Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:54 pm GMT

PDB ID	:	1A0O
Title	:	CHEY-BINDING DOMAIN OF CHEA IN COMPLEX WITH CHEY
Authors	:	Chinardet, N.; Welch, M.; Mourey, L.; Birck, C.; Samama, J.P.
Deposited on	:	1997-12-05
Resolution	:	2.95 Å(reported)

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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 2.95 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		0.235
Clashscore		15
Ramachandran outliers		0.7%
Sidechain outliers		10.1%
RSRZ outliers		0.4%

Worse .... *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
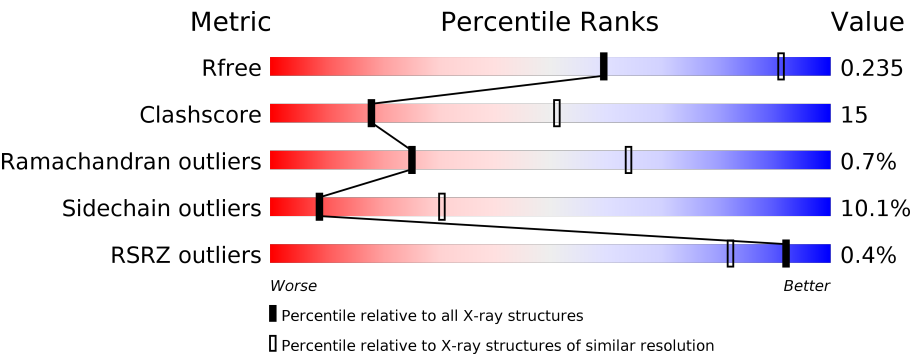
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2395 (3.00-2.92)
Clashscore	112137	2773 (3.00-2.92)
Ramachandran outliers	110173	2680 (3.00-2.92)
Sidechain outliers	110143	2683 (3.00-2.92)
RSRZ outliers	101464	2421 (3.00-2.92)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	128	81% 17% •
1	C	128	80% 16% •
1	E	128	63% 30% 7%
1	G	128	66% 30% 5%
2	B	134	% 31% 19% • 48%
2	D	134	28% 16% 5% 50%

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Mol	Chain	Length	Quality of chain
2	F	134	36% 13% · 49%
2	H	134	% 34% 13% · 50%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 5969 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 CHEY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	128	Total	C	N	O	S	0	0	0
			979	623	162	188	6			
1	C	128	Total	C	N	O	S	0	0	0
			979	623	162	188	6			
1	E	128	Total	C	N	O	S	0	0	0
			979	623	162	188	6			
1	G	128	Total	C	N	O	S	0	0	0
			979	623	162	188	6			

- Molecule 2 is a protein called CHEA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	0	0
			524	329	84	110	1			
2	D	67	Total	C	N	O	S	0	0	0
			505	318	81	105	1			
2	F	69	Total	C	N	O	S	0	0	0
			515	324	83	107	1			
2	H	67	Total	C	N	O	S	0	0	0
			505	318	81	105	1			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	E	1	Total	Mn	0	0
			1	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
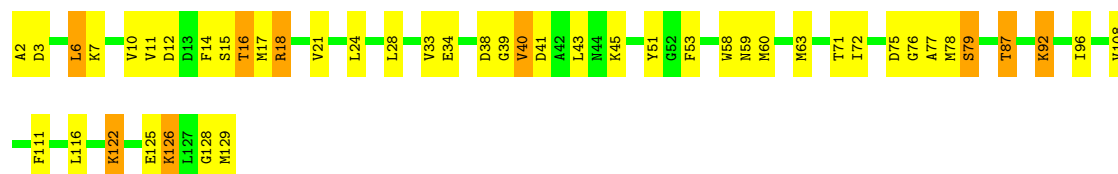
• Molecule 1: CHEY

