Full wwPDB X-ray Structure Validation Report ⓘ

Aug 31, 2020 – 08:23 AM BST

PDB ID	:	1AHJ
Title	:	NITRILE HYDRATASE
Authors	:	Huang, W.; Schneider, G.; Lindqvist, Y.
Deposited on	:	1997-04-05
Resolution	:	2.65 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 following versions of software and data (see references ①) were used in the production of this report:

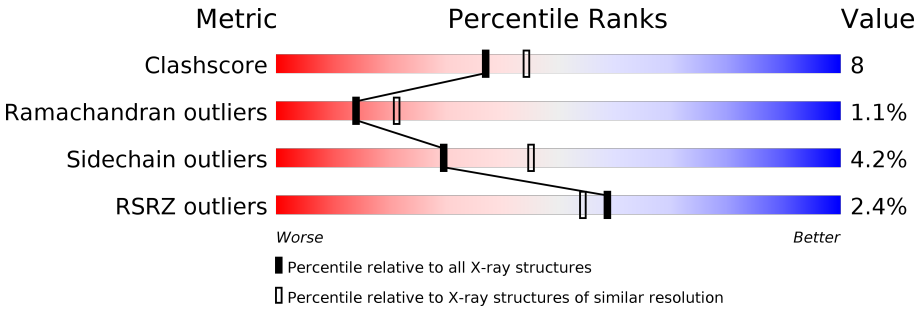
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



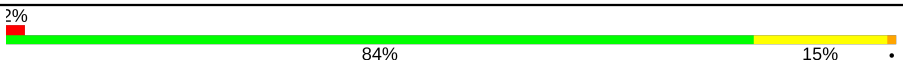
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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	207	3% 72% 22%
1	C	207	4% 74% 21%
1	E	207	2% 67% 27%
1	G	207	4% 74% 21%
2	B	212	% 81% 18%
2	D	212	81% 18%
2	F	212	2% 79% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	212	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12832 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 NITRILE HYDRATASE (SUBUNIT ALPHA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1550	988	261	295	6			
1	C	198	Total	C	N	O	S	0	0	0
			1550	988	261	295	6			
1	E	198	Total	C	N	O	S	0	0	0
			1550	988	261	295	6			
1	G	198	Total	C	N	O	S	0	0	0
			1550	988	261	295	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	PRO	CONFLICT	UNP P13448
C	18	ALA	PRO	CONFLICT	UNP P13448
E	18	ALA	PRO	CONFLICT	UNP P13448
G	18	ALA	PRO	CONFLICT	UNP P13448

- Molecule 2 is a protein called NITRILE HYDRATASE (SUBUNIT BETA).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	212	Total	C	N	O	S	0	0	0
			1657	1050	282	317	8			
2	D	212	Total	C	N	O	S	0	0	0
			1657	1050	282	317	8			
2	F	212	Total	C	N	O	S	0	0	0
			1657	1050	282	317	8			
2	H	212	Total	C	N	O	S	0	0	0
			1657	1050	282	317	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	ASN	CONFLICT	UNP P13449
D	21	ASP	ASN	CONFLICT	UNP P13449
F	21	ASP	ASN	CONFLICT	UNP P13449
H	21	ASP	ASN	CONFLICT	UNP P13449

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

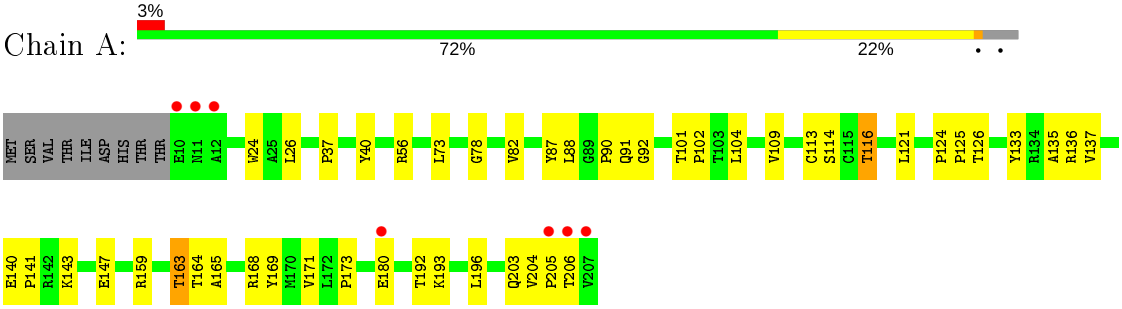
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	C	1	Total Fe 1 1	0	0
3	E	1	Total Fe 1 1	0	0

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.

