WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 12:24 AM EDT

PDB ID	:	1JJI
Title	:	The Crystal Structure of a Hyper-thermophilic Carboxylesterase from the Archaeon Archaeoglobus fulgidus
Authors	:	De Simone, G.; Menchise, V.; Manco, G.; Mandrich, L.; Sorrentino, N.; Lang, D.; Rossi, M.; Pedone, C.
Deposited on	:	2001-07-06
Resolution	:	2.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35
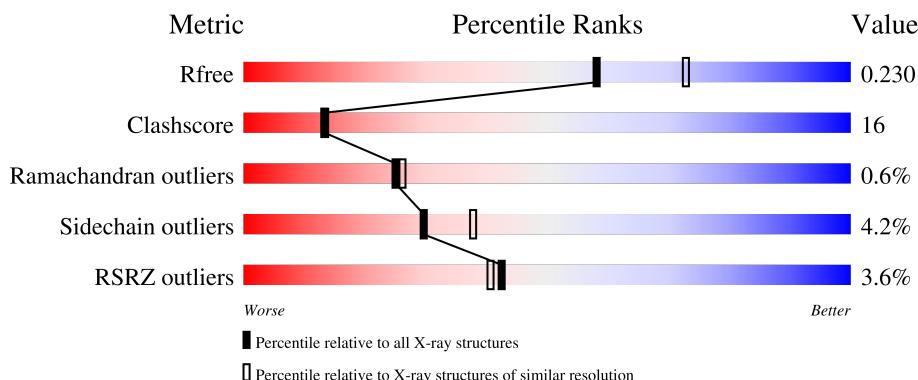
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION
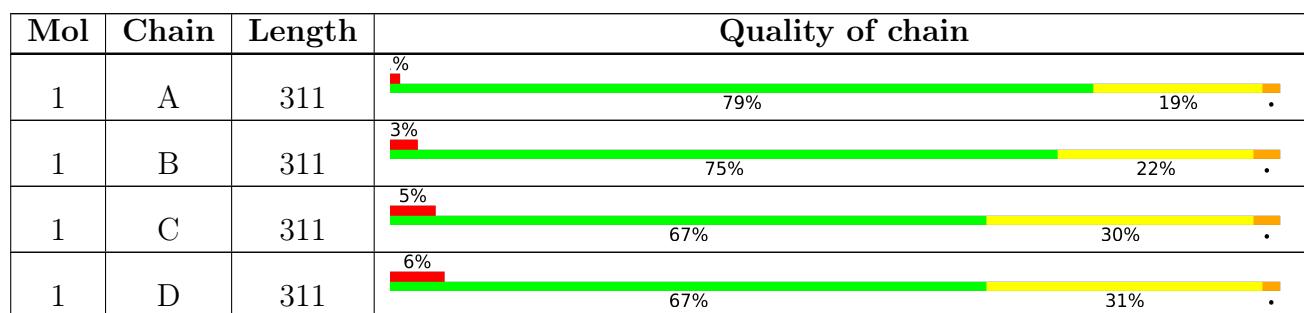
The reported resolution of this entry is 2.20 Å.

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	Percentile Ranks	Value
Rfree		0.230
Clashscore		16
Ramachandran outliers		0.6%
Sidechain outliers		4.2%
RSRZ outliers		3.6%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	311	% 79% 19% •
1	B	311	3% 75% 22% •
1	C	311	5% 67% 30% •
1	D	311	6% 67% 31% •

2 Entry composition ⓘ
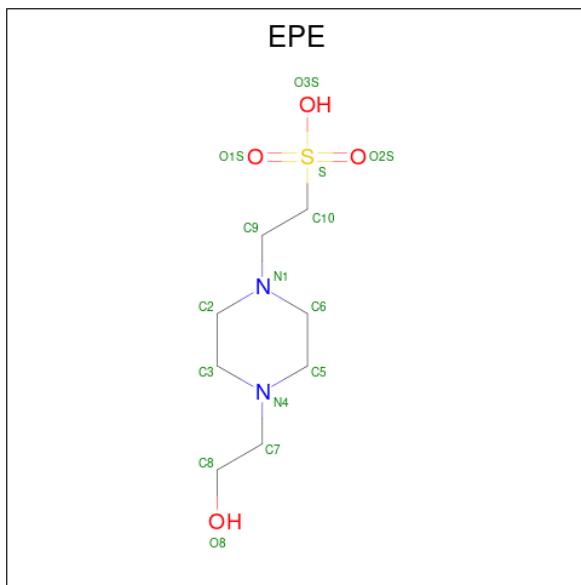
There are 3 unique types of molecules in this entry. The entry contains 10649 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Carboxylesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	53	0	0
			2508	1602	430	468	8			
1	B	311	Total	C	N	O	S	46	0	0
			2508	1602	430	468	8			
1	C	311	Total	C	N	O	S	72	0	0
			2508	1602	430	468	8			
1	D	311	Total	C	N	O	S	54	0	0
			2508	1602	430	468	8			

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).