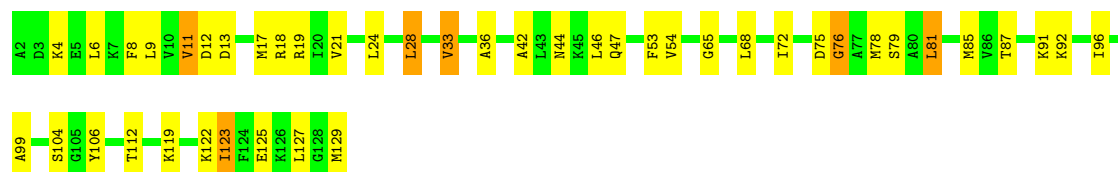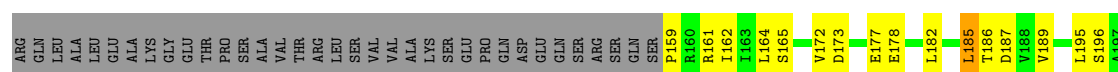Chain A:

• Molecule 1: CHEY

Chain C:

• Molecule 1: CHEY

Chain E:

• Molecule 1: CHEY

Chain G:

• Molecule 2: CHEA

Chain B:

I198 L199 I208 T209 A210 V211 L212 C213 F214 V215 I216 D219 Q220 I221 T225 V226 E227 V228 SER PRO LYS ILE SER THR PRO PRO VAL LEU LYS LEU ALA ALA GLU GLN ALA PRO THR GLY ARG VAL GLU ARG GLU LYS THR THR ARG

● Molecule 2: CHEA

Chain D:

28%   16%   5%   50%

ARG GLN LEU ALA LEU GLU GLU ALA LYS GLY GLU THR PRO SER ALA VAL THR ARG LEU SER VAL VAL ALA LYS SER GLU PRO GLN GLU GLN SER ARG SER GLN SER PRO R160 R161 R166 L167 E171 V172 L175 E176 E177 H181 T184 L185 T186 D187 V188 V189 K190 L195

S196 A197 I198 L199 I208 L212 E217 A218 D219 Q220 I221 T222 F223 E224 T225 V226 GLU VAL SER PRO LYS ILE SER THR PRO PRO VAL LEU LYS LEU ALA ALA GLU GLN ALA PRO THR GLY ARG VAL GLU ARG GLU LYS THR THR ARG

● Molecule 2: CHEA

Chain F:

36%   13%   ·   49%

ARG GLN LEU ALA LEU GLU GLU ALA LYS GLY GLU THR PRO SER ALA VAL THR ARG LEU SER VAL VAL ALA LYS SER GLU GLN PRO GLN ASP GLU GLN SER ARG SER GLN SER P159 R160 R161 I162 I163 L164 S165 R166 L167 V172 L179 D187 A192 S196 A197 I198 D202 E205

D206 V211 L212 C213 T225 V226 E227 VAL SER PRO LYS ILE SER THR PRO PRO VAL LEU LYS LEU ALA ALA GLU GLN ALA PRO THR GLY ARG VAL GLU ARG GLU LYS THR THR ARG

● Molecule 2: CHEA

Chain H:

%
34%   13%   ·   50%

ARG GLN LEU ALA LEU GLU GLU ALA LYS GLY GLU THR PRO SER ALA VAL THR ARG LEU SER VAL VAL ALA LYS SER GLU PRO GLN ASP GLU GLN SER ARG SER GLN SER PRO R160 R161 I162 I163 L164 S165 R166 L167 V172 L182 L195 S196 L199 P200 G201 D202 E205 D206 D207

V211 L212 C213 F214 V215 I216 E217 Q220 I221 T222 F223 E224 T225 V226 GLU VAL SER PRO LYS ILE SER THR PRO PRO VAL LEU LYS LEU ALA ALA GLU GLN ALA PRO THR GLY ARG VAL GLU ARG GLU LYS THR THR ARG

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	53.90Å 156.97Å 65.97Å 90.00° 91.70° 90.00°	Depositor
Resolution (Å)	27.00 – 2.95 26.79 – 2.95	Depositor EDS
% Data completeness (in resolution range)	90.9 (27.00-2.95) 91.0 (26.79-2.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.08 (at 2.94Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , 0.235 0.193 , 0.235	Depositor DCC
R_{free} test set	1073 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 6.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.207 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5969	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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 (i)

5.1 Standard geometry (i)

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

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	0.39	0/991	0.59	0/1332
1	C	0.40	0/991	0.60	0/1332
1	E	0.39	0/991	0.59	0/1332
1	G	0.38	0/991	0.58	0/1332
2	B	0.37	0/527	0.63	1/716 (0.1%)
2	D	0.40	0/508	0.63	0/690
2	F	0.36	0/518	0.68	1/704 (0.1%)
2	H	0.41	0/508	0.66	0/690
All	All	0.39	0/6025	0.61	2/8128 (0.0%)