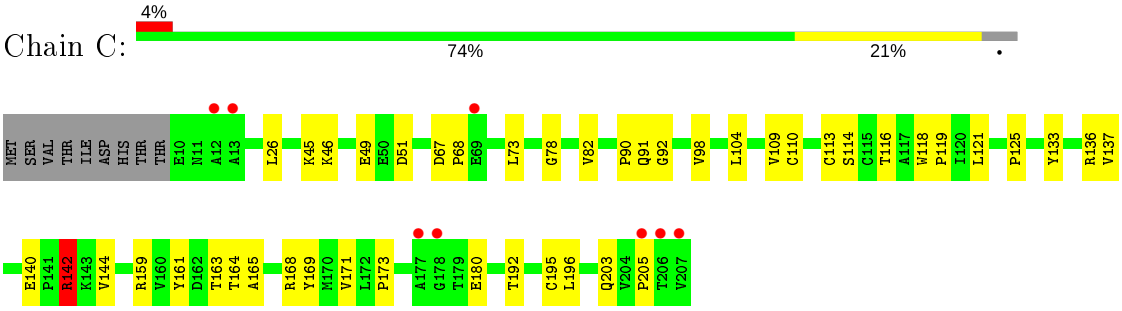
- Molecule 1: NITRILE HYDRATASE (SUBUNIT ALPHA)

Chain A:



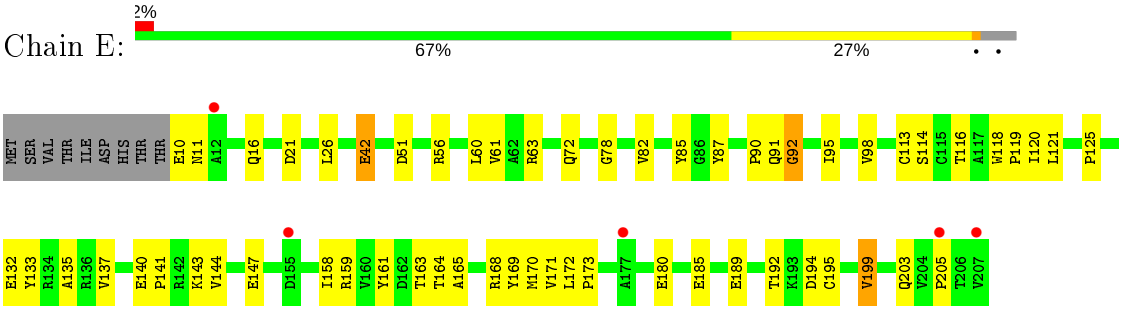
- Molecule 1: NITRILE HYDRATASE (SUBUNIT ALPHA)

Chain C:



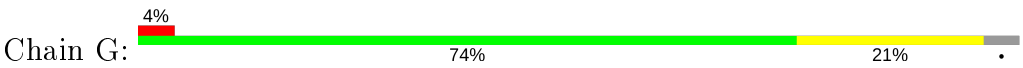
- Molecule 1: NITRILE HYDRATASE (SUBUNIT ALPHA)

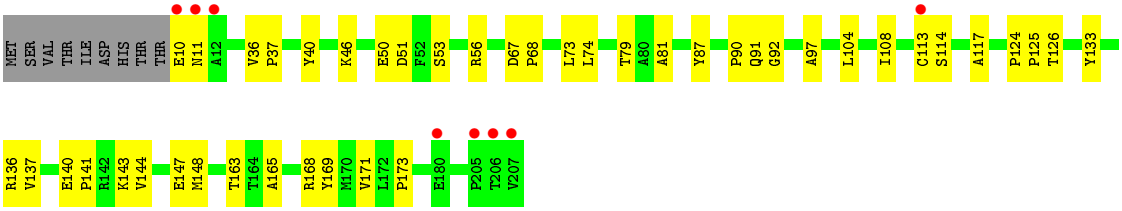
Chain E:



