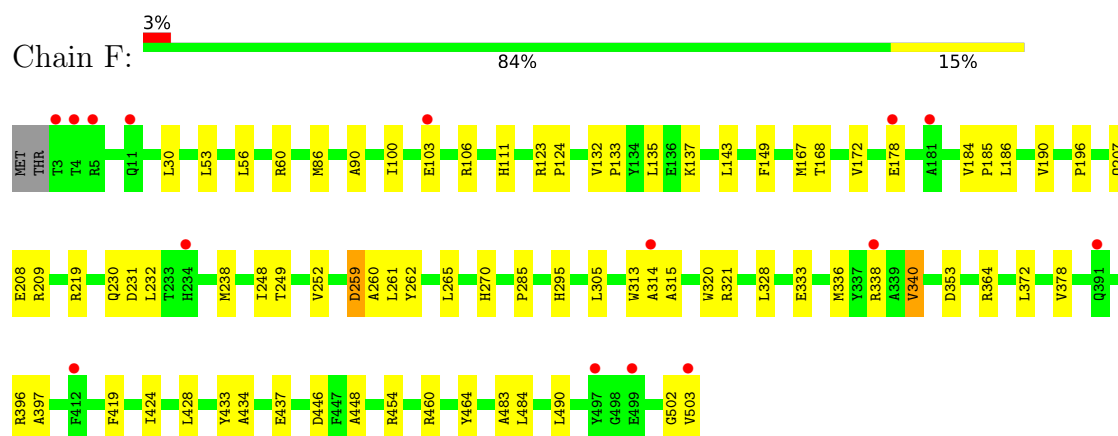
- Molecule 1: Carboxypeptidase 1



- Molecule 1: Carboxypeptidase 1



- Molecule 1: Carboxypeptidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	134.86Å 256.63Å 199.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.97 – 2.40 47.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.97-2.40) 99.9 (47.97-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.07 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.205 , 0.243 0.207 , 0.242	Depositor DCC
R_{free} test set	6746 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtrriage
Anisotropy	0.530	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24483	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3878e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, ZN

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	0.24	0/4007	0.41	0/5438
1	B	0.24	0/4060	0.42	0/5508
1	C	0.23	0/4015	0.41	0/5445
1	D	0.24	0/4021	0.42	0/5456
1	E	0.21	0/4007	0.39	0/5439
1	F	0.21	0/4042	0.39	0/5484
All	All	0.23	0/24152	0.41	0/32770

There are no bond length outliers.

There are no bond angle outliers.

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	3908	0	3689	40	0
1	B	3958	0	3745	41	0
1	C	3916	0	3717	40	0
1	D	3922	0	3708	36	0
1	E	3908	0	3688	60	0
1	F	3943	0	3728	54	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	D	4	3	3	1	0
4	A	176	0	0	1	0
4	B	197	0	0	3	0
4	C	158	0	0	4	0
4	D	197	0	0	0	0
4	E	94	0	0	2	0
4	F	93	0	0	3	0
All	All	24480	3	22278	265	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 (265) 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:86:MET:HE3	1:A:284:THR:HB	1.42	1.02
1:E:86:MET:HE3	1:E:284:THR:HB	1.45	0.98
1:D:136:GLU:HG3	1:D:378:VAL:HG21	1.56	0.86
1:C:446:ASP:OD2	1:C:454:ARG:HD3	1.77	0.83
1:F:103:GLU:OE1	1:F:106:ARG:NH2	2.13	0.80
1:A:328:LEU:HD11	1:A:336:MET:CE	2.15	0.77
1:F:446:ASP:OD2	1:F:454:ARG:HD3	1.87	0.75
1:C:167:MET:HE3	1:C:424:ILE:HD13	1.70	0.74
1:D:136:GLU:HG3	1:D:378:VAL:CG2	2.17	0.74