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
1	E	0	1
1	G	0	1
2	D	0	3
2	F	0	2
2	H	0	1
All	All	0	9

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	159	PRO	N-CA-CB	5.69	110.13	103.30
2	F	159	PRO	N-CA-CB	5.54	109.95	103.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	ARG	Sidechain
2	D	160	ARG	Sidechain
2	D	161	ARG	Sidechain
2	D	166	ARG	Sidechain
1	E	18	ARG	Sidechain
2	F	160	ARG	Sidechain
2	F	166	ARG	Sidechain
1	G	19	ARG	Sidechain
2	H	160	ARG	Sidechain

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	979	0	999	22	0
1	C	979	0	999	19	0
1	E	979	0	999	37	0
1	G	979	0	999	38	0
2	B	524	0	520	16	0
2	D	505	0	510	27	0
2	F	515	0	514	11	0
2	H	505	0	510	17	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
All	All	5969	0	6050	182	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 15.

All (182) 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)
2:D:225:THR:O	2:D:226:VAL:HG12	1.28	1.23
1:E:92:LYS:HD3	1:E:96:ILE:HD11	1.26	1.17
1:E:92:LYS:HD3	1:E:96:ILE:CD1	1.79	1.11
1:C:84:LEU:HD11	1:C:107:VAL:HG12	1.29	1.08
2:D:225:THR:O	2:D:226:VAL:CG1	2.01	1.08
1:G:106:TYR:O	1:G:119:LYS:HE3	1.64	0.97
2:D:185:LEU:N	2:D:185:LEU:HD22	1.79	0.96
2:F:162:ILE:HD13	2:F:164:LEU:HD21	1.44	0.96
1:E:28:LEU:CD1	1:E:116:LEU:HD23	2.06	0.86
1:E:28:LEU:HD11	1:E:116:LEU:HD23	1.56	0.85
1:A:72:ILE:HG12	1:A:78:MET:CE	2.07	0.85
1:C:84:LEU:HD11	1:C:107:VAL:CG1	2.09	0.82
2:F:162:ILE:CD1	2:F:164:LEU:HD21	2.09	0.82
2:D:185:LEU:N	2:D:185:LEU:CD2	2.43	0.81
2:H:182:LEU:HD11	2:H:211:VAL:HG21	1.64	0.80
1:C:7:LYS:HE2	1:C:34:GLU:HG3	1.64	0.78
1:A:72:ILE:HA	1:A:78:MET:CE	2.12	0.78
1:A:6:LEU:HD11	1:A:52:GLY:HA3	1.66	0.78
2:D:190:LYS:HG2	2:D:195:LEU:HD12	1.64	0.77
2:H:160:ARG:NH1	2:H:205:GLU:OE1	2.18	0.76
2:D:186:THR:HB	2:D:198:ILE:HG13	1.68	0.76
1:A:72:ILE:HG12	1:A:78:MET:HE3	1.68	0.75
1:G:75:ASP:OD2	1:G:78:MET:HG2	1.87	0.75
2:D:225:THR:C	2:D:226:VAL:CG1	2.51	0.74
1:G:17:MET:O	1:G:21:VAL:HG23	1.88	0.74
1:G:68:LEU:O	1:G:72:ILE:HG13	1.88	0.74
1:C:84:LEU:CD1	1:C:107:VAL:HG12	2.15	0.72
1:E:24:LEU:O	1:E:28:LEU:HG	1.90	0.71
1:E:92:LYS:HD3	1:E:96:ILE:HD12	1.68	0.71
1:E:58:TRP:HD1	1:E:59:ASN:OD1	1.74	0.70
1:E:92:LYS:CD	1:E:96:ILE:CD1	2.67	0.70
2:F:162:ILE:HD13	2:F:164:LEU:CD2	2.21	0.68
1:A:72:ILE:HG12	1:A:78:MET:HE1	1.73	0.67
2:H:217:GLU:H	2:H:220:GLN:NE2	1.93	0.66
1:E:34:GLU:OE1	1:E:51:TYR:OH	2.10	0.66
2:D:208:ILE:O	2:D:212:LEU:HG	1.96	0.66