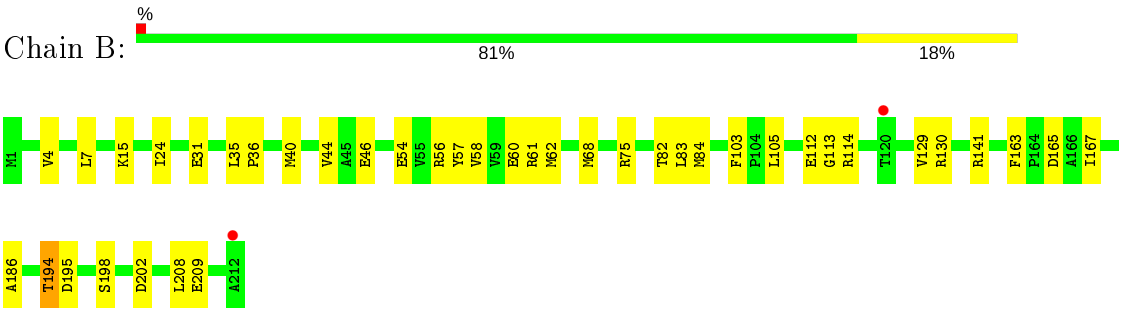
- Molecule 1: NITRILE HYDRATASE (SUBUNIT ALPHA)

Chain G:

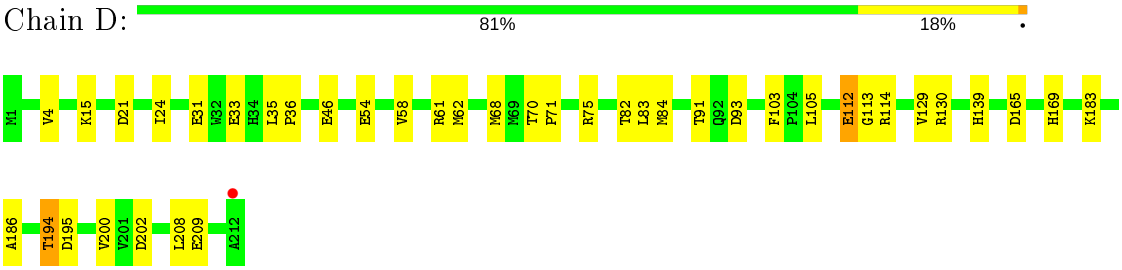




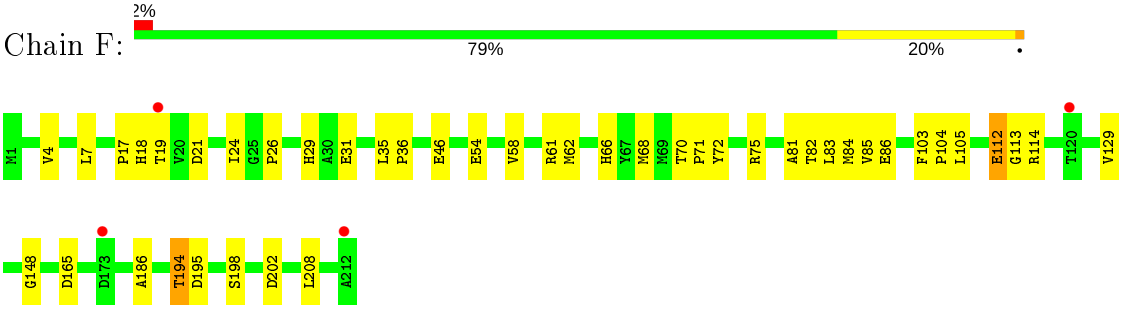
• Molecule 2: NITRILE HYDRATASE (SUBUNIT BETA)