1:A:17:TRP:CZ3	1:A:86:MET:HE2	2.23	0.74
1:D:71:ASP:OD1	1:D:91:ARG:NH1	2.22	0.73
1:E:17:TRP:CZ3	1:E:86:MET:HE2	2.24	0.73
1:B:494:ARG:HD3	4:B:809:HOH:O	1.89	0.72
1:A:320:TRP:HE1	1:A:336:MET:HE3	1.56	0.71
1:A:86:MET:CE	1:A:284:THR:HB	2.20	0.71
1:B:240:ARG:NH1	1:B:274:GLU:OE2	2.23	0.71
1:C:219:ARG:HD2	4:C:731:HOH:O	1.92	0.69
1:A:238:MET:CE	1:A:270:HIS:HB3	2.22	0.69
1:A:103:GLU:HB2	4:A:770:HOH:O	1.91	0.69
1:A:170:GLU:O	1:A:174:GLN:HG3	1.93	0.69
1:C:366:GLU:HG2	1:C:369:ARG:NH2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:320:TRP:CD1	1:E:328:LEU:HD21	2.29	0.67
1:A:310:ARG:NH2	1:A:499:GLU:OE1	2.27	0.66
1:B:167:MET:HE3	1:B:424:ILE:HD13	1.77	0.66
1:E:136:GLU:HG3	1:E:378:VAL:HG21	1.76	0.66
1:D:123:ARG:HB3	1:D:124:PRO:HD3	1.77	0.66
1:B:111:HIS:CE1	1:B:137:LYS:HD3	2.31	0.65
1:F:396:ARG:NH1	1:F:397:ALA:O	2.29	0.65
1:B:60:ARG:NH2	1:F:56:LEU:HD21	2.11	0.65
1:E:86:MET:CE	1:E:284:THR:HB	2.24	0.65
1:E:136:GLU:HG3	1:E:378:VAL:CG2	2.26	0.65
1:E:310:ARG:HD3	1:E:337:TYR:CD2	2.32	0.65
1:D:167:MET:HE3	1:D:424:ILE:HD13	1.80	0.64
1:A:238:MET:HE2	1:A:270:HIS:HB3	1.79	0.64
1:C:60:ARG:NH2	1:E:56:LEU:HD21	2.14	0.63
1:E:317:PHE:CE1	1:E:328:LEU:HD23	2.32	0.63
1:D:111:HIS:ND1	1:D:137:LYS:HD3	2.14	0.63
1:E:7:ASP:O	1:E:10:TRP:HB3	1.98	0.63
1:C:100:ILE:HD11	1:C:149:PHE:HE1	1.64	0.63
1:E:396:ARG:NH1	1:E:397:ALA:O	2.33	0.62
1:A:56:LEU:O	1:A:60:ARG:HG2	1.99	0.62
1:C:240:ARG:NH1	1:C:274:GLU:OE1	2.34	0.61
1:B:111:HIS:ND1	1:B:137:LYS:HD3	2.15	0.61
1:E:86:MET:HG2	1:E:286:LEU:HG	1.82	0.61
1:C:319:ASP:OD2	1:C:450:LYS:NZ	2.31	0.60
1:E:238:MET:CE	1:E:270:HIS:HB3	2.32	0.60
1:B:230:GLN:HA	1:B:248:ILE:O	2.01	0.59
1:B:428:LEU:HD21	1:B:484:LEU:HD13	1.84	0.59
1:E:320:TRP:HD1	1:E:328:LEU:HD21	1.66	0.59
1:F:123:ARG:HB3	1:F:124:PRO:HD3	1.83	0.59
1:A:320:TRP:NE1	1:A:336:MET:HE3	2.17	0.59
1:C:334:GLU:OE2	1:C:338:ARG:NH1	2.36	0.59
1:B:123:ARG:HB3	1:B:124:PRO:HD3	1.83	0.59
1:C:230:GLN:HA	1:C:248:ILE:O	2.04	0.58
1:C:209:ARG:NH1	1:C:323:THR:O	2.36	0.58
1:F:196:PRO:HB3	1:F:338:ARG:HE	1.69	0.58