1:C:59:ASN:OD1	1:C:59:ASN:N	2.22	0.65
2:D:186:THR:HG22	2:D:187:ASP:N	2.11	0.65
1:G:53:PHE:CE2	1:G:123:ILE:HG21	2.31	0.65
2:D:187:ASP:H	2:D:198:ILE:HG12	1.61	0.65
2:D:171:GLU:O	2:D:175:LEU:HD12	1.97	0.65
2:B:172:VAL:HG23	2:B:195:LEU:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ALA:N	1:E:129:MET:OXT	2.31	0.63
1:C:64:ASP:OD1	1:C:67:GLU:HG3	1.99	0.63
2:D:190:LYS:HG2	2:D:195:LEU:CD1	2.29	0.63
2:B:162:ILE:HB	2:B:199:LEU:HD11	1.80	0.62
1:G:9:LEU:HD23	1:G:46:LEU:HD21	1.79	0.62
2:D:185:LEU:H	2:D:185:LEU:CD2	2.12	0.62
1:G:42:ALA:O	1:G:46:LEU:HG	1.99	0.62
2:H:182:LEU:HD23	2:H:182:LEU:N	2.14	0.62
1:A:7:LYS:HB3	1:A:51:TYR:HA	1.82	0.62
1:C:6:LEU:HD23	1:C:8:PHE:CE1	2.34	0.61
2:B:185:LEU:H	2:B:185:LEU:HD12	1.65	0.61
2:H:182:LEU:HD11	2:H:211:VAL:CG2	2.31	0.60
1:E:17:MET:O	1:E:21:VAL:HG23	2.00	0.60
2:B:164:LEU:HD12	2:B:195:LEU:HD23	1.83	0.60
1:E:92:LYS:CD	1:E:96:ILE:HD12	2.29	0.60
1:G:127:LEU:HD13	1:G:129:MET:HE1	1.84	0.59
1:G:75:ASP:OD1	1:G:76:GLY:N	2.35	0.59
1:E:40:VAL:HG12	1:E:41:ASP:N	2.18	0.59
2:D:219:ASP:C	2:D:219:ASP:OD1	2.42	0.58
1:G:127:LEU:HD13	1:G:129:MET:CE	2.33	0.58
1:G:53:PHE:HE2	1:G:123:ILE:HG21	1.68	0.58
2:D:225:THR:C	2:D:226:VAL:HG13	2.23	0.57
2:H:160:ARG:NH1	2:H:205:GLU:CD	2.58	0.57
1:E:75:ASP:O	1:E:79:SER:HB2	2.05	0.57
1:A:72:ILE:HA	1:A:78:MET:HE2	1.85	0.57
1:E:28:LEU:HD12	1:E:116:LEU:HD23	1.83	0.57
1:G:54:VAL:HG23	1:G:81:LEU:HD12	1.85	0.57
2:B:208:ILE:HG22	2:B:212:LEU:HD22	1.85	0.57
1:G:8:PHE:HB2	1:G:33:VAL:HG13	1.86	0.56
1:E:75:ASP:OD2	1:E:78:MET:CE	2.53	0.56
1:C:7:LYS:HE2	1:C:34:GLU:CG	2.36	0.55
2:D:221:ILE:HD11	2:D:223:PHE:CZ	2.42	0.55
1:G:9:LEU:CD2	1:G:46:LEU:HD21	2.37	0.55
1:G:4:LYS:NZ	1:G:28:LEU:O	2.39	0.55
2:F:179:LEU:HD21	2:F:212:LEU:HD11	1.88	0.55
1:A:6:LEU:HD21	1:A:53:PHE:HB2	1.89	0.54
1:G:75:ASP:O	1:G:79:SER:HB3	2.07	0.54
1:A:53:PHE:HA	1:A:82:PRO:HG2	1.88	0.54
1:G:122:LYS:NZ	1:G:125:GLU:OE2	2.40	0.54
2:B:182:LEU:HD21	2:B:211:VAL:HG21	1.90	0.54
1:G:6:LEU:HD21	1:G:53:PHE:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:184:THR:C	2:D:185:LEU:HD22	2.28	0.54
1:C:67:GLU:O	1:C:71:THR:OG1	2.26	0.53
1:E:75:ASP:OD2	1:E:78:MET:HE3	2.07	0.53
1:G:127:LEU:CD1	1:G:129:MET:HE1	2.38	0.53
2:B:161:ARG:HB2	2:B:198:ILE:HD13	1.90	0.53
1:G:127:LEU:CD1	1:G:129:MET:CE	2.87	0.53
1:A:72:ILE:HG23	1:A:78:MET:HE3	1.90	0.52
1:C:122:LYS:HE2	1:C:122:LYS:HA	1.90	0.52
1:E:14:PHE:HD2	1:E:17:MET:HB2	1.75	0.52
