



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 2F9Z / pdb_00002f9z
Title : Complex between the chemotaxis deamidase CheD and the chemotaxis phosphatase CheC from *Thermotoga maritima*
Authors : Chao, X.; Park, S.Y.; Bilwes, A.M.; Crane, B.R.
Deposited on : 2005-12-06
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
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

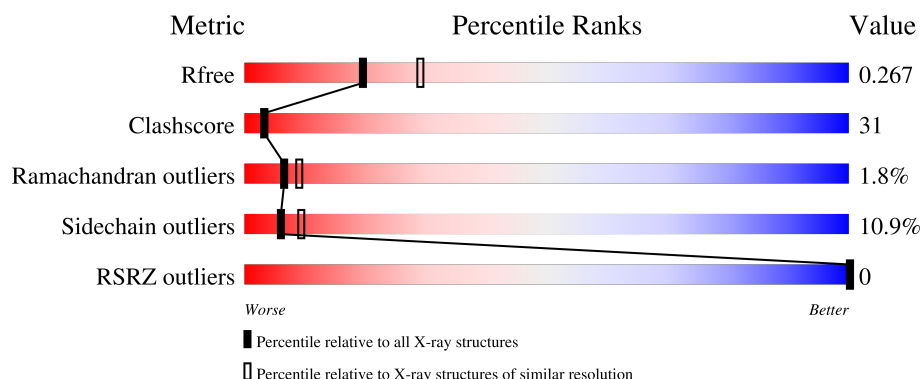
1 Overall quality at a glance

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	205	
1	B	205	
2	C	159	
2	D	159	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5552 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 chemotaxis protein CheC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1452	939	222	281	10			
1	B	190	Total	C	N	O	S	0	0	0
			1433	930	224	268	11			

- Molecule 2 is a protein called PROTEIN (chemotaxis methylation protein).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	154	Total	C	N	O	S	0	0	0
			1140	719	201	210	10			
2	D	154	Total	C	N	O	S	0	0	0
			1135	715	202	209	9			

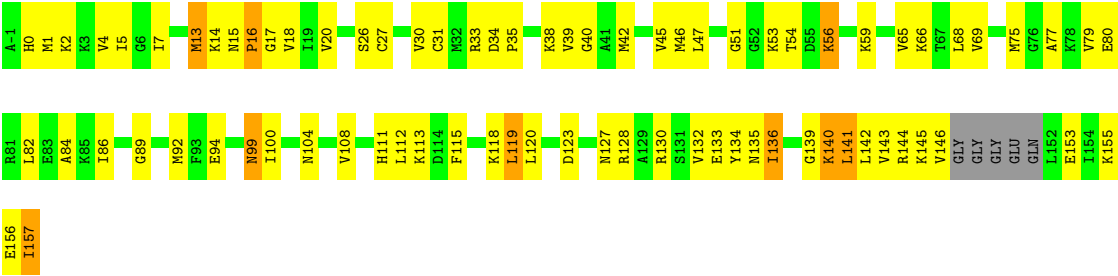
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ALA	-	cloning artifact	UNP Q9X005
C	0	HIS	-	cloning artifact	UNP Q9X005
D	-1	ALA	-	cloning artifact	UNP Q9X005
D	0	HIS	-	cloning artifact	UNP Q9X005

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	111	Total	O	0	0
			111	111		
3	B	100	Total	O	0	0
			100	100		
3	C	94	Total	O	0	0
			94	94		
3	D	87	Total	O	0	0
			87	87		

● Molecule 2: PROTEIN (chemotaxis methylation protein)