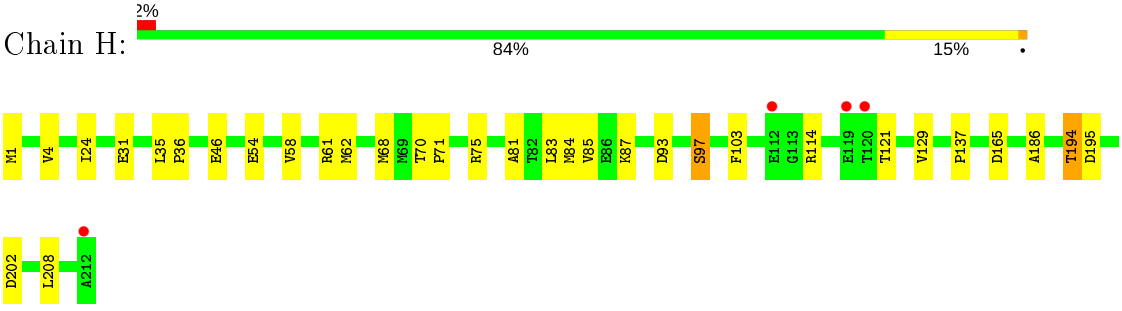
• Molecule 2: NITRILE HYDRATASE (SUBUNIT BETA)



• Molecule 2: NITRILE HYDRATASE (SUBUNIT BETA)



• Molecule 2: NITRILE HYDRATASE (SUBUNIT BETA)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.85Å 144.24Å 159.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 2.65 29.01 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.0 (7.50-2.65) 87.9 (29.01-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.43 (at 2.64Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.264 , 0.289 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.544	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12832	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FE

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	0.36	0/1588	0.58	0/2168
1	C	0.36	0/1588	0.61	1/2168 (0.0%)
1	E	0.37	0/1588	0.58	0/2168
1	G	0.37	0/1588	0.57	0/2168
2	B	0.37	0/1705	0.58	0/2318
2	D	0.37	0/1705	0.58	0/2318
2	F	0.36	0/1705	0.58	0/2318
2	H	0.36	0/1705	0.59	0/2318
All	All	0.37	0/13172	0.58	1/17944 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	142	ARG	NE-CZ-NH1	5.10	122.85	120.30

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	1550	0	1523	29	0
1	C	1550	0	1522	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1550	0	1522	33	0
1	G	1550	0	1522	31	0
2	B	1657	0	1570	28	0
2	D	1657	0	1570	27	0
2	F	1657	0	1570	27	0
2	H	1657	0	1570	19	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	12832	0	12369	197	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 8.