1:A:6:LEU:CD1	1:A:52:GLY:HA3	2.36	0.52
1:E:11:VAL:HG12	1:E:60:MET:SD	2.50	0.52
2:B:209:THR:HG23	2:B:221:ILE:HD12	1.92	0.52
2:F:167:LEU:HD12	2:F:172:VAL:HG22	1.92	0.52
1:A:6:LEU:HD11	1:A:52:GLY:CA	2.38	0.51
2:B:162:ILE:O	2:B:196:SER:HA	2.10	0.51
2:F:187:ASP:HB2	2:F:198:ILE:HD12	1.93	0.51
1:A:126:LYS:O	1:A:127:LEU:HD23	2.11	0.50
1:E:12:ASP:O	1:E:18:ARG:HD3	2.11	0.50
2:H:207:ASP:O	2:H:211:VAL:HG13	2.11	0.50
2:D:167:LEU:HD12	2:D:172:VAL:HG22	1.94	0.50
1:A:85:MET:O	1:A:106:TYR:HA	2.12	0.49
1:A:122:LYS:HD3	1:A:122:LYS:O	2.12	0.49
1:A:89:GLU:CG	1:A:91:LYS:HG2	2.41	0.49
1:A:89:GLU:HG2	1:A:91:LYS:HG2	1.94	0.49
2:B:162:ILE:HB	2:B:199:LEU:CD1	2.42	0.49
2:H:225:THR:O	2:H:226:VAL:HG12	2.11	0.49
1:C:75:ASP:OD1	1:C:77:ALA:N	2.46	0.49
2:B:185:LEU:N	2:B:185:LEU:HD12	2.28	0.48
2:B:213:CYS:HA	2:B:216:ILE:O	2.13	0.48
2:H:167:LEU:HD12	2:H:172:VAL:HG22	1.94	0.48
1:C:7:LYS:HG2	1:C:51:TYR:CD2	2.49	0.48
2:H:217:GLU:HB2	2:H:220:GLN:HE21	1.78	0.48
2:H:162:ILE:HD11	2:H:221:ILE:HG23	1.94	0.47
1:G:12:ASP:HB3	1:G:18:ARG:HG2	1.96	0.47
1:G:99:ALA:HB2	2:H:214:PHE:CZ	2.49	0.47
1:C:11:VAL:HG12	1:C:60:MET:SD	2.54	0.47
1:A:43:LEU:HD21	1:A:71:THR:HG21	1.97	0.47
1:E:111:PHE:CE1	1:E:116:LEU:HD13	2.50	0.47
1:E:38:ASP:HA	1:E:60:MET:SD	2.54	0.47
1:E:122:LYS:HA	1:E:122:LYS:HD3	1.44	0.46
1:A:122:LYS:HE3	2:B:215:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:ASP:O	1:E:6:LEU:HB2	2.16	0.46
1:G:9:LEU:CD2	1:G:46:LEU:CD2	2.94	0.46
1:A:72:ILE:CG1	1:A:78:MET:CE	2.89	0.46
1:C:75:ASP:O	1:C:79:SER:HB3	2.15	0.46
1:G:28:LEU:HD12	1:G:28:LEU:HA	1.75	0.46
2:D:219:ASP:OD1	2:D:220:GLN:N	2.50	0.45
2:F:187:ASP:O	2:F:197:ALA:HA	2.17	0.45
2:F:160:ARG:HD3	2:F:205:GLU:OE2	2.17	0.45
2:H:160:ARG:HH12	2:H:205:GLU:CD	2.18	0.45
1:C:92:LYS:HB3	2:D:181:HIS:O	2.16	0.45
1:G:65:GLY:HA3	1:G:85:MET:HE3	1.99	0.45
1:E:14:PHE:CE2	1:E:16:THR:HB	2.52	0.44
1:A:2:ALA:N	1:A:129:MET:O	2.51	0.44
1:E:76:GLY:O	1:E:77:ALA:HB3	2.17	0.44
2:F:162:ILE:O	2:F:196:SER:HA	2.18	0.44
1:G:68:LEU:HG	1:G:72:ILE:HD11	2.00	0.44
1:G:9:LEU:HD22	1:G:46:LEU:CD2	2.48	0.44
1:E:126:LYS:NZ	2:F:213:CYS:O	2.47	0.43
1:G:4:LYS:HA	1:G:4:LYS:HD3	1.70	0.43
1:C:122:LYS:HE3	1:C:122:LYS:HB2	1.84	0.43
1:C:75:ASP:OD1	1:C:75:ASP:C	2.57	0.43
2:D:217:GLU:H	2:D:220:GLN:NE2	2.16	0.43
1:G:11:VAL:HG13	1:G:36:ALA:HB3	2.00	0.43
2:H:162:ILE:O	2:H:196:SER:HA	2.18	0.43
1:C:124:PHE:O	1:C:128:GLY:N	2.51	0.42
2:D:189:VAL:HG23	2:D:196:SER:OG	2.20	0.42