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	66.08Å 66.08Å 161.76Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.00-2.40) 53.0 (30.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.275 0.211 , 0.267	Depositor DCC
R_{free} test set	1635 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.186 for -h,-k,l 0.319 for h,-h-k,-l 0.217 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5552	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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	0.49	0/1468	1.07	5/1987 (0.3%)
1	B	0.56	0/1450	1.08	8/1961 (0.4%)
2	C	0.51	1/1149 (0.1%)	0.98	4/1531 (0.3%)
2	D	0.46	0/1145	1.10	8/1527 (0.5%)
All	All	0.51	1/5212 (0.0%)	1.06	25/7006 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	157	ILE	C-OXT	-5.39	1.12	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	SER	N-CA-C	-10.17	101.00	113.41
2	D	17	GLY	N-CA-C	8.97	126.95	111.16
1	B	164	GLN	N-CA-C	-8.03	94.48	108.69
1	B	93	GLY	CA-C-O	-7.81	114.97	121.76
2	D	16	PRO	CA-C-N	-7.55	116.34	122.16
2	D	16	PRO	C-N-CA	-7.55	116.34	122.16
1	B	99	LEU	N-CA-C	6.87	121.12	112.87
2	D	47	LEU	CA-C-N	6.46	126.04	119.19
2	D	47	LEU	C-N-CA	6.46	126.04	119.19
1	A	87	ILE	N-CA-C	-6.27	106.82	111.90
2	C	154	ILE	N-CA-C	6.26	118.49	108.85
2	C	114	ASP	CB-CA-C	-6.19	97.54	110.17
1	B	83	VAL	N-CA-C	6.00	116.18	110.42
1	A	13	GLU	N-CA-C	-5.96	104.87	111.36
1	A	160	ASN	N-CA-C	5.94	117.55	108.52
1	B	195	VAL	N-CA-C	-5.75	104.91	110.72
2	C	145	LYS	N-CA-C	-5.70	99.95	109.24
2	D	68	LEU	N-CA-C	-5.54	106.20	113.12
1	B	55	ASP	CA-C-N	5.21	124.71	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	55	ASP	C-N-CA	5.21	124.71	119.19
2	D	56	LYS	CA-C-N	5.17	124.79	119.05
2	D	56	LYS	C-N-CA	5.17	124.79	119.05
1	A	42	GLU	N-CA-C	5.16	117.23	109.23
1	A	182	THR	N-CA-C	5.12	117.72	110.50
2	C	15	ASN	N-CA-C	5.02	120.91	109.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1452	0	1504	98	0
1	B	1433	0	1518	103	0
2	C	1140	0	1220	69	0
2	D	1135	0	1202	63	0
3	A	111	0	0	10	0
3	B	100	0	0	18	0
3	C	94	0	0	6	0
3	D	87	0	0	7	0
All	All	5552	0	5444	325	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 31.