All (197) 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:E:192:THR:HG22	1:E:195:CYS:SG	2.00	1.00
1:C:192:THR:HG22	1:C:195:CYS:SG	2.22	0.80
2:B:58:VAL:HG21	2:B:83:LEU:HG	1.65	0.78
2:F:129:VAL:HG11	2:F:208:LEU:HB3	1.66	0.77
2:H:186:ALA:HB1	2:H:194:THR:HG21	1.67	0.77
1:E:91:GLN:HE22	1:E:168:ARG:HH21	1.31	0.76
1:E:192:THR:CG2	1:E:195:CYS:SG	2.75	0.74
2:H:58:VAL:HG21	2:H:83:LEU:HG	1.68	0.74
1:G:91:GLN:HE22	1:G:168:ARG:HH21	1.34	0.74
2:F:58:VAL:HG21	2:F:83:LEU:HG	1.71	0.73
2:D:58:VAL:HG21	2:D:83:LEU:HG	1.71	0.73
2:D:186:ALA:HB1	2:D:194:THR:HG21	1.71	0.71
1:A:121:LEU:HD22	1:A:196:LEU:HB3	1.73	0.71
1:A:171:VAL:O	1:A:173:PRO:HD3	1.93	0.68
1:C:171:VAL:O	1:C:173:PRO:HD3	1.93	0.68
1:A:104:LEU:HD21	1:A:159:ARG:HD3	1.74	0.68
2:D:129:VAL:HG11	2:D:208:LEU:HB3	1.75	0.67
1:G:143:LYS:O	1:G:147:GLU:HG3	1.96	0.66
1:G:171:VAL:O	1:G:173:PRO:HD3	1.95	0.66
2:B:186:ALA:HB1	2:B:194:THR:HG21	1.77	0.66
2:F:186:ALA:HB1	2:F:194:THR:HG21	1.79	0.65
2:B:54:GLU:O	2:B:58:VAL:HG23	1.98	0.64
1:E:171:VAL:O	1:E:173:PRO:HD3	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:VAL:HG11	2:H:208:LEU:HB3	1.80	0.63
1:E:63:ARG:HD3	1:E:85:TYR:OH	1.99	0.63
2:B:129:VAL:HG11	2:B:208:LEU:HB3	1.81	0.62
2:F:129:VAL:CG1	2:F:208:LEU:HB3	2.30	0.61
2:F:58:VAL:HG22	2:F:61:ARG:NH1	2.15	0.61
1:C:165:ALA:HB3	2:D:202:ASP:OD2	2.01	0.61
1:C:142:ARG:HH11	1:C:142:ARG:HB2	1.65	0.61
1:A:91:GLN:HE22	1:A:168:ARG:HH21	1.48	0.61
1:A:159:ARG:HG2	2:B:198:SER:OG	2.01	0.60
2:B:4:VAL:HG11	2:B:68:MET:SD	2.41	0.60
1:C:91:GLN:HE22	1:C:168:ARG:HH21	1.49	0.60
2:D:54:GLU:O	2:D:58:VAL:HG23	2.02	0.60
2:H:4:VAL:HG11	2:H:68:MET:SD	2.41	0.60
2:H:54:GLU:O	2:H:58:VAL:HG23	2.03	0.59
2:B:114:ARG:HB3	2:B:165:ASP:HB3	1.84	0.59
1:C:133:TYR:CE2	1:C:137:VAL:HG21	2.38	0.59
1:G:163:THR:HG22	1:G:169:TYR:HD2	1.68	0.59
1:E:10:GLU:HG2	1:E:11:ASN:OD1	2.02	0.58
1:E:203:GLN:O	1:E:205:PRO:HD3	2.02	0.58
1:C:121:LEU:HD22	1:C:196:LEU:HB3	1.86	0.58
1:A:137:VAL:O	1:A:141:PRO:HG3	2.04	0.57
1:G:56:ARG:HD2	1:G:87:TYR:CE1	2.39	0.57
2:F:114:ARG:HB3	2:F:165:ASP:HB3	1.87	0.57
1:G:133:TYR:CE1	1:G:137:VAL:HG21	2.41	0.56
2:H:62:MET:SD	2:H:75:ARG:HG2	2.46	0.55
1:G:144:VAL:HG12	1:G:148:MET:CE	2.37	0.55
1:E:194:ASP:HB3	1:E:199:VAL:HG12	1.87	0.55
1:A:136:ARG:HH21	2:B:15:LYS:HA	1.71	0.55
2:F:54:GLU:O	2:F:58:VAL:HG23	2.06	0.55