EPE

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	3	0
			14	8	2	3	1		
2	B	1	Total	C	N	O	S	3	0
			14	8	2	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total 14	C 8	N 2	O 3	S 1	3	0
2	D	1	Total 14	C 8	N 2	O 3	S 1	3	0
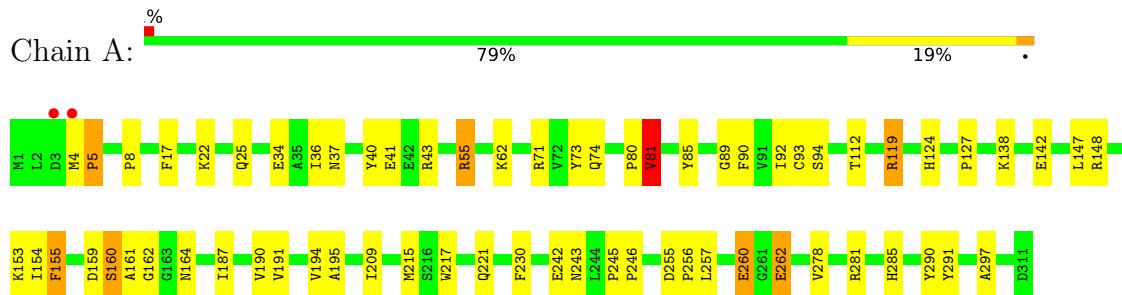
• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	165	Total 165	O 165	0	0
3	B	180	Total 180	O 180	0	0
3	C	108	Total 108	O 108	0	0
3	D	108	Total 108	O 108	0	0
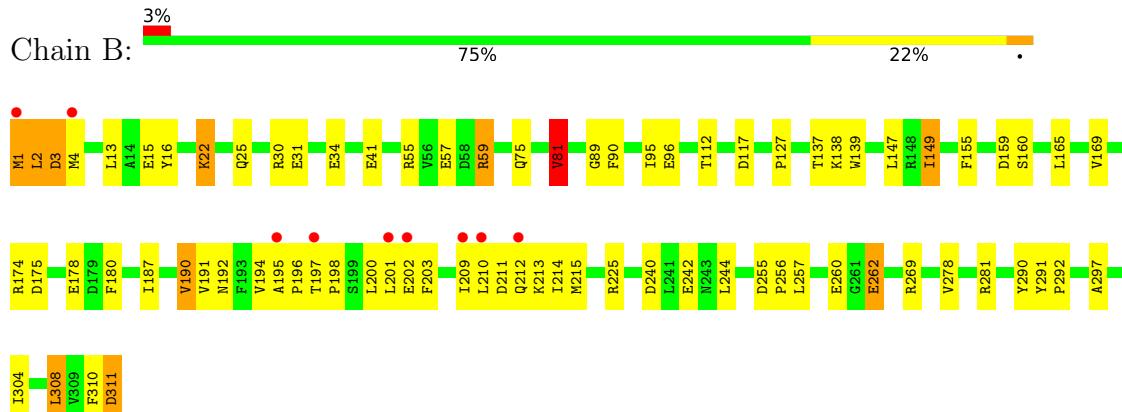
3 Residue-property plots ⓘ

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 as grey.
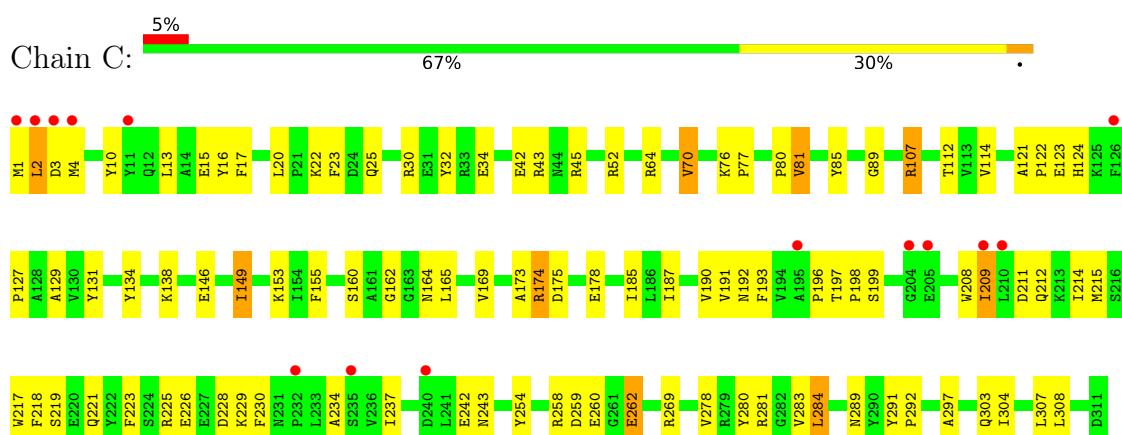
• Molecule 1: Carboxylesterase
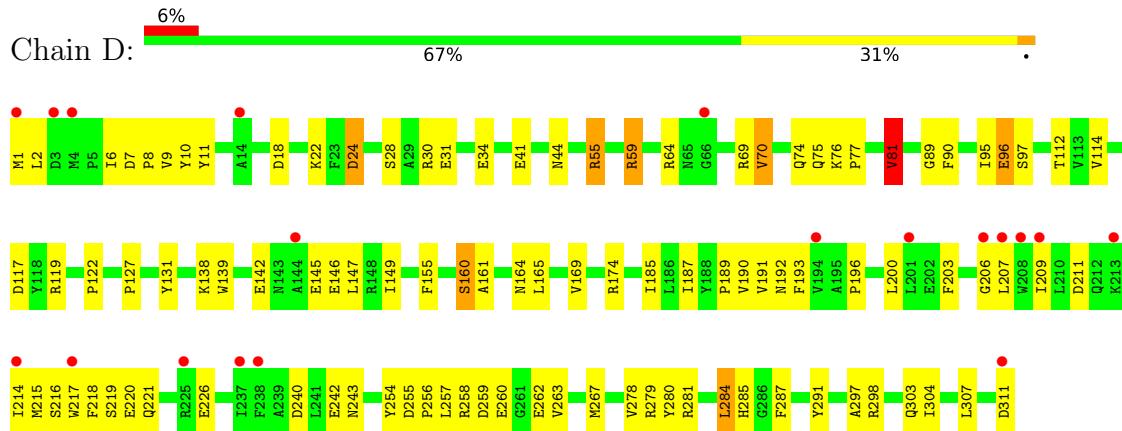
Chain A:

• Molecule 1: Carboxylesterase

Chain B:

• Molecule 1: Carboxylesterase

Chain C:

• Molecule 1: Carboxylesterase

Chain D:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α, β, γ	169.05Å 169.05Å 104.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.3 (8.00-2.20) 98.7 (19.99-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 2.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.235 0.198 , 0.230	Depositor DCC
R_{free} test set	4236 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 46.3	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10649	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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 ⓘ