All (325) 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:45:PRO:HB3	1:A:163:ASP:HB3	1.33	1.11
1:A:190:LYS:HB3	1:A:191:PRO:HD2	1.41	1.00
1:A:66:PRO:HG2	1:A:136:LEU:HB2	1.49	0.94
2:D:39:VAL:HG21	2:D:75:MET:HG2	1.51	0.91
2:C:7:ILE:H	2:C:7:ILE:HD12	1.36	0.90
2:C:13:MET:HG2	2:C:17:GLY:HA3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:HD13	1:A:59:ILE:H	1.36	0.89
1:B:49:VAL:HG21	1:B:165:ILE:HD11	1.54	0.88
1:A:158:GLU:HG2	1:A:159:ASP:H	1.39	0.85
2:D:1:MET:SD	2:D:16:PRO:HB2	2.17	0.84
1:B:26:ILE:HD12	1:B:36:ILE:HD11	1.59	0.83
2:C:135:ASN:HD21	2:C:137:GLU:HB3	1.44	0.82
1:B:165:ILE:HD12	1:B:186:MET:SD	2.19	0.81
2:D:42:MET:HG2	3:D:1237:HOH:O	1.82	0.80
1:B:77:LEU:HD23	1:B:114:GLY:HA2	1.63	0.80
2:C:127:ASN:HD22	2:C:127:ASN:H	1.29	0.79
1:B:78:ILE:HB	1:B:184:TYR:HB2	1.65	0.78
1:B:63:VAL:HG11	1:B:114:GLY:HA3	1.68	0.75
1:B:41:VAL:HG12	1:B:168:VAL:HG22	1.69	0.75
1:A:13:GLU:O	1:A:17:ILE:HG12	1.87	0.75
2:D:99:ASN:H	2:D:99:ASN:ND2	1.82	0.75
1:B:190:LYS:HB3	1:B:191:PRO:HD2	1.69	0.74
2:D:14:LYS:C	2:D:16:PRO:HD2	2.12	0.74
1:A:171:LEU:HD11	1:A:180:PRO:HB2	1.67	0.74
1:B:12:LYS:HD3	1:B:40:ASN:HA	1.70	0.73
1:B:46:ILE:HD13	1:B:46:ILE:H	1.53	0.73
2:D:99:ASN:N	2:D:99:ASN:HD22	1.86	0.72
1:A:89:GLU:HB3	3:A:1187:HOH:O	1.91	0.70
2:C:43:ALA:HB1	3:C:1067:HOH:O	1.92	0.70
1:B:133:ILE:HG13	3:B:1357:HOH:O	1.92	0.70
2:D:86:ILE:HG23	2:D:119:LEU:HD21	1.72	0.70
1:B:34:VAL:HB	3:B:1104:HOH:O	1.91	0.70
1:A:190:LYS:HB3	1:A:191:PRO:CD	2.20	0.69
1:B:77:LEU:CD2	1:B:114:GLY:HA2	2.22	0.69
1:B:99:LEU:HB3	1:B:142:ILE:HD13	1.74	0.69
1:B:167:PHE:CD1	1:B:186:MET:HB3	2.27	0.69
1:A:60:VAL:HG21	1:A:78:ILE:HG23	1.75	0.69
1:A:45:PRO:CB	1:A:163:ASP:HB3	2.18	0.69
1:A:41:VAL:HG22	1:A:168:VAL:HG13	1.75	0.68
1:B:151:GLU:HG3	2:D:92:MET:SD	2.34	0.68
2:D:99:ASN:H	2:D:99:ASN:HD22	1.40	0.68
2:C:135:ASN:HD22	2:C:138:THR:H	1.40	0.68
1:A:136:LEU:HB3	1:A:137:PRO:HD2	1.76	0.68
1:B:44:VAL:HG23	3:B:1151:HOH:O	1.93	0.68
2:C:10:TYR:HD2	2:C:68:LEU:HD12	1.60	0.67
1:B:81:THR:HG22	1:B:85:LYS:HE2	1.75	0.67
1:A:74:SER:HB3	3:A:1365:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:127:ASN:HD22	2:C:127:ASN:N	1.92	0.67
1:B:190:LYS:HB2	1:B:193:TYR:CD2	2.31	0.66
1:A:64:LYS:HE2	3:A:1365:HOH:O	1.96	0.65
2:D:18:VAL:HG11	2:D:133:GLU:HB3	1.79	0.65
1:A:109:ALA:O	1:A:113:ILE:HG13	1.96	0.65
2:D:27:CYS:HA	3:D:1165:HOH:O	1.95	0.65
1:B:89:GLU:O	1:B:91:LEU:N	2.30	0.65
2:C:19:ILE:HG13	3:C:1057:HOH:O	1.97	0.65
1:A:88:LEU:HD21	1:A:106:SER:OG	1.97	0.64
2:C:24:LEU:HD11	2:C:29:ALA:HB2	1.78	0.64
1:B:148:ILE:HB	3:B:1253:HOH:O	1.98	0.64
2:D:15:ASN:N	2:D:16:PRO:HD2	2.13	0.64
1:A:39:PRO:HD3	3:A:1220:HOH:O	1.97	0.63
1:A:45:PRO:HA	1:A:163:ASP:O	1.98	0.63
1:B:3:ILE:HA	3:B:1116:HOH:O	1.99	0.62
2:D:31:CYS:SG	2:D:42:MET:HG3	2.40	0.62
1:B:102:LEU:HD13	3:B:1236:HOH:O	2.00	0.62
2:C:15:ASN:HB2	2:C:38:LYS:HB3	1.80	0.62
1:B:89:GLU:HG3	1:B:94:ARG:HA	1.82	0.61
2:D:141:LEU:HD12	2:D:157:ILE:HD11	1.82	0.61
1:B:89:GLU:C	1:B:91:LEU:H	2.08	0.61
1:B:141:VAL:HG13	1:B:148:ILE:HD13	1.82	0.61
1:A:106:SER:O	1:A:110:LEU:HB2	2.01	0.61
1:A:45:PRO:HG2	1:A:48:LYS:CB	2.31	0.61
1:B:34:VAL:HG22	1:B:35:GLU:H	1.66	0.61
1:B:193:TYR:HA	1:B:196:LYS:HB2	1.83	0.61
1:B:86:LYS:HG3	1:B:90:ILE:HD13	1.82	0.60
1:B:60:VAL:O	1:B:142:ILE:HA	2.01	0.60
1:A:190:LYS:CB	1:A:191:PRO:HD2	2.24	0.60
1:B:34:VAL:HG22	1:B:35:GLU:N	2.17	0.60
1:B:95:ALA:N	1:B:96:PRO:CD	2.65	0.60
1:A:59:ILE:HD13	1:A:59:ILE:N	2.11	0.60
1:B:29:MET:HG2	3:B:1304:HOH:O	2.02	0.60
1:A:82:THR:O	1:A:86:LYS:HG2	2.02	0.59