1:E:43:LEU:HD21	1:E:71:THR:HG21	2.01	0.42
1:G:92:LYS:O	1:G:96:ILE:HG12	2.19	0.42
2:H:212:LEU:HD23	2:H:212:LEU:HA	1.79	0.42
2:H:205:GLU:HG3	2:H:223:PHE:CE2	2.55	0.42
2:D:161:ARG:HH11	2:D:226:VAL:HG11	1.83	0.42
2:B:177:GLU:HG3	2:B:178:GLU:N	2.35	0.42
2:D:189:VAL:CG2	2:D:196:SER:OG	2.68	0.42
1:G:12:ASP:HB3	1:G:18:ARG:CG	2.50	0.41
2:B:219:ASP:OD1	2:B:219:ASP:C	2.58	0.41
1:E:58:TRP:CE3	1:E:87:THR:HG23	2.55	0.41
1:G:122:LYS:HE3	2:H:215:VAL:O	2.21	0.41
1:E:6:LEU:CD1	1:E:53:PHE:HB2	2.51	0.41
1:E:6:LEU:HD11	1:E:53:PHE:HB2	2.02	0.41
1:G:127:LEU:CB	1:G:129:MET:HE3	2.51	0.41
1:E:7:LYS:HB3	1:E:51:TYR:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:LYS:HE3	1:E:125:GLU:OE1	2.21	0.41
1:G:127:LEU:CD1	1:G:129:MET:HE3	2.51	0.41
2:D:186:THR:O	2:D:188:VAL:HG23	2.21	0.41
2:D:198:ILE:O	2:D:198:ILE:HG13	2.21	0.41
1:G:44:ASN:O	1:G:47:GLN:HB2	2.20	0.41
1:E:126:LYS:HB3	1:E:126:LYS:HE2	1.85	0.41
2:F:160:ARG:NH1	2:F:205:GLU:OE2	2.44	0.41
1:E:72:ILE:HG23	1:E:78:MET:HB3	2.03	0.40
1:E:10:VAL:CG2	1:E:33:VAL:CG1	2.99	0.40
1:G:12:ASP:O	1:G:18:ARG:HD3	2.22	0.40
2:B:172:VAL:HG13	2:B:173:ASP:N	2.36	0.40
1:E:39:GLY:HA3	1:E:63:MET:HB3	2.03	0.40
1:G:13:ASP:N	1:G:13:ASP:OD1	2.52	0.40
1:G:92:LYS:HB3	1:G:92:LYS:HE2	1.86	0.40
1:A:11:VAL:HG12	1:A:60:MET:SD	2.61	0.40
1:C:93:GLU:H	1:C:93:GLU:CD	2.24	0.40
2:D:187:ASP:H	2:D:198:ILE:CG1	2.32	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	126/128 (98%)	117 (93%)	9 (7%)	0	100	100
1	C	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
1	E	126/128 (98%)	117 (93%)	7 (6%)	2 (2%)	11	42
1	G	126/128 (98%)	120 (95%)	5 (4%)	1 (1%)	22	61
2	B	68/134 (51%)	64 (94%)	4 (6%)	0	100	100
2	D	65/134 (48%)	59 (91%)	6 (9%)	0	100	100
2	F	67/134 (50%)	59 (88%)	6 (9%)	2 (3%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	65/134 (48%)	57 (88%)	8 (12%)	0	100	100
All	All	769/1048 (73%)	713 (93%)	51 (7%)	5 (1%)	25	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	79	SER
2	F	192	ALA
1	E	128	GLY
1	G	76	GLY
2	F	202	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	102/102 (100%)	98 (96%)	4 (4%)	37	73
1	C	102/102 (100%)	92 (90%)	10 (10%)	9	32
1	E	102/102 (100%)	92 (90%)	10 (10%)	9	32
1	G	102/102 (100%)	92 (90%)	10 (10%)	9	32
2	B	57/115 (50%)	48 (84%)	9 (16%)	3	12
2	D	56/115 (49%)	48 (86%)	8 (14%)	4	16
2	F	56/115 (49%)	50 (89%)	6 (11%)	8	27
2	H	56/115 (49%)	49 (88%)	7 (12%)	5	20
All	All	633/868 (73%)	569 (90%)	64 (10%)	9	30