1:F:321:ARG:HA	1:F:328:LEU:HD13	1.85	0.58
1:D:111:HIS:CE1	1:D:137:LYS:HB3	2.39	0.58
1:D:238:MET:HE2	1:D:270:HIS:HB3	1.86	0.58
1:E:358:ASN:O	1:E:362:ILE:HG13	2.04	0.57
1:F:259:ASP:HB3	4:F:704:HOH:O	2.04	0.57
1:A:86:MET:HG2	1:A:286:LEU:HG	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:ARG:NE	1:B:469:ARG:O	2.38	0.57
1:D:238:MET:CE	1:D:270:HIS:HB3	2.33	0.57
1:C:461:GLU:OE2	1:C:465:ARG:NH2	2.37	0.56
1:E:179:LEU:HD23	1:E:490:LEU:HD21	1.88	0.56
1:E:35:SER:O	1:E:233:THR:HG22	2.06	0.55
1:B:345:ARG:HD3	1:B:393:LEU:O	2.06	0.55
1:E:310:ARG:HD3	1:E:337:TYR:CE2	2.42	0.55
1:A:238:MET:HE3	1:A:270:HIS:HB3	1.89	0.55
1:E:386:HIS:O	1:E:390:GLU:HG3	2.08	0.54
1:E:26:ILE:CG2	1:E:53:LEU:HD21	2.38	0.54
1:E:26:ILE:HG22	1:E:53:LEU:HD21	1.88	0.54
1:B:428:LEU:CD2	1:B:484:LEU:HD13	2.38	0.54
1:F:135:LEU:CB	1:F:378:VAL:HG11	2.37	0.54
1:C:27:GLU:OE1	1:C:57:ARG:HD3	2.08	0.54
1:D:136:GLU:CG	1:D:378:VAL:HG21	2.35	0.54
1:D:396:ARG:NH1	1:D:397:ALA:O	2.41	0.54
1:F:167:MET:HE3	1:F:424:ILE:HD13	1.90	0.54
1:E:82:GLU:OE2	1:E:469:ARG:NH1	2.41	0.54
1:C:87:VAL:O	1:C:91:ARG:HG3	2.07	0.53
1:E:160:ILE:CD1	1:E:169:ALA:HA	2.37	0.53
1:B:427:VAL:CG2	1:B:484:LEU:HD11	2.39	0.53
1:D:111:HIS:CE1	1:D:137:LYS:HD3	2.44	0.53
1:E:76:ARG:HH21	1:E:78:ASP:CB	2.21	0.53
1:A:230:GLN:HA	1:A:248:ILE:O	2.09	0.53
1:E:26:ILE:HG22	1:E:53:LEU:CD2	2.39	0.52
1:B:111:HIS:CE1	1:B:137:LYS:HB3	2.45	0.52
1:D:123:ARG:HA	1:D:405:LEU:HD13	1.90	0.52
1:E:240:ARG:NH1	1:E:274:GLU:OE1	2.42	0.52
1:F:207:GLN:NE2	1:F:232:LEU:HD11	2.25	0.52
1:E:10:TRP:CZ2	1:E:83:GLN:HG2	2.44	0.52
1:E:238:MET:HE2	1:E:270:HIS:HB3	1.92	0.52
1:C:238:MET:CE	1:C:270:HIS:HB3	2.41	0.51
1:F:262:TYR:OH	1:F:340:VAL:HG11	2.11	0.51
1:A:315:ALA:HB2	1:A:448:ALA:HA	1.93	0.51
1:A:184:VAL:HB	1:A:185:PRO:HD3	1.92	0.51
1:D:238:MET:H	3:D:602:ACT:H2	1.75	0.51
1:D:26:ILE:CG2	1:D:53:LEU:HD11	2.42	0.50
1:F:90:ALA:HB2	1:F:285:PRO:HG2	1.93	0.50
1:C:334:GLU:O	1:C:338:ARG:HG3	2.11	0.50
1:B:135:LEU:HB2	1:B:378:VAL:HG11	1.94	0.50
1:B:427:VAL:HG21	1:B:484:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:MET:HE3	1:E:270:HIS:HB3	1.94	0.50