2:D:84:ALA:H	2:D:120:LEU:HD13	1.67	0.59
2:D:65:VAL:O	2:D:69:VAL:HG13	2.03	0.59
1:B:39:PRO:HG2	1:B:169:GLU:HG3	1.85	0.59
2:D:7:ILE:HG22	2:D:46:MET:HE2	1.85	0.59
1:A:189:PRO:HB2	1:A:193:TYR:HB2	1.84	0.58
2:C:22:LEU:HD23	3:C:1356:HOH:O	2.03	0.58
1:A:99:LEU:HG	1:A:142:ILE:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLU:HG3	1:A:157:LEU:H	1.67	0.58
1:B:164:GLN:O	1:B:194:LEU:HD22	2.03	0.58
2:C:7:ILE:H	2:C:7:ILE:CD1	2.12	0.58
1:A:41:VAL:HG13	1:A:168:VAL:HG22	1.85	0.58
1:B:44:VAL:HB	1:B:45:PRO:HD2	1.83	0.58
2:D:77:ALA:HB1	2:D:82:LEU:HD11	1.85	0.58
2:C:32:MET:HA	2:C:83:GLU:O	2.03	0.58
2:D:133:GLU:HB2	2:D:142:LEU:HB3	1.86	0.58
1:B:11:LEU:HB2	1:B:41:VAL:HG21	1.85	0.58
2:C:128:ARG:HH12	2:C:152:LEU:HD13	1.69	0.58
1:B:131:PHE:CZ	1:B:200:ARG:HG3	2.39	0.57
1:B:190:LYS:HB2	1:B:193:TYR:HD2	1.68	0.57
2:C:19:ILE:HG21	2:C:42:MET:HB3	1.85	0.57
2:C:109:LYS:HE3	2:C:119:LEU:HD12	1.86	0.57
1:B:27:SER:HB2	1:B:34:VAL:HG12	1.86	0.57
1:A:63:VAL:CG1	1:A:138:PRO:HB2	2.34	0.57
1:A:64:LYS:HD3	1:A:139:GLN:NE2	2.19	0.57
1:B:89:GLU:C	1:B:91:LEU:N	2.63	0.57
1:B:149:PHE:CZ	1:B:186:MET:HE3	2.40	0.57
2:D:30:VAL:HG22	2:D:108:VAL:HG21	1.86	0.57
1:A:156:GLU:HG3	1:A:157:LEU:N	2.20	0.57
1:A:59:ILE:H	1:A:59:ILE:CD1	2.07	0.56
2:D:145:LYS:HG2	3:D:1031:HOH:O	2.05	0.56
1:B:26:ILE:HG22	3:B:1104:HOH:O	2.03	0.56
1:A:9:ASP:O	1:A:13:GLU:HG3	2.05	0.56
1:B:95:ALA:N	1:B:96:PRO:HD2	2.20	0.56
1:B:50:ILE:HA	3:B:1303:HOH:O	2.05	0.56
1:A:43:ILE:HG12	1:A:198:PHE:HZ	1.70	0.56
2:D:145:LYS:O	2:D:153:GLU:HG3	2.06	0.56
1:B:96:PRO:HA	3:B:1236:HOH:O	2.06	0.55
2:D:123:ASP:OD2	2:D:143:VAL:HG11	2.05	0.55
1:A:45:PRO:HA	1:A:163:ASP:C	2.31	0.55
1:B:39:PRO:HD2	1:B:169:GLU:O	2.06	0.55
1:A:60:VAL:HG23	1:A:79:MET:O	2.06	0.55
1:B:60:VAL:HG21	3:B:1253:HOH:O	2.07	0.55
2:D:135:ASN:O	2:D:139:GLY:N	2.40	0.55
1:A:171:LEU:N	3:A:1220:HOH:O	2.40	0.55
1:A:84:VAL:HG13	1:A:110:LEU:HD11	1.89	0.54
1:B:91:LEU:HD23	1:B:92:THR:HG23	1.89	0.54
1:A:70:ASP:CG	1:A:132:LYS:H	2.16	0.54
1:B:145:ILE:HA	3:B:1253:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:VAL:HA	2:D:20:VAL:O	2.07	0.54
1:A:70:ASP:HB3	1:A:131:PHE:CD2	2.43	0.54
1:A:170:THR:OG1	1:A:183:SER:HB2	2.08	0.54
1:B:125:LEU:HD22	1:B:187:MET:HE1	1.90	0.54
2:D:1:MET:HE1	3:D:1154:HOH:O	2.08	0.54
1:A:55:ASP:O	1:A:145:ILE:HG21	2.07	0.53
2:C:61:ALA:O	2:C:65:VAL:HG12	2.07	0.53
1:A:46:ILE:HD13	1:A:46:ILE:H	1.74	0.53
1:A:70:ASP:HB3	1:A:131:PHE:HD2	1.73	0.53
1:A:159:ASP:HA	2:C:46:MET:CE	2.39	0.53
1:A:112:GLU:O	1:A:116:ILE:HG13	2.09	0.53
2:C:32:MET:HE3	2:C:68:LEU:HD23	1.90	0.53
2:D:111:HIS:O	2:D:115:PHE:HD1	1.91	0.53
2:D:1:MET:SD	2:D:16:PRO:CB	2.93	0.52
1:A:4:SER:O	1:A:8:LYS:HG3	2.09	0.52
1:A:158:GLU:HG2	1:A:159:ASP:N	2.16	0.52
1:A:171:LEU:HB2	3:A:1220:HOH:O	2.09	0.52
1:A:91:LEU:HD22	1:A:105:PHE:CE1	2.45	0.52
1:A:111:ARG:HD3	1:A:140:LEU:HB2	1.91	0.52
1:A:144:MET:HE1	2:C:131:SER:HB2	1.92	0.52
2:D:51:GLY:H	2:D:53:LYS:HE2	1.74	0.52
1:A:63:VAL:HG12	1:A:138:PRO:HB2	1.92	0.52
2:C:40:GLY:HA3	2:C:136:ILE:HD12	1.90	0.51
1:A:59:ILE:HB	1:A:99:LEU:HD11	1.91	0.51
1:B:88:LEU:HD13	1:B:102:LEU:HD21	1.91	0.51
2:C:47:LEU:HA	2:C:104:ASN:HD21	1.75	0.51
2:C:47:LEU:HB3	2:C:48:PRO:HD2	1.92	0.51
1:A:7:GLN:HB3	3:A:1207:HOH:O	2.10	0.51
2:C:65:VAL:HG11	2:C:111:HIS:HB2	1.91	0.51
2:C:144:ARG:HH21	2:C:154:ILE:HD13	1.75	0.51
1:B:60:VAL:HB	3:B:1169:HOH:O	2.09	0.51
1:B:115:ASN:HB2	1:B:138:PRO:HG3	1.93	0.51
2:C:4:VAL:HA	2:C:20:VAL:O	2.10	0.51
2:C:135:ASN:ND2	2:C:137:GLU:HB3	2.21	0.51
2:D:5:ILE:HD11	2:D:42:MET:HE2	1.93	0.51