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

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	0.64	2/2568 (0.1%)	0.72	1/3482 (0.0%)
1	B	0.63	1/2568 (0.0%)	0.75	4/3482 (0.1%)
1	C	0.58	2/2568 (0.1%)	0.70	2/3482 (0.1%)
1	D	0.57	1/2568 (0.0%)	0.67	2/3482 (0.1%)
All	All	0.61	6/10272 (0.1%)	0.71	9/13928 (0.1%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	GLU	CD-OE2	-6.30	1.18	1.25
1	B	262	GLU	CD-OE1	-6.25	1.18	1.25
1	A	262	GLU	CD-OE2	-6.14	1.19	1.25
1	C	262	GLU	CD-OE1	-5.19	1.20	1.25
1	C	146	GLU	CD-OE1	-5.17	1.20	1.25
1	A	260	GLU	CB-CG	-5.01	1.42	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	107	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	81	VAL	CB-CA-C	-7.18	97.76	111.40
1	A	81	VAL	CB-CA-C	-6.74	98.59	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	107	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	81	VAL	CB-CA-C	-5.71	100.54	111.40
1	B	190	VAL	CB-CA-C	-5.37	101.20	111.40
1	B	3	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	D	298	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	2	LEU	CA-CB-CG	-5.12	103.53	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	290	TYR	Sidechain

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	2508	0	2449	51	0
1	B	2508	0	2449	93	0
1	C	2508	0	2449	96	0
1	D	2508	0	2449	97	0
2	A	14	0	17	3	0
2	B	14	0	17	5	0
2	C	14	0	17	6	0
2	D	14	0	17	3	0
3	A	165	0	0	7	0
3	B	180	0	0	2	0
3	C	108	0	0	8	0
3	D	108	0	0	3	0
All	All	10649	0	9864	313	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 16.