1:F:135:LEU:HB3	1:F:378:VAL:HG11	1.92	0.50
1:C:238:MET:HE3	1:C:270:HIS:HB3	1.94	0.49
1:A:320:TRP:HE1	1:A:336:MET:CE	2.23	0.49
1:A:123:ARG:HA	1:A:405:LEU:HD13	1.93	0.49
1:A:26:ILE:HG22	1:A:53:LEU:HD11	1.93	0.49
1:D:26:ILE:HG22	1:D:53:LEU:HD11	1.95	0.49
1:E:66:TYR:CZ	1:E:70:LEU:HD11	2.47	0.49
1:B:227:ARG:NH2	1:B:275:GLN:O	2.45	0.49
1:C:473:GLY:O	1:C:477:GLU:HG3	2.13	0.49
1:A:111:HIS:ND1	1:A:137:LYS:HD3	2.28	0.49
1:A:26:ILE:CG2	1:A:53:LEU:HD11	2.42	0.48
1:A:305:LEU:HD13	1:A:433:TYR:CB	2.43	0.48
1:D:251:ARG:NH1	1:D:259:ASP:OD2	2.46	0.48
1:B:123:ARG:HA	1:B:405:LEU:HD13	1.96	0.48
1:D:230:GLN:HA	1:D:248:ILE:O	2.14	0.48
1:C:251:ARG:O	1:C:251:ARG:HG3	2.13	0.48
1:F:208:GLU:HG3	1:F:209:ARG:N	2.29	0.48
1:F:252:VAL:HA	1:F:260:ALA:HB2	1.94	0.48
1:F:143:LEU:CD2	1:F:372:LEU:HD22	2.43	0.48
1:B:417:GLY:HA2	1:B:420:GLN:OE1	2.14	0.48
1:C:252:VAL:HA	1:C:260:ALA:HB2	1.95	0.48
1:F:320:TRP:CD1	1:F:328:LEU:HD11	2.49	0.48
1:E:179:LEU:CD2	1:E:490:LEU:HD21	2.43	0.48
1:F:186:LEU:O	1:F:190:VAL:HG23	2.14	0.47
1:F:230:GLN:HA	1:F:248:ILE:O	2.14	0.47
1:A:26:ILE:HG22	1:A:53:LEU:CD1	2.43	0.47
1:D:238:MET:CE	1:D:295:HIS:CE1	2.98	0.47
1:C:60:ARG:HH22	1:E:56:LEU:HD21	1.78	0.47
1:E:417:GLY:HA2	1:E:420:GLN:OE1	2.14	0.47
1:F:238:MET:CE	1:F:270:HIS:HB3	2.45	0.47
1:B:70:LEU:HB3	1:B:91:ARG:HG2	1.97	0.47
1:E:218:ILE:HA	1:E:221:TYR:HB2	1.97	0.47
1:A:328:LEU:HD11	1:A:336:MET:HE3	1.92	0.47
1:D:136:GLU:CG	1:D:378:VAL:CG2	2.90	0.47
1:E:123:ARG:O	1:E:401:VAL:HG22	2.14	0.47
1:A:111:HIS:CE1	1:A:137:LYS:HB3	2.50	0.47
1:E:286:LEU:HA	1:E:468:ARG:HB2	1.95	0.47
1:B:85:ARG:NH1	1:B:88:GLN:OE1	2.46	0.46
1:E:304:ASN:HB3	1:E:354:GLU:OE1	2.15	0.46
1:C:26:ILE:CG2	1:C:53:LEU:HD21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:GLU:HG2	1:F:490:LEU:HD11	1.97	0.46
1:F:184:VAL:HB	1:F:185:PRO:HD3	1.97	0.46
1:A:474:GLU:O	1:A:478:ARG:HG3	2.16	0.46
1:C:417:GLY:HA2	1:C:420:GLN:OE1	2.15	0.46
1:B:227:ARG:HD2	1:B:244:HIS:ND1	2.31	0.46
1:B:238:MET:C	1:B:238:MET:HE2	2.41	0.46