2:H:58:VAL:HG22	2:H:61:ARG:NH1	2.22	0.54
2:H:58:VAL:HG21	2:H:83:LEU:CG	2.37	0.54
1:A:101:THR:HB	1:A:102:PRO:HD2	1.90	0.54
2:D:4:VAL:HG11	2:D:68:MET:SD	2.48	0.54
1:E:165:ALA:HB3	2:F:202:ASP:OD2	2.08	0.53
1:C:98:VAL:HG11	1:C:161:TYR:CE2	2.44	0.53
2:D:58:VAL:HG21	2:D:83:LEU:CG	2.37	0.53
2:D:129:VAL:HG13	2:D:209:GLU:O	2.09	0.53
1:G:91:GLN:HE22	1:G:168:ARG:NH2	2.05	0.53
2:F:58:VAL:HG21	2:F:83:LEU:CG	2.37	0.53
2:B:58:VAL:HG21	2:B:83:LEU:CG	2.37	0.52
2:F:82:THR:OG1	2:F:105:LEU:HB3	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:ASP:O	2:H:97:SER:HB3	2.10	0.52
2:D:58:VAL:HG22	2:D:61:ARG:NH1	2.25	0.52
1:E:133:TYR:CE1	1:E:137:VAL:HG21	2.45	0.52
1:C:45:LYS:HG2	1:C:49:GLU:OE1	2.10	0.51
1:G:125:PRO:HB3	2:H:24:ILE:HD13	1.92	0.51
1:C:142:ARG:HB3	2:D:195:ASP:OD2	2.10	0.51
2:D:62:MET:SD	2:D:75:ARG:HG2	2.51	0.51
1:A:125:PRO:HB3	2:B:24:ILE:HD13	1.91	0.51
1:A:192:THR:HG22	1:A:193:LYS:H	1.76	0.51
2:D:129:VAL:CG1	2:D:208:LEU:HB3	2.41	0.51
1:E:56:ARG:HH21	1:E:87:TYR:HA	1.75	0.51
2:F:35:LEU:N	2:F:36:PRO:HD2	2.26	0.51
1:E:143:LYS:O	1:E:147:GLU:HG3	2.11	0.50
1:E:140:GLU:O	1:E:144:VAL:HG23	2.12	0.50
1:C:137:VAL:HG22	1:C:144:VAL:HG11	1.94	0.50
1:E:140:GLU:HA	2:F:195:ASP:HB3	1.93	0.50
1:E:78:GLY:O	1:E:82:VAL:HG23	2.10	0.50
1:C:125:PRO:HB3	2:D:24:ILE:HD13	1.94	0.50
2:H:114:ARG:HB3	2:H:165:ASP:HB3	1.94	0.50
1:A:204:VAL:O	1:A:204:VAL:HG23	2.10	0.50
1:E:192:THR:HG21	2:F:21:ASP:OD1	2.12	0.50
2:F:4:VAL:HG11	2:F:68:MET:SD	2.51	0.49
2:F:62:MET:SD	2:F:75:ARG:HG2	2.53	0.49
1:A:165:ALA:HB3	2:B:202:ASP:OD2	2.13	0.49
1:E:125:PRO:HB3	2:F:24:ILE:HD13	1.95	0.49
1:E:163:THR:HG22	1:E:169:TYR:CD2	2.48	0.49
1:E:16:GLN:OE1	2:F:66:HIS:NE2	2.46	0.49
2:B:82:THR:OG1	2:B:105:LEU:HB3	2.12	0.49
1:A:203:GLN:O	1:A:205:PRO:HD3	2.13	0.49
2:H:1:MET:HB2	2:H:137:PRO:O	2.12	0.49
1:G:165:ALA:HB3	2:H:202:ASP:OD2	2.12	0.49
2:H:35:LEU:N	2:H:36:PRO:HD2	2.28	0.48
2:B:129:VAL:CG1	2:B:208:LEU:HB3	2.41	0.48
1:A:56:ARG:HG2	1:A:87:TYR:CZ	2.48	0.48
1:G:133:TYR:O	1:G:137:VAL:HG23	2.13	0.48
2:F:72:TYR:O	2:F:75:ARG:HB2	2.14	0.48
1:G:108:ILE:HD11	1:G:171:VAL:HG23	1.96	0.48
1:A:133:TYR:O	1:A:137:VAL:HG12	2.14	0.47
1:G:91:GLN:NE2	1:G:168:ARG:HH21	2.08	0.47
1:E:163:THR:HG22	1:E:169:TYR:HD2	1.79	0.47