All (313) 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:D:41:GLU:HG2	1:D:96:GLU:HB2	1.23	1.16
1:C:174:ARG:HG2	1:C:174:ARG:HH11	1.14	1.10
1:B:174:ARG:HH11	1:B:174:ARG:HG2	1.22	1.02
1:D:122:PRO:HG3	1:D:221:GLN:HE21	1.23	1.00
1:B:191:VAL:HG22	1:B:260:GLU:HG2	1.47	0.94
1:B:2:LEU:HD22	1:C:237:ILE:HD13	1.50	0.90
1:D:174:ARG:HH11	1:D:174:ARG:HG2	1.39	0.87
1:C:174:ARG:HH11	1:C:174:ARG:CG	1.87	0.87
1:B:194:VAL:HG23	1:B:195:ALA:H	1.40	0.86
1:B:41:GLU:HG2	1:B:96:GLU:HB2	1.56	0.86
1:B:57:GLU:HG3	3:B:610:HOH:O	1.76	0.83
1:C:191:VAL:HG22	1:C:260:GLU:HG2	1.59	0.83
1:B:198:PRO:O	1:B:202:GLU:HG3	1.79	0.82
1:D:191:VAL:HG22	1:D:260:GLU:HG2	1.59	0.82
1:C:260:GLU:HB2	3:C:469:HOH:O	1.80	0.80
1:C:174:ARG:HG3	3:C:555:HOH:O	1.80	0.80
1:B:15:GLU:CG	1:C:230:PHE:HB2	2.12	0.79
1:B:112:THR:HG21	1:B:149:ILE:HD11	1.65	0.77
1:C:81:VAL:HG11	1:C:149:ILE:CD1	2.14	0.77
1:D:263:VAL:HG12	1:D:267:MET:CE	2.14	0.77
1:C:81:VAL:HG13	1:C:112:THR:HB	1.67	0.76
1:D:263:VAL:HG12	1:D:267:MET:HE3	1.68	0.74
1:C:174:ARG:NH1	1:C:175:ASP:OD1	2.19	0.72
1:D:6:ILE:HG22	1:D:254:TYR:CE2	2.24	0.72
1:D:260:GLU:HB2	3:D:485:HOH:O	1.90	0.72
1:D:95:ILE:HD11	1:D:117:ASP:HB2	1.71	0.71
1:C:22:LYS:O	1:C:25:GLN:HG2	1.90	0.71
1:B:194:VAL:HG23	1:B:195:ALA:N	2.05	0.71
1:D:30:ARG:O	1:D:34:GLU:HG2	1.91	0.71
1:D:41:GLU:CG	1:D:96:GLU:HB2	2.12	0.71
1:A:281:ARG:NH1	1:B:262:GLU:OE1	2.22	0.70
1:C:52:ARG:HG3	1:C:52:ARG:HH11	1.56	0.70
1:C:89:GLY:HA2	2:C:455:EPE:H62	1.71	0.70
1:A:262:GLU:OE1	1:B:281:ARG:NH1	2.22	0.70
1:A:242:GLU:HG2	1:A:243:ASN:ND2	2.07	0.69
1:B:81:VAL:HG22	1:B:149:ILE:HG13	1.73	0.69
1:B:196:PRO:HA	1:B:200:LEU:HD23	1.75	0.69
1:D:122:PRO:HG3	1:D:221:GLN:NE2	2.04	0.69
1:D:41:GLU:HG2	1:D:96:GLU:CB	2.13	0.69
1:D:81:VAL:HG11	1:D:149:ILE:CD1	2.23	0.68
1:B:225:ARG:HG2	1:B:225:ARG:HH11	1.57	0.68
1:D:207:LEU:HD21	1:D:254:TYR:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PRO:HG3	1:C:221:GLN:HB3	1.75	0.68
1:C:174:ARG:HG2	1:C:174:ARG:NH1	1.96	0.67
1:B:174:ARG:HH11	1:B:174:ARG:CG	1.99	0.67
1:B:291:TYR:HA	1:B:297:ALA:HB3	1.77	0.67
1:C:1:MET:HG2	1:C:2:LEU:N	2.09	0.67
1:D:187:ILE:HD11	1:D:304:ILE:HD11	1.77	0.66
1:C:81:VAL:HG11	1:C:149:ILE:HD11	1.78	0.66
1:D:95:ILE:CD1	1:D:117:ASP:HB2	2.24	0.66
1:C:209:ILE:HD12	1:C:284:LEU:HD12	1.76	0.66
1:C:191:VAL:CG2	1:C:260:GLU:HG2	2.26	0.66
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.09	0.66
1:B:174:ARG:CD	1:B:242:GLU:O	2.43	0.65
1:C:2:LEU:C	1:C:4:MET:H	1.99	0.65
1:D:242:GLU:HG2	1:D:243:ASN:ND2	2.12	0.65
1:C:173:ALA:O	1:C:178:GLU:HB2	1.96	0.64
1:D:81:VAL:CG1	1:D:112:THR:HB	2.27	0.64
1:A:22:LYS:HB2	1:A:25:GLN:HG3	1.78	0.64
1:B:15:GLU:HG3	1:C:230:PHE:HB2	1.77	0.64
1:D:81:VAL:HG13	1:D:112:THR:HB	1.80	0.64
1:B:174:ARG:HG2	1:B:174:ARG:NH1	2.01	0.64
1:B:174:ARG:HD2	1:B:242:GLU:O	1.98	0.64
1:B:30:ARG:NH1	1:B:31:GLU:OE2	2.32	0.63
1:C:80:PRO:HG3	1:C:153:LYS:HD2	1.80	0.63
1:D:211:ASP:O	1:D:215:MET:HG3	1.99	0.63
1:C:281:ARG:NH1	1:D:262:GLU:OE1	2.31	0.62
1:D:155:PHE:HE2	1:D:307:LEU:HB3	1.64	0.62
1:D:89:GLY:O	1:D:90:PHE:HB2	1.99	0.62
1:B:2:LEU:HD12	1:C:197:THR:CG2	2.29	0.62
1:B:55:ARG:NH2	1:B:57:GLU:OE1	2.34	0.61
1:D:122:PRO:CG	1:D:221:GLN:HE21	2.07	0.61
1:C:242:GLU:HG2	1:C:243:ASN:ND2	2.15	0.61
1:B:15:GLU:HG2	1:C:230:PHE:HB2	1.82	0.60
1:C:214:ILE:HG12	1:C:218:PHE:CE2	2.36	0.60
1:C:215:MET:HG2	2:C:455:EPE:H31	1.84	0.60
1:A:191:VAL:HG22	1:A:260:GLU:HG2	1.83	0.60
1:A:260:GLU:HB2	3:A:486:HOH:O	2.01	0.60
1:C:217:TRP:O	1:C:221:GLN:HG2	2.03	0.59