1:C:167:MET:HE2	1:C:167:MET:HB2	1.84	0.46
1:D:11:GLN:O	1:D:15:GLU:HG3	2.16	0.46
1:E:9:GLN:HG3	1:E:10:TRP:N	2.31	0.45
1:F:428:LEU:HD21	1:F:484:LEU:HD13	1.98	0.45
1:B:366:GLU:HG2	1:B:369:ARG:NH2	2.31	0.45
1:F:314:ALA:HA	1:F:333:GLU:CD	2.41	0.45
1:F:502:GLY:O	1:F:503:VAL:O	2.35	0.45
1:B:53:LEU:HD12	1:B:53:LEU:HA	1.77	0.45
1:D:191:ILE:HD13	1:D:345:ARG:HG3	1.98	0.45
1:F:434:ALA:HA	1:F:437:GLU:HG2	1.99	0.45
1:F:502:GLY:O	1:F:503:VAL:HG22	2.15	0.45
1:C:9:GLN:N	4:C:709:HOH:O	2.50	0.45
1:D:56:LEU:O	1:D:60:ARG:HG2	2.17	0.45
1:E:184:VAL:HB	1:E:185:PRO:HD3	1.97	0.45
1:A:238:MET:HE1	1:A:295:HIS:CE1	2.52	0.45
1:C:73:ALA:HA	1:C:76:ARG:HG3	1.98	0.45
1:B:338:ARG:HG2	1:B:500:LEU:CD2	2.46	0.45
1:A:17:TRP:CZ3	1:A:86:MET:CE	2.97	0.45
1:B:473:GLY:O	1:B:477:GLU:HG3	2.16	0.45
1:F:53:LEU:HD23	1:F:53:LEU:HA	1.71	0.45
1:B:184:VAL:HB	1:B:185:PRO:HD3	1.99	0.45
1:E:103:GLU:OE1	1:E:106:ARG:NH2	2.50	0.45
1:E:219:ARG:HD3	4:E:708:HOH:O	2.16	0.45
1:B:36:THR:HG22	1:B:233:THR:CG2	2.47	0.44
1:C:60:ARG:HH22	1:E:56:LEU:CD2	2.29	0.44
1:E:252:VAL:HA	1:E:260:ALA:HB2	1.98	0.44
1:B:367:LEU:HG	4:B:799:HOH:O	2.17	0.44
1:C:86:MET:HE3	1:C:86:MET:HB2	1.87	0.44
1:D:252:VAL:HA	1:D:260:ALA:HB2	2.00	0.44
1:F:261:LEU:O	1:F:265:LEU:HG	2.18	0.44
1:F:314:ALA:HA	1:F:333:GLU:OE2	2.17	0.44
1:D:466:HIS:O	1:D:469:ARG:HB3	2.17	0.44
1:F:100:ILE:HD11	1:F:149:PHE:HE1	1.83	0.44
1:A:428:LEU:HD21	1:A:484:LEU:HD13	1.99	0.44
1:B:86:MET:HG2	1:B:286:LEU:HG	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:301:LEU:C	1:E:301:LEU:HD23	2.42	0.44
1:F:483:ALA:HB1	4:F:732:HOH:O	2.18	0.44
1:B:60:ARG:HH22	1:F:56:LEU:HD21	1.81	0.44
1:E:390:GLU:OE1	1:E:396:ARG:HD2	2.18	0.44
1:A:30:LEU:HD12	1:A:53:LEU:HD12	1.99	0.43
1:F:111:HIS:ND1	1:F:137:LYS:HD3	2.33	0.43
1:B:358:ASN:ND2	4:B:710:HOH:O	2.51	0.43
1:D:286:LEU:HA	1:D:468:ARG:HB2	1.99	0.43
1:B:427:VAL:HA	1:B:489:TYR:CG	2.53	0.43
1:C:428:LEU:HD21	1:C:484:LEU:HD13	2.00	0.43
1:F:313:TRP:CH2	1:F:336:MET:HE2	2.54	0.43
1:C:261:LEU:O	1:C:265:LEU:HG	2.18	0.43