1:A:140:GLU:HA	2:B:195:ASP:HB3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:VAL:HG12	1:G:148:MET:HE2	1.97	0.47
1:G:163:THR:HG22	1:G:169:TYR:CD2	2.50	0.47
2:B:62:MET:SD	2:B:75:ARG:HG2	2.55	0.47
1:C:161:TYR:CD1	2:D:200:VAL:HB	2.50	0.47
1:C:133:TYR:CZ	1:C:137:VAL:HG21	2.50	0.46
2:B:40:MET:O	2:B:44:VAL:HG23	2.14	0.46
1:C:140:GLU:O	1:C:144:VAL:HG23	2.14	0.46
1:G:37:PRO:HB2	1:G:40:TYR:HB2	1.96	0.46
1:E:141:PRO:HB2	1:E:158:ILE:HG21	1.98	0.46
1:G:140:GLU:HA	2:H:195:ASP:HB3	1.97	0.46
1:G:140:GLU:O	1:G:144:VAL:HG23	2.16	0.46
2:F:112:GLU:HG2	2:F:113:GLY:N	2.31	0.45
1:A:109:VAL:HG21	1:A:137:VAL:CG1	2.46	0.45
1:A:163:THR:HG23	1:A:169:TYR:HD2	1.81	0.45
1:C:192:THR:CG2	1:C:195:CYS:SG	2.99	0.45
1:A:135:ALA:HB2	2:B:7:LEU:HB3	1.98	0.45
1:G:133:TYR:CZ	1:G:137:VAL:HG21	2.52	0.45
1:A:109:VAL:HG21	1:A:137:VAL:HG13	1.99	0.45
2:B:112:GLU:HG2	2:B:113:GLY:N	2.32	0.45
2:F:17:PRO:O	2:F:18:HIS:HB2	2.16	0.45
2:F:81:ALA:O	2:F:85:VAL:HG23	2.17	0.45
1:G:46:LYS:HD3	1:G:50:GLU:OE2	2.17	0.44
2:B:35:LEU:N	2:B:36:PRO:HD2	2.32	0.44
2:H:129:VAL:CG1	2:H:208:LEU:HB3	2.47	0.44
1:A:143:LYS:O	1:A:147:GLU:HG3	2.16	0.44
1:C:78:GLY:O	1:C:82:VAL:HG23	2.16	0.44
1:E:61:VAL:HG13	1:E:172:LEU:HD22	1.99	0.44
1:G:137:VAL:O	1:G:141:PRO:HG3	2.17	0.44
1:C:142:ARG:HB3	2:D:195:ASP:CG	2.37	0.44
1:C:109:VAL:HG12	1:C:110:CYS:N	2.33	0.44
1:C:163:THR:HG22	1:C:169:TYR:HD1	1.83	0.44
1:E:159:ARG:HG2	2:F:198:SER:OG	2.18	0.44
2:F:82:THR:O	2:F:86:GLU:HG3	2.18	0.44
1:G:137:VAL:HG22	1:G:144:VAL:HG11	2.00	0.44
1:A:136:ARG:NH2	2:B:15:LYS:HA	2.31	0.44
2:B:141:ARG:HA	2:B:141:ARG:HD2	1.85	0.44
1:A:116:THR:HG21	1:A:124:PRO:HB3	1.98	0.43
2:D:112:GLU:HG2	2:D:113:GLY:N	2.33	0.43
1:G:73:LEU:HG	1:G:81:ALA:HB2	2.00	0.43
2:D:114:ARG:HB3	2:D:165:ASP:HB3	2.00	0.43
1:C:192:THR:HG21	2:D:21:ASP:OD1	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:81:ALA:O	2:H:85:VAL:HG23	2.17	0.43
2:B:57:TYR:CE2	2:B:61:ARG:HD2	2.53	0.43
1:A:78:GLY:O	1:A:82:VAL:HG23	2.18	0.43
1:A:56:ARG:HG2	1:A:87:TYR:CE1	2.53	0.43
2:B:129:VAL:HG13	2:B:209:GLU:O	2.18	0.43
1:E:121:LEU:HD11	1:E:170:MET:HG3	2.01	0.43
1:C:118:TRP:N	1:C:119:PRO:HD2	2.34	0.43
2:D:35:LEU:N	2:D:36:PRO:HD2	2.34	0.43
1:G:36:VAL:HA	1:G:37:PRO:HD3	1.87	0.43
2:H:70:THR:HA	2:H:71:PRO:HD3	1.86	0.43
1:C:159:ARG:HH11	2:D:183:LYS:HE2	1.84	0.43
1:E:185:GLU:CD	1:E:185:GLU:N	2.72	0.43