1:D:174:ARG:HG2	1:D:174:ARG:NH1	2.13	0.59
1:D:10:TYR:CE2	1:D:284:LEU:HG	2.37	0.59
1:C:291:TYR:HA	1:C:297:ALA:HB3	1.85	0.59
1:D:203:PHE:HD1	1:D:207:LEU:HD11	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG13	1:A:112:THR:HB	1.85	0.58
1:C:81:VAL:CG1	1:C:112:THR:HB	2.32	0.57
1:A:291:TYR:HA	1:A:297:ALA:HB3	1.85	0.57
1:C:226:GLU:OE2	1:C:229:LYS:HD2	2.04	0.57
1:D:263:VAL:HG12	1:D:267:MET:HE2	1.86	0.57
1:C:291:TYR:CG	1:C:292:PRO:HD3	2.40	0.57
1:B:81:VAL:HG22	1:B:149:ILE:CG1	2.35	0.57
1:C:13:LEU:HD23	1:C:17:PHE:CZ	2.40	0.57
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.70	0.56
1:B:194:VAL:CG2	1:B:195:ALA:H	2.15	0.56
1:C:258:ARG:HD2	1:C:259:ASP:OD1	2.05	0.56
1:A:155:PHE:HD1	1:A:155:PHE:N	2.03	0.56
1:B:190:VAL:CG2	2:B:455:EPE:H22	2.36	0.56
1:D:217:TRP:O	1:D:221:GLN:HG2	2.06	0.56
1:A:278:VAL:HG12	1:B:278:VAL:CG1	2.36	0.56
1:B:95:ILE:CD1	1:B:117:ASP:HB2	2.35	0.56
1:C:303:GLN:HG2	1:D:303:GLN:HG2	1.88	0.56
1:C:52:ARG:HG3	1:C:52:ARG:NH1	2.21	0.56
1:B:191:VAL:CG2	1:B:260:GLU:HG2	2.31	0.56
1:B:192:ASN:HD21	1:B:195:ALA:HB3	1.70	0.55
1:C:10:TYR:CE2	1:C:283:VAL:HA	2.41	0.55
1:C:43:ARG:NH1	3:C:490:HOH:O	2.40	0.55
1:D:55:ARG:NH1	1:D:74:GLN:OE1	2.39	0.55
1:C:124:HIS:NE2	3:C:544:HOH:O	2.30	0.55
1:C:129:ALA:HB2	3:C:513:HOH:O	2.06	0.55
1:A:62:LYS:HG2	3:A:543:HOH:O	2.06	0.55
1:A:217:TRP:O	1:A:221:GLN:HG2	2.06	0.55
1:A:43:ARG:HD3	3:A:494:HOH:O	2.07	0.54
1:A:55:ARG:HD2	3:A:572:HOH:O	2.06	0.54
1:C:164:ASN:HB2	1:C:190:VAL:O	2.07	0.54
1:D:190:VAL:HG21	2:D:455:EPE:H22	1.90	0.54
1:A:278:VAL:CG1	1:B:278:VAL:CG1	2.85	0.54
1:B:13:LEU:O	1:B:16:TYR:N	2.40	0.54
1:B:215:MET:HE3	1:B:257:LEU:HD21	1.88	0.54
1:C:30:ARG:O	1:C:34:GLU:HG3	2.06	0.54
1:A:119:ARG:HG2	1:A:124:HIS:CG	2.42	0.54
1:C:70:VAL:HG13	1:C:114:VAL:HG13	1.88	0.54
1:D:207:LEU:N	1:D:207:LEU:HD12	2.23	0.54
1:C:174:ARG:CG	1:C:174:ARG:NH1	2.55	0.54
1:D:7:ASP:OD1	1:D:9:VAL:HG23	2.08	0.54
1:B:59:ARG:HG3	1:B:59:ARG:NH1	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:PHE:O	1:B:256:PRO:HG3	2.08	0.53
1:B:2:LEU:HD12	1:C:197:THR:HG22	1.90	0.53
1:D:174:ARG:HH11	1:D:174:ARG:CG	2.16	0.53
1:A:119:ARG:HG2	1:A:124:HIS:CE1	2.44	0.53
1:D:164:ASN:HB2	1:D:190:VAL:O	2.08	0.53
1:A:119:ARG:HG2	1:A:124:HIS:CD2	2.44	0.53
1:C:165:LEU:O	1:C:169:VAL:HG23	2.08	0.52
1:A:155:PHE:N	1:A:155:PHE:CD1	2.76	0.52
1:C:218:PHE:HB2	2:C:455:EPE:H51	1.91	0.52
1:B:89:GLY:HA2	2:B:455:EPE:H91	1.91	0.52
1:D:81:VAL:HG11	1:D:149:ILE:HD13	1.90	0.52
1:B:225:ARG:HG2	1:B:225:ARG:NH1	2.25	0.52
1:C:187:ILE:HD11	1:C:304:ILE:HD11	1.91	0.52
1:C:223:PHE:O	3:C:529:HOH:O	2.19	0.52
1:A:17:PHE:HE1	1:A:290:TYR:OH	1.93	0.52
1:D:174:ARG:NH2	1:D:240:ASP:O	2.42	0.51
1:D:190:VAL:HG23	1:D:257:LEU:HD13	1.93	0.51
1:D:196:PRO:HA	1:D:200:LEU:HD23	1.93	0.51
1:A:257:LEU:HD11	2:A:455:EPE:H22	1.93	0.51
1:B:192:ASN:HD21	1:B:195:ALA:CA	2.23	0.51
1:D:291:TYR:HA	1:D:297:ALA:HB3	1.93	0.51
1:C:13:LEU:HB3	1:C:17:PHE:CE2	2.46	0.51
1:D:145:GLU:HA	3:D:506:HOH:O	2.09	0.51
1:C:215:MET:HE3	2:C:455:EPE:H32	1.91	0.51
1:D:174:ARG:CD	1:D:242:GLU:O	2.59	0.51
1:D:207:LEU:CD2	1:D:254:TYR:HB3	2.41	0.51
1:B:215:MET:HG2	2:B:455:EPE:H31	1.93	0.50
1:D:138:LYS:O	1:D:142:GLU:HG3	2.10	0.50
1:B:95:ILE:HD12	1:B:117:ASP:HB2	1.92	0.50
1:D:70:VAL:HG13	1:D:114:VAL:HG13	1.94	0.50
1:B:197:THR:O	1:B:201:LEU:HG	2.12	0.50
1:A:154:ILE:C	1:A:155:PHE:HD1	2.15	0.49
1:C:16:TYR:CZ	1:C:20:LEU:HD21	2.47	0.49
1:A:92:ILE:O	1:A:93:CYS:HB2	2.12	0.49
1:C:1:MET:HG2	1:C:2:LEU:H	1.76	0.49