1:F:168:THR:O	1:F:172:VAL:HG23	2.18	0.43
1:F:364:ARG:HD3	1:F:419:PHE:CD1	2.53	0.43
1:F:305:LEU:HD13	1:F:433:TYR:CB	2.49	0.43
1:C:100:ILE:HD11	1:C:149:PHE:CE1	2.49	0.43
1:D:240:ARG:NH1	1:D:274:GLU:OE2	2.51	0.43
1:E:7:ASP:O	1:E:11:GLN:N	2.47	0.43
1:A:123:ARG:O	1:A:401:VAL:HG22	2.19	0.43
1:D:103:GLU:HG2	1:D:104:PHE:N	2.34	0.43
1:E:460:ARG:HA	1:E:464:TYR:HB2	2.01	0.43
1:F:460:ARG:HA	1:F:464:TYR:HB2	1.99	0.43
1:B:56:LEU:HD21	1:F:60:ARG:HH21	1.83	0.43
1:C:301:LEU:C	1:C:301:LEU:HD23	2.44	0.43
1:D:26:ILE:HG22	1:D:53:LEU:CD1	2.49	0.43
1:E:209:ARG:NE	4:E:704:HOH:O	2.44	0.43
1:E:191:ILE:HD13	1:E:345:ARG:HG3	2.00	0.42
1:B:208:GLU:H	1:B:208:GLU:CD	2.27	0.42
1:C:337:TYR:CE2	1:C:500:LEU:HD21	2.54	0.42
1:E:489:TYR:CZ	1:E:493:LEU:HD11	2.54	0.42
1:F:86:MET:HE3	1:F:86:MET:HB2	1.93	0.42
1:C:26:ILE:HG22	1:C:53:LEU:CD2	2.49	0.42
1:C:315:ALA:HB2	1:C:448:ALA:HA	2.00	0.42
1:F:167:MET:HE2	1:F:167:MET:HB2	1.94	0.42
1:F:238:MET:CE	1:F:295:HIS:CE1	3.02	0.42
1:C:90:ALA:HB2	1:C:285:PRO:HG2	2.02	0.42
1:E:390:GLU:HG2	1:E:396:ARG:HB2	2.00	0.42
1:A:460:ARG:HA	1:A:464:TYR:HB2	2.01	0.42
1:F:315:ALA:HB2	1:F:448:ALA:HA	2.01	0.42
1:B:19:GLU:OE1	1:B:60:ARG:NE	2.40	0.42
1:F:135:LEU:HB2	1:F:378:VAL:HG11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ALA:HB3	4:C:810:HOH:O	2.19	0.42
1:E:132:VAL:N	1:E:133:PRO:HD2	2.34	0.42
1:E:11:GLN:O	1:E:15:GLU:HG3	2.20	0.41
1:F:231:ASP:O	1:F:249:THR:HA	2.19	0.41
1:D:417:GLY:HA2	1:D:420:GLN:OE1	2.19	0.41
1:E:19:GLU:OE1	1:E:60:ARG:HD3	2.19	0.41
1:F:340:VAL:O	1:F:340:VAL:CG1	2.66	0.41
1:A:286:LEU:HA	1:A:468:ARG:HB2	2.00	0.41
1:C:427:VAL:HG13	1:C:486:ALA:HA	2.02	0.41
1:E:111:HIS:CE1	1:E:137:LYS:HD3	2.56	0.41
1:F:305:LEU:HD13	1:F:433:TYR:HB2	2.03	0.41
1:B:301:LEU:HD21	1:B:455:LEU:HD21	2.02	0.41
1:D:238:MET:HE1	1:D:295:HIS:CE1	2.56	0.41
1:F:353:ASP:HB2	4:F:723:HOH:O	2.20	0.41
1:D:184:VAL:HB	1:D:185:PRO:HD3	2.02	0.41
1:F:132:VAL:N	1:F:133:PRO:HD2	2.35	0.41
1:B:23:PHE:CE2	1:B:60:ARG:HD3	2.55	0.41
1:A:252:VAL:HA	1:A:260:ALA:HB2	2.03	0.41