2:C:14:LYS:HG2	2:C:15:ASN:H	1.75	0.51
1:A:45:PRO:O	1:A:49:VAL:HB	2.11	0.50
2:C:87:ALA:HA	2:C:123:ASP:O	2.11	0.50
2:D:30:VAL:O	2:D:42:MET:HA	2.11	0.50
1:A:39:PRO:CD	3:A:1220:HOH:O	2.59	0.50
1:A:6:ARG:O	1:A:10:LEU:HD23	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLY:HA2	1:A:190:LYS:HG3	1.94	0.49
2:C:21:THR:HG23	2:C:21:THR:O	2.11	0.49
2:D:35:PRO:O	2:D:38:LYS:HG3	2.11	0.49
1:A:81:THR:OG1	1:A:99:LEU:HD13	2.12	0.49
2:D:104:ASN:O	2:D:108:VAL:HG12	2.12	0.49
2:C:101:GLY:O	2:C:105:VAL:HG23	2.13	0.49
2:C:13:MET:HB3	3:C:1057:HOH:O	2.12	0.49
2:C:20:VAL:HG12	2:C:21:THR:N	2.28	0.49
1:A:39:PRO:HD2	1:A:169:GLU:O	2.13	0.49
2:C:60:TYR:HB2	2:C:63:THR:HG22	1.94	0.49
2:C:144:ARG:HE	2:C:154:ILE:HG12	1.77	0.48
2:D:4:VAL:HG12	2:D:20:VAL:HB	1.95	0.48
2:D:94:GLU:HG2	3:D:1294:HOH:O	2.13	0.48
1:A:46:ILE:HA	1:A:49:VAL:CG1	2.43	0.48
2:D:113:LYS:HD2	3:D:1037:HOH:O	2.12	0.48
1:A:45:PRO:O	1:A:49:VAL:N	2.46	0.48
2:C:65:VAL:HG11	2:C:111:HIS:CB	2.44	0.48
2:C:155:LYS:O	2:C:155:LYS:HG3	2.13	0.48
2:D:140:LYS:HG3	2:D:156:GLU:HB3	1.95	0.48
1:B:108:SER:HA	1:B:111:ARG:NH1	2.29	0.48
1:B:65:MET:HB3	1:B:75:VAL:HG23	1.94	0.48
1:B:91:LEU:HB3	1:B:92:THR:H	1.34	0.48
1:B:94:ARG:C	1:B:96:PRO:CD	2.87	0.48
1:B:66:PRO:HG2	1:B:136:LEU:HB2	1.95	0.48
1:A:46:ILE:HA	1:A:49:VAL:HG12	1.94	0.48
1:B:72:GLU:HB2	1:B:193:TYR:CE2	2.49	0.48
1:B:91:LEU:C	1:B:93:GLY:H	2.22	0.48
2:D:157:ILE:HD13	2:D:157:ILE:H	1.79	0.48
1:A:166:VAL:O	1:A:186:MET:HA	2.14	0.47
1:B:45:PRO:HA	1:B:164:GLN:HG2	1.96	0.47
1:B:193:TYR:O	1:B:197:ILE:HG13	2.14	0.47
1:A:15:GLY:C	1:A:38:VAL:HG21	2.40	0.47
2:C:12:VAL:HG22	2:C:41:ALA:HB2	1.96	0.47
2:C:14:LYS:HG2	2:C:15:ASN:N	2.29	0.47
2:D:46:MET:SD	2:D:59:LYS:HE3	2.54	0.47
2:C:90:ALA:HB2	3:C:1330:HOH:O	2.14	0.47
1:A:27:SER:HB2	1:A:34:VAL:HG12	1.97	0.47
1:B:86:LYS:HG3	1:B:90:ILE:CD1	2.44	0.47
1:A:60:VAL:HG21	1:A:78:ILE:CG2	2.42	0.47
1:A:60:VAL:HG22	1:A:61:VAL:N	2.30	0.47
2:C:27:CYS:SG	2:C:46:MET:HA	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ILE:HD12	1:B:36:ILE:CD1	2.39	0.46
2:D:132:VAL:HA	2:D:142:LEU:O	2.14	0.46
1:A:99:LEU:HD23	1:A:100:LEU:H	1.80	0.46
1:B:167:PHE:HD1	1:B:186:MET:HB3	1.77	0.46
1:A:99:LEU:HD23	1:A:100:LEU:N	2.31	0.46
1:B:17:ILE:HD11	3:B:1287:HOH:O	2.15	0.46
1:B:86:LYS:CG	1:B:90:ILE:HD13	2.46	0.46
2:C:20:VAL:HG13	2:C:133:GLU:HG2	1.98	0.46
2:C:83:GLU:HB3	2:C:120:LEU:HD22	1.98	0.46
2:C:108:VAL:O	2:C:112:LEU:HG	2.16	0.46
2:D:0:HIS:HB3	2:D:2:LYS:NZ	2.31	0.46
1:B:148:ILE:HA	2:D:92:MET:HE1	1.98	0.46
1:B:49:VAL:O	1:B:52:ILE:HG22	2.15	0.46
1:A:45:PRO:HB3	1:A:163:ASP:CB	2.24	0.45
2:D:14:LYS:O	2:D:136:ILE:HD11	2.17	0.45
2:D:75:MET:O	2:D:75:MET:HE3	2.16	0.45
1:B:149:PHE:CE2	1:B:186:MET:HE3	2.51	0.45
2:D:13:MET:HE2	2:D:13:MET:HB2	1.87	0.45
1:B:60:VAL:HG21	1:B:145:ILE:HA	1.99	0.45
2:C:53:LYS:HG3	2:C:54:THR:N	2.31	0.45
1:A:60:VAL:O	1:A:142:ILE:HA	2.15	0.45
1:A:179:GLU:CB	1:A:180:PRO:HD2	2.46	0.45
2:C:7:ILE:HD12	2:C:7:ILE:N	2.19	0.45
2:D:33:ARG:HA	2:D:40:GLY:HA2	1.99	0.45
2:D:128:ARG:HH11	2:D:145:LYS:HE3	1.81	0.45
1:A:162:GLU:OE1	1:A:162:GLU:HA	2.16	0.45
1:B:94:ARG:O	1:B:95:ALA:HB3	2.17	0.45
1:B:117:MET:O	1:B:185:MET:HE1	2.17	0.45
2:C:48:PRO:O	2:C:61:ALA:HB3	2.17	0.45
1:A:160:ASN:H	2:C:46:MET:HE1	1.82	0.45
2:C:41:ALA:CB	2:C:68:LEU:HG	2.47	0.45
1:A:116:ILE:O	1:A:120:THR:HG23	2.17	0.44
2:C:118:LYS:HA	2:C:118:LYS:HD2	1.81	0.44
1:A:46:ILE:CG2	1:A:186:MET:HE1	2.47	0.44
1:A:75:VAL:CG1	1:A:118:CYS:HB3	2.47	0.44
2:D:84:ALA:O	2:D:119:LEU:HD23	2.17	0.44
1:B:14:ILE:HD13	1:B:125:LEU:HD12	1.99	0.44