1:D:190:VAL:HG21	2:D:455:EPE:H92	1.94	0.49
1:D:191:VAL:CG2	1:D:260:GLU:HG2	2.37	0.49
1:D:216:SER:O	1:D:220:GLU:HG3	2.13	0.49
1:A:4:MET:N	1:A:5:PRO:HD2	2.25	0.49
1:B:215:MET:CE	1:B:257:LEU:HD21	2.43	0.49
1:C:10:TYR:HE2	1:C:283:VAL:HA	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:ASN:ND2	1:B:195:ALA:O	2.46	0.48
1:C:81:VAL:HG13	1:C:149:ILE:HG12	1.96	0.48
1:D:193:PHE:HE2	2:D:455:EPE:H52	1.78	0.48
1:D:280:TYR:OH	1:D:303:GLN:NE2	2.46	0.48
1:A:191:VAL:CG2	1:A:260:GLU:HG2	2.43	0.48
1:A:209:ILE:HD12	3:A:606:HOH:O	2.12	0.48
1:B:15:GLU:HG3	1:C:230:PHE:CB	2.42	0.48
1:D:214:ILE:HG12	1:D:218:PHE:CE2	2.47	0.48
1:C:225:ARG:HB2	1:C:228:ASP:OD2	2.14	0.48
1:C:242:GLU:CG	1:C:243:ASN:ND2	2.77	0.48
1:D:75:GLN:O	1:D:76:LYS:HG2	2.13	0.48
1:C:64:ARG:NH1	1:C:131:TYR:CD1	2.82	0.48
1:B:2:LEU:HD22	1:C:237:ILE:CD1	2.34	0.48
1:C:192:ASN:O	3:C:461:HOH:O	2.20	0.48
1:B:190:VAL:HG22	2:B:455:EPE:H22	1.95	0.47
1:D:190:VAL:CG2	1:D:257:LEU:HD13	2.45	0.47
1:D:119:ARG:HG3	1:D:119:ARG:HH11	1.80	0.47
1:A:4:MET:HB2	1:A:5:PRO:HD3	1.96	0.47
1:A:147:LEU:O	1:A:148:ARG:HB2	2.14	0.47
1:B:196:PRO:HA	1:B:200:LEU:CD2	2.43	0.47
1:C:134:TYR:OH	1:C:138:LYS:HD2	2.14	0.47
1:B:192:ASN:HD21	1:B:195:ALA:N	2.12	0.47
1:B:1:MET:CG	1:B:1:MET:O	2.61	0.47
1:B:139:TRP:CZ3	1:B:147:LEU:HD11	2.49	0.47
1:B:191:VAL:HG22	1:B:260:GLU:CG	2.34	0.47
1:B:210:LEU:HG	1:B:215:MET:SD	2.55	0.47
1:D:64:ARG:NH1	1:D:131:TYR:CD2	2.83	0.47
1:D:81:VAL:HG11	1:D:149:ILE:HD11	1.96	0.47
1:A:36:ILE:HG13	1:A:40:TYR:CE2	2.50	0.47
1:B:291:TYR:CG	1:B:292:PRO:HD3	2.49	0.47
1:A:37:ASN:O	1:A:41:GLU:HG3	2.15	0.47
1:C:81:VAL:HG11	1:C:149:ILE:HD13	1.94	0.47
1:B:155:PHE:CD2	1:B:308:LEU:HD12	2.49	0.46
1:C:218:PHE:CB	2:C:455:EPE:H51	2.46	0.46
1:D:59:ARG:NH1	1:D:59:ARG:HG2	2.30	0.46
1:B:174:ARG:NH1	1:B:175:ASP:OD1	2.41	0.46
1:C:174:ARG:HH12	1:C:175:ASP:CG	2.17	0.46
1:D:81:VAL:HG13	1:D:149:ILE:HG12	1.97	0.46
1:C:278:VAL:HG13	1:D:278:VAL:CG1	2.45	0.46
1:A:160:SER:HB3	1:A:161:ALA:H	1.56	0.46
1:C:278:VAL:CG1	1:D:278:VAL:CG1	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:MET:SD	2:A:455:EPE:H32	2.56	0.46
1:B:2:LEU:CD2	1:C:237:ILE:HD13	2.35	0.46
1:B:81:VAL:HG13	1:B:112:THR:HB	1.97	0.45
1:C:280:TYR:OH	1:C:303:GLN:NE2	2.49	0.45
1:C:291:TYR:CD2	1:C:292:PRO:HD3	2.51	0.45
1:C:121:ALA:HB1	1:C:221:GLN:O	2.16	0.45
1:A:89:GLY:O	1:A:90:PHE:HB2	2.16	0.45
1:B:174:ARG:CG	1:B:174:ARG:NH1	2.65	0.45
1:B:192:ASN:ND2	1:B:195:ALA:HB3	2.31	0.45
1:C:122:PRO:O	1:C:123:GLU:C	2.55	0.45
1:D:22:LYS:C	1:D:24:ASP:N	2.68	0.45
1:B:22:LYS:HB2	1:B:25:GLN:HG3	1.98	0.45
1:A:195:ALA:HB2	1:D:1:MET:HE2	1.99	0.45
1:D:44:ASN:ND2	1:D:97:SER:O	2.50	0.45
1:C:2:LEU:C	1:C:4:MET:N	2.67	0.45
1:A:80:PRO:HG3	1:A:153:LYS:HD2	1.98	0.45
1:D:64:ARG:CZ	1:D:131:TYR:CD2	2.99	0.45
1:D:185:ILE:HG21	1:D:304:ILE:HG12	1.98	0.45
1:B:165:LEU:O	1:B:169:VAL:HG23	2.17	0.44
1:C:284:LEU:N	1:C:284:LEU:HD23	2.33	0.44
1:B:112:THR:CG2	1:B:149:ILE:HD11	2.42	0.44
1:D:59:ARG:HG2	1:D:59:ARG:HH11	1.83	0.44
1:D:263:VAL:CG1	1:D:267:MET:HE2	2.47	0.44
1:D:76:LYS:HA	1:D:77:PRO:HD3	1.76	0.44
1:C:155:PHE:CE2	1:C:308:LEU:HD23	2.52	0.44
1:A:215:MET:HG2	2:A:455:EPE:H31	1.99	0.44
1:D:139:TRP:CZ3	1:D:147:LEU:HD11	2.52	0.44
1:D:174:ARG:NH1	1:D:174:ARG:CG	2.76	0.44
1:D:263:VAL:CG1	1:D:267:MET:CE	2.93	0.44
1:A:138:LYS:HE2	1:A:142:GLU:OE2	2.18	0.44
1:D:259:ASP:O	1:D:263:VAL:HG23	2.17	0.44
1:B:2:LEU:HD23	1:B:2:LEU:HA	1.62	0.43
1:B:137:THR:HG22	1:B:180:PHE:HE1	1.83	0.43
1:B:211:ASP:OD1	1:B:213:LYS:HB2	2.19	0.43