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	47	GLN
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	91	LYS
2	B	165	SER
2	B	185	LEU
2	B	186	THR
2	B	187	ASP
2	B	189	VAL
2	B	212	LEU
2	B	219	ASP
2	B	225	THR
2	B	226	VAL
1	C	16	THR
1	C	37	GLU
1	C	57	ASP
1	C	59	ASN
1	C	71	THR
1	C	81	LEU
1	C	92	LYS
1	C	107	VAL
1	C	112	THR
1	C	122	LYS
2	D	177	GLU
2	D	184	THR
2	D	185	LEU
2	D	188	VAL
2	D	189	VAL
2	D	199	LEU
2	D	225	THR
2	D	226	VAL
1	E	6	LEU
1	E	15	SER
1	E	16	THR
1	E	40	VAL
1	E	45	LYS
1	E	87	THR
1	E	92	LYS
1	E	108	VAL
1	E	122	LYS
1	E	126	LYS
2	F	162	ILE
2	F	165	SER
2	F	166	ARG
2	F	206	ASP

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Mol	Chain	Res	Type
2	F	211	VAL
2	F	225	THR
1	G	11	VAL
1	G	24	LEU
1	G	28	LEU
1	G	33	VAL
1	G	81	LEU
1	G	87	THR
1	G	91	LYS
1	G	104	SER
1	G	112	THR
1	G	123	ILE
2	H	163	ILE
2	H	165	SER
2	H	195	LEU
2	H	199	LEU
2	H	205	GLU
2	H	211	VAL
2	H	226	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	32	ASN
1	A	94	ASN
2	B	220	GLN
1	C	47	GLN
2	D	220	GLN
1	E	121	ASN
2	H	220	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	128/128 (100%)	-0.76	0	100	100	8, 23, 53, 88	0
1	C	128/128 (100%)	-0.79	0	100	100	8, 24, 53, 68	0
1	E	128/128 (100%)	-0.64	0	100	100	8, 24, 60, 80	0
1	G	128/128 (100%)	-0.70	0	100	100	9, 22, 59, 82	0
2	B	70/134 (52%)	-0.31	1 (1%)	75	58	17, 40, 81, 117	0
2	D	67/134 (50%)	-0.56	0	100	100	15, 38, 65, 101	0
2	F	69/134 (51%)	-0.41	0	100	100	16, 44, 82, 107	0
2	H	67/134 (50%)	-0.57	2 (2%)	51	32	13, 38, 74, 95	0
All	All	785/1048 (74%)	-0.63	3 (0%)	92	82	8, 28, 68, 117	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	228	VAL	4.5
2	H	201	GLY	2.7
2	H	202	ASP	2.2

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
3	MN	A	130	1/1	0.96	0.10	-1.64	28,28,28,28	0
3	MN	E	130	1/1	0.97	0.09	-1.84	25,25,25,25	0
3	MN	C	1	1/1	0.96	0.06	-2.20	28,28,28,28	0
3	MN	G	130	1/1	0.97	0.07	-	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.