1:B:190:LYS:HB3	1:B:191:PRO:CD	2.44	0.44
2:C:65:VAL:HG13	2:C:66:LYS:N	2.33	0.44
2:C:66:LYS:HD2	3:C:1143:HOH:O	2.17	0.44
2:C:30:VAL:HB	2:C:43:ALA:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:LEU:HD12	2:D:120:LEU:N	2.32	0.44
1:B:136:LEU:HB3	1:B:137:PRO:HD2	1.99	0.44
1:B:167:PHE:CE1	1:B:186:MET:HB3	2.52	0.44
2:C:70:GLU:O	2:C:74:LYS:HG3	2.18	0.44
1:A:85:LYS:O	1:A:87:ILE:N	2.51	0.44
1:B:4:SER:HB3	1:B:7:GLN:HG3	1.99	0.44
1:B:58:GLU:HG2	1:B:59:ILE:N	2.33	0.44
1:B:63:VAL:O	1:B:76:LEU:HD12	2.18	0.44
1:A:65:MET:HE1	1:A:119:GLY:HA2	2.00	0.43
1:B:148:ILE:HA	2:D:92:MET:CE	2.48	0.43
1:A:159:ASP:HA	2:C:46:MET:HE1	2.00	0.43
1:A:60:VAL:CG2	1:A:78:ILE:HG23	2.46	0.43
1:B:76:LEU:HB3	1:B:186:MET:HG3	1.99	0.43
2:C:98:MET:HG3	2:C:98:MET:O	2.18	0.43
1:A:46:ILE:C	1:A:48:LYS:H	2.26	0.43
2:C:30:VAL:HG22	2:C:108:VAL:HG11	2.00	0.43
1:A:63:VAL:HA	1:A:139:GLN:O	2.17	0.43
2:D:69:VAL:HG21	2:D:115:PHE:CE2	2.54	0.43
1:A:145:ILE:HG23	1:A:146:SER:N	2.33	0.43
1:B:23:ALA:HB1	1:B:34:VAL:HG13	2.01	0.43
2:D:144:ARG:HA	2:D:153:GLU:O	2.18	0.43
1:A:46:ILE:C	1:A:48:LYS:N	2.77	0.43
1:A:85:LYS:C	1:A:87:ILE:H	2.27	0.43
2:D:18:VAL:HA	2:D:134:TYR:O	2.18	0.43
2:C:73:LYS:C	2:C:75:MET:H	2.27	0.42
2:C:135:ASN:O	2:C:139:GLY:N	2.51	0.42
1:B:49:VAL:HG12	3:B:1103:HOH:O	2.19	0.42
1:B:59:ILE:HD12	2:D:146:VAL:HG12	2.01	0.42
1:B:62:GLY:N	1:B:141:VAL:O	2.52	0.42
1:B:83:VAL:HG22	1:B:181:LEU:HD13	2.02	0.42
1:B:98:ASN:O	1:B:102:LEU:HB2	2.20	0.42
2:C:127:ASN:N	2:C:127:ASN:ND2	2.64	0.42
1:B:7:GLN:NE2	1:B:198:PHE:CG	2.87	0.42
1:A:145:ILE:HD13	3:A:1363:HOH:O	2.19	0.42
1:B:87:ILE:HG21	1:B:113:ILE:CD1	2.49	0.42
2:C:26:SER:HB2	2:C:101:GLY:CA	2.50	0.42
2:D:26:SER:O	2:D:89:GLY:HA2	2.20	0.42
1:B:61:VAL:HG22	1:B:99:LEU:HD13	2.02	0.42
1:B:191:PRO:HA	3:B:1336:HOH:O	2.18	0.42
2:D:66:LYS:HA	2:D:69:VAL:HG22	2.02	0.42
2:D:53:LYS:H	2:D:53:LYS:HG2	1.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:VAL:O	1:A:199:GLU:HG2	2.19	0.42
2:D:100:ILE:H	2:D:100:ILE:HG13	1.54	0.42
1:A:62:GLY:HA2	1:A:77:LEU:O	2.19	0.41
1:B:89:GLU:O	1:B:90:ILE:C	2.63	0.41
2:C:26:SER:HB2	2:C:101:GLY:HA2	2.02	0.41
1:A:189:PRO:HB2	1:A:193:TYR:CB	2.50	0.41
1:A:171:LEU:CB	3:A:1220:HOH:O	2.66	0.41
1:B:193:TYR:HA	1:B:196:LYS:CB	2.50	0.41
1:B:199:GLU:C	1:B:201:MET:H	2.28	0.41
1:B:29:MET:HE1	1:B:112:GLU:HG3	2.02	0.41
2:C:4:VAL:HG23	2:C:21:THR:HA	2.03	0.41
1:A:84:VAL:O	1:A:88:LEU:HB2	2.21	0.41
2:C:48:PRO:HD3	2:C:104:ASN:ND2	2.35	0.41
2:D:79:VAL:HA	2:D:82:LEU:HD13	2.02	0.41
1:A:137:PRO:HA	1:A:138:PRO:HD2	1.89	0.41
1:B:32:LYS:HG2	3:B:1018:HOH:O	2.20	0.41
2:C:53:LYS:HG3	2:C:54:THR:H	1.86	0.41
2:D:143:VAL:HB	2:D:155:LYS:HG3	2.02	0.41
1:B:145:ILE:HG23	1:B:146:SER:N	2.36	0.41
2:C:94:GLU:HA	2:C:94:GLU:OE2	2.21	0.41
2:C:100:ILE:H	2:C:100:ILE:HG12	1.71	0.41
1:A:26:ILE:HD12	1:A:36:ILE:HD11	2.03	0.40
2:D:128:ARG:HE	2:D:145:LYS:CE	2.33	0.40
1:B:68:THR:HG22	3:B:1285:HOH:O	2.21	0.40
1:B:104:GLU:H	1:B:104:GLU:HG2	1.55	0.40
1:A:46:ILE:HG22	1:A:186:MET:HE1	2.03	0.40
1:A:179:GLU:HB3	1:A:180:PRO:HD2	2.03	0.40
1:B:65:MET:SD	1:B:75:VAL:CG2	3.10	0.40
2:D:34:ASP:OD1	2:D:77:ALA:HA	2.21	0.40
2:D:56:LYS:HG2	3:D:1228:HOH:O	2.21	0.40
1:B:46:ILE:HG21	1:B:165:ILE:HD13	2.03	0.40
2:C:31:CYS:O	2:C:84:ALA:HA	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	187/205 (91%)	169 (90%)	14 (8%)	4 (2%)	5	7
1	B	184/205 (90%)	159 (86%)	19 (10%)	6 (3%)	3	2
2	C	150/159 (94%)	131 (87%)	17 (11%)	2 (1%)	9	14
2	D	150/159 (94%)	137 (91%)	13 (9%)	0	100	100
All	All	671/728 (92%)	596 (89%)	63 (9%)	12 (2%)	6	9