1:C:9:GLN:N	4:C:712:HOH:O	2.54	0.41
1:D:241:LEU:N	1:D:241:LEU:HD12	2.35	0.41
1:F:364:ARG:HD3	1:F:419:PHE:CE1	2.56	0.41
1:A:65:GLY:O	1:A:69:LEU:CD1	2.69	0.41
1:A:305:LEU:HD13	1:A:433:TYR:HB2	2.03	0.41
1:E:9:GLN:OE1	1:E:76:ARG:HD2	2.20	0.41
1:F:30:LEU:CD1	1:F:53:LEU:HD12	2.51	0.41
1:A:96:LYS:HE2	1:A:96:LYS:HB3	1.92	0.40
1:C:279:ALA:HA	1:C:282:LEU:HG	2.04	0.40
1:D:460:ARG:HA	1:D:464:TYR:HB2	2.02	0.40
1:E:90:ALA:HB2	1:E:285:PRO:HG2	2.03	0.40
1:B:252:VAL:HA	1:B:260:ALA:HB2	2.02	0.40
1:F:111:HIS:CE1	1:F:137:LYS:HB3	2.55	0.40
1:A:334:GLU:OE1	1:A:338:ARG:NH1	2.53	0.40
1:B:427:VAL:HG22	1:B:428:LEU:N	2.36	0.40
1:E:111:HIS:ND1	1:E:137:LYS:HD3	2.36	0.40
1:E:156:LEU:CD2	1:E:369:ARG:HG3	2.52	0.40
1:A:65:GLY:O	1:A:69:LEU:HD13	2.22	0.40
1:D:90:ALA:HB2	1:D:285:PRO:HG2	2.03	0.40
1:D:323:THR:C	1:D:325:PRO:HD3	2.46	0.40
1:E:111:HIS:CE1	1:E:137:LYS:HB3	2.56	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	495/503 (98%)	488 (99%)	7 (1%)	0	100	100
1	B	500/503 (99%)	491 (98%)	9 (2%)	0	100	100
1	C	493/503 (98%)	487 (99%)	6 (1%)	0	100	100
1	D	495/503 (98%)	489 (99%)	6 (1%)	0	100	100
1	E	495/503 (98%)	487 (98%)	8 (2%)	0	100	100
1	F	499/503 (99%)	491 (98%)	8 (2%)	0	100	100
All	All	2977/3018 (99%)	2933 (98%)	44 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	380/392 (97%)	376 (99%)	4 (1%)	65	82
1	B	388/392 (99%)	382 (98%)	6 (2%)	57	77
1	C	384/392 (98%)	383 (100%)	1 (0%)	86	93
1	D	383/392 (98%)	380 (99%)	3 (1%)	73	86
1	E	380/392 (97%)	374 (98%)	6 (2%)	55	76
1	F	384/392 (98%)	381 (99%)	3 (1%)	73	86
All	All	2299/2352 (98%)	2276 (99%)	23 (1%)	68	84

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	GLU
1	A	259	ASP
1	A	295	HIS
1	A	310	ARG
1	B	14	THR
1	B	151	GLU
1	B	238	MET
1	B	310	ARG
1	B	321	ARG
1	B	427	VAL
1	C	340	VAL
1	D	14	THR
1	D	321	ARG
1	D	340	VAL
1	E	167	MET
1	E	259	ASP
1	E	310	ARG
1	E	340	VAL
1	E	378	VAL
1	E	477	GLU
1	F	219	ARG
1	F	259	ASP
1	F	340	VAL

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	12	GLN
1	A	50	GLN
1	A	235	HIS
1	A	298	GLN
1	B	235	HIS