1:D:64:ARG:NH1	1:D:131:TYR:CE2	2.87	0.43
1:D:258:ARG:HD3	1:D:279:ARG:HH21	1.83	0.43
1:A:195:ALA:CB	1:D:1:MET:HE2	2.49	0.43
1:A:278:VAL:CG1	1:B:278:VAL:HG12	2.47	0.43
1:B:75:GLN:HA	1:B:75:GLN:OE1	2.19	0.43
1:B:194:VAL:CG2	1:B:195:ALA:N	2.75	0.43
1:A:194:VAL:HG11	1:A:230:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PHE:O	1:C:229:LYS:HD3	2.19	0.43
1:B:138:LYS:NZ	1:B:178:GLU:OE2	2.45	0.43
1:D:284:LEU:O	1:D:287:PHE:HB3	2.18	0.43
1:B:3:ASP:O	1:B:4:MET:C	2.57	0.43
1:D:81:VAL:HG22	1:D:149:ILE:HG23	2.01	0.43
1:A:71:ARG:HG2	1:A:73:TYR:CE1	2.54	0.43
1:B:192:ASN:HD21	1:B:195:ALA:CB	2.30	0.43
1:D:81:VAL:HG12	1:D:112:THR:HB	1.98	0.43
1:B:244:LEU:HD23	1:B:244:LEU:HA	1.88	0.42
1:C:1:MET:CG	1:C:2:LEU:N	2.77	0.42
1:A:245:PRO:HA	1:A:246:PRO:HD3	1.90	0.42
1:A:43:ARG:NE	3:A:537:HOH:O	2.52	0.42
1:C:23:PHE:HA	1:C:32:TYR:CD1	2.53	0.42
1:C:269:ARG:NH2	1:D:8:PRO:HG2	2.35	0.42
1:D:59:ARG:HH11	1:D:59:ARG:CG	2.33	0.42
1:A:159:ASP:HA	1:A:187:ILE:HB	2.01	0.42
1:B:41:GLU:CG	1:B:96:GLU:HB2	2.38	0.42
1:A:8:PRO:HG2	1:B:269:ARG:NH2	2.34	0.42
1:B:174:ARG:NH2	1:B:240:ASP:O	2.51	0.42
1:B:187:ILE:HD11	1:B:304:ILE:HD11	2.01	0.42
1:B:211:ASP:O	1:B:214:ILE:HG22	2.19	0.42
1:B:291:TYR:N	1:B:292:PRO:CD	2.82	0.42
1:C:190:VAL:O	1:C:190:VAL:HG13	2.19	0.42
1:A:255:ASP:OD1	1:A:256:PRO:HD2	2.20	0.42
1:B:159:ASP:HA	1:B:187:ILE:HB	2.01	0.42
1:D:174:ARG:HD2	1:D:242:GLU:O	2.19	0.42
1:B:225:ARG:HD3	3:B:631:HOH:O	2.20	0.42
1:D:22:LYS:C	1:D:24:ASP:H	2.22	0.42
1:D:28:SER:OG	1:D:31:GLU:HG3	2.19	0.42
1:D:89:GLY:O	1:D:90:PHE:CB	2.65	0.42
1:D:41:GLU:HB3	3:D:548:HOH:O	2.19	0.42
1:B:225:ARG:NH1	1:B:225:ARG:CG	2.81	0.42
1:B:155:PHE:HD2	1:B:308:LEU:CD1	2.33	0.41
1:C:254:TYR:HB2	1:C:284:LEU:HD22	2.00	0.41
1:A:74:GLN:HG3	1:A:112:THR:OG1	2.20	0.41
1:B:89:GLY:O	1:B:90:PHE:HB2	2.19	0.41
1:C:198:PRO:HG2	1:C:259:ASP:OD2	2.19	0.41
1:D:257:LEU:HD12	1:D:285:HIS:CE1	2.55	0.41
1:D:255:ASP:HA	1:D:256:PRO:HD3	1.91	0.41
1:A:85:TYR:O	1:A:162:GLY:HA3	2.21	0.41
1:C:85:TYR:O	1:C:162:GLY:HA3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ARG:NH2	1:D:311:ASP:O	2.52	0.41
1:D:165:LEU:O	1:D:169:VAL:HG23	2.20	0.41
1:D:258:ARG:HD2	1:D:259:ASP:OD1	2.20	0.41
1:C:127:PRO:CG	1:C:131:TYR:CE2	3.04	0.41
1:C:234:ALA:HA	3:C:472:HOH:O	2.21	0.41
1:B:310:PHE:O	1:B:311:ASP:OD1	2.38	0.41
1:D:2:LEU:HD12	1:D:2:LEU:O	2.20	0.41
1:C:42:GLU:HA	1:C:45:ARG:NH1	2.36	0.41
1:D:1:MET:HE2	1:D:11:TYR:HE1	1.86	0.41
1:B:174:ARG:HD3	1:B:242:GLU:O	2.19	0.41
1:C:185:ILE:HD11	1:C:307:LEU:HD12	2.02	0.41
1:A:164:ASN:HB2	1:A:190:VAL:O	2.20	0.40
1:B:255:ASP:HA	1:B:256:PRO:HD3	1.95	0.40
1:C:89:GLY:HA2	2:C:455:EPE:H91	2.03	0.40
1:C:185:ILE:CD1	1:C:307:LEU:HD12	2.51	0.40
1:D:160:SER:HB3	1:D:161:ALA:H	1.54	0.40
1:B:190:VAL:HG21	2:B:455:EPE:H22	2.04	0.40
1:C:262:GLU:OE1	1:D:281:ARG:NH1	2.55	0.40
1:D:190:VAL:CG2	1:D:257:LEU:CD1	3.00	0.40
1:A:94:SER:HB2	3:A:569:HOH:O	2.21	0.40
1:A:255:ASP:OD2	1:A:285:HIS:ND1	2.54	0.40
1:C:43:ARG:NH2	1:C:289:ASN:O	2.54	0.40
1:C:199:SER:HB3	1:C:259:ASP:CG	2.42	0.40
1:B:30:ARG:HH11	1:B:30:ARG:HG2	1.86	0.40
1:C:76:LYS:HA	1:C:77:PRO:HD3	1.83	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	309/311 (99%)	293 (95%)	15 (5%)	1 (0%)	41	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	309/311 (99%)	293 (95%)	15 (5%)	1 (0%)	41	46
1	C	309/311 (99%)	288 (93%)	18 (6%)	3 (1%)	15	14
1	D	309/311 (99%)	283 (92%)	24 (8%)	2 (1%)	25	26
All	All	1236/1244 (99%)	1157 (94%)	72 (6%)	7 (1%)	25	26