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	90	ILE
1	B	91	LEU
1	B	94	ARG
1	B	95	ALA
1	A	163	ASP
1	A	54	LYS
1	A	86	LYS
1	B	126	ALA
1	A	190	LYS
1	B	46	ILE
2	C	74	LYS
2	C	153	GLU

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	162/179 (90%)	145 (90%)	17 (10%)	6	10
1	B	161/179 (90%)	141 (88%)	20 (12%)	4	6
2	C	119/122 (98%)	109 (92%)	10 (8%)	10	17
2	D	117/122 (96%)	103 (88%)	14 (12%)	5	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	559/602 (93%)	498 (89%)	61 (11%)	6 9

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ILE
1	A	31	ASN
1	A	40	ASN
1	A	46	ILE
1	A	49	VAL
1	A	52	ILE
1	A	59	ILE
1	A	77	LEU
1	A	91	LEU
1	A	99	LEU
1	A	104	GLU
1	A	140	LEU
1	A	143	ASP
1	A	155	GLU
1	A	156	GLU
1	A	162	GLU
1	A	181	LEU
1	B	2	LYS
1	B	10	LEU
1	B	31	ASN
1	B	43	ILE
1	B	46	ILE
1	B	49	VAL
1	B	52	ILE
1	B	57	GLU
1	B	70	ASP
1	B	75	VAL
1	B	91	LEU
1	B	94	ARG
1	B	97	ASP
1	B	110	LEU
1	B	112	GLU
1	B	125	LEU
1	B	139	GLN
1	B	185	MET
1	B	196	LYS
1	B	199	GLU