1	B	298	GLN
1	C	50	GLN
1	D	298	GLN
1	D	462	ASN
1	E	50	GLN
1	E	298	GLN
1	E	358	ASN
1	E	426	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](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
3	ACT	D	602	2	3,3,3	0.78	0	3,3,3	1.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	602	ACT	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	497/503 (98%)	-0.19	7 (1%) 73 69	17, 24, 45, 66	0
1	B	501/503 (99%)	-0.20	3 (0%) 85 83	12, 24, 42, 64	1 (0%)
1	C	495/503 (98%)	-0.07	4 (0%) 82 80	20, 28, 42, 65	0
1	D	497/503 (98%)	-0.11	6 (1%) 76 73	18, 25, 45, 65	0
1	E	497/503 (98%)	0.26	17 (3%) 48 44	21, 35, 57, 78	0
1	F	501/503 (99%)	0.23	15 (2%) 52 48	19, 34, 52, 64	0
All	All	2988/3018 (99%)	-0.01	52 (1%) 69 65	12, 28, 49, 78	1 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	7	ASP	4.7
1	D	77	SER	4.2
1	A	8	THR	3.7
1	E	412	PHE	3.6
1	B	3	THR	3.4
1	E	78	ASP	3.3
1	A	7	ASP	3.3
1	D	8	THR	3.1
1	C	234	HIS	3.0
1	F	4	THR	2.8
1	A	234	HIS	2.8
1	E	461	GLU	2.7
1	D	234	HIS	2.7
1	F	3	THR	2.7
1	E	502	GLY	2.6
1	E	8	THR	2.6
1	F	178	GLU	2.6
1	F	499	GLU	2.6
1	E	9	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	76	ARG	2.5
1	F	412	PHE	2.5
1	C	235	HIS	2.5
1	F	338	ARG	2.5
1	B	412	PHE	2.5
1	E	77	SER	2.5
1	C	391	GLN	2.4
1	E	396	ARG	2.4
1	C	444	GLU	2.4
1	E	208	GLU	2.4
1	A	9	GLN	2.3
1	D	7	ASP	2.3
1	E	72	ALA	2.3
1	E	342	THR	2.3
1	E	170	GLU	2.2
1	D	412	PHE	2.2
1	F	503	VAL	2.2
1	F	11	GLN	2.2
1	F	234	HIS	2.2
1	F	314	ALA	2.2
1	B	114	GLN	2.1
1	F	103	GLU	2.1
1	E	391	GLN	2.1
1	F	391	GLN	2.1
1	F	5	ARG	2.1
1	A	444	GLU	2.1
1	A	208	GLU	2.1
1	E	96	LYS	2.1
1	E	503	VAL	2.0
1	F	497	TYR	2.0
1	D	114	GLN	2.0
1	F	181	ALA	2.0
1	A	235	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	D	602	4/4	0.91	0.11	20,20,32,32	0
2	ZN	F	601	1/1	0.98	0.03	30,30,30,30	0
2	ZN	E	601	1/1	0.98	0.03	33,33,33,33	0
2	ZN	D	601	1/1	0.99	0.02	25,25,25,25	0
2	ZN	A	601	1/1	0.99	0.03	24,24,24,24	0
2	ZN	B	601	1/1	1.00	0.01	25,25,25,25	0
2	ZN	C	601	1/1	1.00	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.