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	209	ILE
1	B	209	ILE
1	D	209	ILE
1	A	5	PRO
1	C	3	ASP
1	D	206	GLY
1	C	196	PRO

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	266/266 (100%)	259 (97%)	7 (3%)	46	58
1	B	266/266 (100%)	255 (96%)	11 (4%)	30	39
1	C	266/266 (100%)	254 (96%)	12 (4%)	27	34
1	D	266/266 (100%)	251 (94%)	15 (6%)	21	25
All	All	1064/1064 (100%)	1019 (96%)	45 (4%)	30	38

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLU
1	A	55	ARG
1	A	81	VAL
1	A	119	ARG

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Mol	Chain	Res	Type
1	A	127	PRO
1	A	155	PHE
1	A	160	SER
1	B	1	MET
1	B	22	LYS
1	B	34	GLU
1	B	59	ARG
1	B	81	VAL
1	B	127	PRO
1	B	149	ILE
1	B	160	SER
1	B	212	GLN
1	B	308	LEU
1	B	311	ASP
1	C	2	LEU
1	C	15	GLU
1	C	70	VAL
1	C	81	VAL
1	C	149	ILE
1	C	160	SER
1	C	174	ARG
1	C	208	TRP
1	C	211	ASP
1	C	212	GLN
1	C	219	SER
1	C	284	LEU
1	D	18	ASP
1	D	24	ASP
1	D	55	ARG
1	D	59	ARG
1	D	69	ARG
1	D	70	VAL
1	D	81	VAL
1	D	96	GLU
1	D	127	PRO
1	D	160	SER
1	D	189	PRO
1	D	192	ASN
1	D	219	SER
1	D	226	GLU
1	D	284	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	183	HIS
1	A	243	ASN
1	A	289	ASN
1	A	303	GLN
1	B	143	ASN
1	B	192	ASN
1	B	266	GLN
1	B	303	GLN
1	C	243	ASN
1	C	289	ASN
1	C	303	GLN
1	D	212	GLN
1	D	221	GLN
1	D	243	ASN
1	D	266	GLN
1	D	303	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	EPE	B	455	1	11,14,15	1.34	1 (9%)	15,17,20	1.58	1 (6%)
2	EPE	A	455	1	11,14,15	1.29	1 (9%)	15,17,20	1.56	1 (6%)
2	EPE	D	455	1	11,14,15	1.69	2 (18%)	15,17,20	1.22	1 (6%)
2	EPE	C	455	1	11,14,15	1.12	1 (9%)	15,17,20	1.61	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	B	455	1	-	2/8/18/19	0/1/1/1
2	EPE	A	455	1	-	3/8/18/19	0/1/1/1
2	EPE	D	455	1	-	2/8/18/19	0/1/1/1
2	EPE	C	455	1	-	2/8/18/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	455	EPE	C7-N4	3.58	1.55	1.47
2	B	455	EPE	C7-N4	3.13	1.54	1.47
2	D	455	EPE	C9-N1	2.98	1.54	1.47
2	A	455	EPE	C7-N4	2.86	1.54	1.47
2	C	455	EPE	C7-N4	2.60	1.53	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
2	A	455	EPE	O1S-S-C10	5.35	115.29	105.50
2	B	455	EPE	O1S-S-C10	5.07	114.79	105.50
2	C	455	EPE	O1S-S-C10	4.47	113.69	105.50
2	D	455	EPE	O1S-S-C10	3.43	111.77	105.50
2	C	455	EPE	C10-C9-N1	-3.09	106.04	113.17

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	455	EPE	C9-C10-S-O1S
2	A	455	EPE	C9-C10-S-O2S
2	B	455	EPE	C9-C10-S-O1S
2	B	455	EPE	C9-C10-S-O2S
2	C	455	EPE	C9-C10-S-O1S
2	A	455	EPE	N4-C7-C8-O8
2	D	455	EPE	C9-C10-S-O1S
2	C	455	EPE	C10-C9-N1-C6
2	D	455	EPE	C10-C9-N1-C6

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	455	EPE	5	0
2	A	455	EPE	3	0
2	D	455	EPE	3	0
2	C	455	EPE	6	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(Å²)	Q<0.9
1	A	309/311 (99%)	0.02	2 (0%)	89	88	24, 34, 53, 64	9 (2%)
1	B	308/311 (99%)	0.12	9 (2%)	51	49	25, 36, 58, 76	5 (1%)
1	C	307/311 (98%)	0.39	14 (4%)	32	31	28, 45, 64, 82	11 (3%)
1	D	311/311 (100%)	0.33	19 (6%)	21	20	32, 47, 66, 82	13 (4%)
All	All	1235/1244 (99%)	0.21	44 (3%)	42	41	24, 41, 62, 82	38 (3%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	ILE	7.3
1	D	209	ILE	6.8
1	D	207	LEU	6.4
1	B	201	LEU	6.1
1	B	209	ILE	4.8
1	D	194	VAL	4.6
1	D	208	TRP	4.5
1	A	3	ASP	4.3
1	B	1	MET	4.3
1	C	2	LEU	4.1
1	C	3	ASP	4.0
1	C	1	MET	3.6
1	C	205	GLU	3.5
1	C	235	SER	3.5
1	C	4	MET	3.4
1	D	3	ASP	3.3
1	D	206	GLY	3.3
1	D	225	ARG	3.2
1	D	66	GLY	3.1
1	D	1	MET	3.1
1	C	11	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	195	ALA	2.6
1	C	195	ALA	2.6
1	C	240	ASP	2.6
1	C	210	LEU	2.4
1	D	201	LEU	2.4
1	B	210	LEU	2.3
1	D	237	ILE	2.3
1	D	311	ASP	2.3
1	B	4	MET	2.2
1	D	238	PHE	2.2
1	D	214	ILE	2.2
1	B	212	GLN	2.2
1	C	204	GLY	2.2
1	C	126	PHE	2.1
1	C	232	PRO	2.1
1	D	213	LYS	2.1
1	D	14	ALA	2.1
1	B	202	GLU	2.1
1	D	217	TRP	2.1
1	A	4	MET	2.0
1	D	4	MET	2.0
1	B	197	THR	2.0
1	D	144	ALA	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 monosaccharides in this entry.

6.4 Ligands ⓘ

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EPE	D	455	14/15	0.62	0.32	60,67,67,67	3
2	EPE	A	455	14/15	0.74	0.29	54,56,58,58	3
2	EPE	B	455	14/15	0.77	0.23	55,60,61,61	3
2	EPE	C	455	14/15	0.81	0.46	60,65,65,65	3

6.5 Other polymers (i)

There are no such residues in this entry.