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Mol	Chain	Res	Type
2	C	4	VAL
2	C	7	ILE
2	C	10	TYR
2	C	13	MET
2	C	69	VAL
2	C	78	LYS
2	C	85	LYS
2	C	95	SER
2	C	98	MET
2	C	127	ASN
2	D	13	MET
2	D	45	VAL
2	D	54	THR
2	D	80	GLU
2	D	99	ASN
2	D	112	LEU
2	D	118	LYS
2	D	119	LEU
2	D	127	ASN
2	D	130	ARG
2	D	136	ILE
2	D	140	LYS
2	D	141	LEU
2	D	157	ILE

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

Mol	Chain	Res	Type
1	B	98	ASN
2	C	15	ASN
2	C	104	ASN
2	C	127	ASN
2	C	135	ASN
2	D	99	ASN

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	193/205 (94%)	-1.43	0 100 100	15, 50, 94, 115	0
1	B	190/205 (92%)	-1.41	0 100 100	20, 48, 113, 120	0
2	C	154/159 (96%)	-1.54	0 100 100	8, 30, 63, 85	0
2	D	154/159 (96%)	-1.53	0 100 100	14, 32, 78, 108	0
All	All	691/728 (94%)	-1.47	0 100 100	8, 40, 99, 120	0

There are no RSRZ outliers to report.

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.