1:G:67:ASP:HA	1:G:68:PRO:HD2	1.90	0.43
2:D:82:THR:OG1	2:D:105:LEU:HB3	2.19	0.42
2:D:139:HIS:H	2:D:169:HIS:HE1	1.67	0.42
1:A:88:LEU:HD23	1:A:88:LEU:HA	1.88	0.42
1:E:92:GLY:O	1:E:95:ILE:HD11	2.19	0.42
1:G:74:LEU:HD22	1:G:97:ALA:HB2	2.01	0.42
2:B:58:VAL:HG22	2:B:61:ARG:NH1	2.34	0.42
2:H:83:LEU:O	2:H:87:LYS:HG2	2.19	0.42
1:A:37:PRO:HB2	1:A:40:TYR:HB2	2.02	0.42
2:D:91:THR:HG22	2:D:93:ASP:H	1.84	0.42
1:E:16:GLN:HG2	2:F:104:PRO:HG3	2.01	0.42
1:G:136:ARG:HH22	1:G:147:GLU:CD	2.22	0.42
1:C:163:THR:HG22	1:C:169:TYR:CD1	2.55	0.42
1:C:140:GLU:HA	2:D:195:ASP:HB3	2.01	0.42
1:C:136:ARG:NH2	2:D:15:LYS:HA	2.35	0.42
2:D:70:THR:HA	2:D:71:PRO:HD3	1.85	0.42
1:A:192:THR:HG22	1:A:193:LYS:N	2.35	0.41
1:G:53:SER:O	1:G:56:ARG:HG3	2.19	0.41
1:A:24:TRP:CZ3	2:B:35:LEU:HD11	2.55	0.41
1:C:163:THR:CG2	1:C:169:TYR:HD1	2.33	0.41
1:G:10:GLU:HB3	1:G:11:ASN:H	1.76	0.41
2:F:26:PRO:HD2	2:F:29:HIS:CE1	2.56	0.41
1:C:67:ASP:HA	1:C:68:PRO:HD2	1.87	0.41
2:D:130:ARG:O	2:D:209:GLU:HG2	2.21	0.41
1:G:124:PRO:HA	1:G:125:PRO:HD3	1.70	0.41
1:C:142:ARG:CB	1:C:142:ARG:HH11	2.31	0.41
2:B:56:ARG:O	2:B:60:GLU:HG3	2.20	0.41
1:C:203:GLN:O	1:C:205:PRO:HD3	2.20	0.41
1:E:120:ILE:HG22	1:E:121:LEU:HD12	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:VAL:HG11	1:E:161:TYR:CZ	2.56	0.41
1:E:135:ALA:HB2	2:F:7:LEU:HB3	2.03	0.41
1:G:117:ALA:HB2	1:G:168:ARG:HB3	2.02	0.41
1:C:98:VAL:HG11	1:C:161:TYR:CZ	2.56	0.40
1:E:42:GLU:HG2	1:E:42:GLU:H	1.62	0.40
2:B:130:ARG:O	2:B:209:GLU:HG2	2.21	0.40
2:B:163:PHE:O	2:B:167:ILE:HG22	2.21	0.40
1:E:118:TRP:N	1:E:119:PRO:HD2	2.37	0.40
1:E:60:LEU:HD21	1:E:82:VAL:HG22	2.03	0.40
2:F:70:THR:HA	2:F:71:PRO:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	196/207 (95%)	184 (94%)	8 (4%)	4 (2%)	7	10
1	C	196/207 (95%)	184 (94%)	8 (4%)	4 (2%)	7	10
1	E	196/207 (95%)	180 (92%)	12 (6%)	4 (2%)	7	10
1	G	196/207 (95%)	183 (93%)	9 (5%)	4 (2%)	7	10
2	B	210/212 (99%)	196 (93%)	14 (7%)	0	100	100
2	D	210/212 (99%)	199 (95%)	10 (5%)	1 (0%)	29	43
2	F	210/212 (99%)	196 (93%)	13 (6%)	1 (0%)	29	43
2	H	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
All	All	1624/1676 (97%)	1519 (94%)	87 (5%)	18 (1%)	14	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	33	GLU
1	A	113	CYS
1	A	114	SER
1	C	113	CYS
1	E	113	CYS
1	E	114	SER
1	G	113	CYS
1	G	114	SER
1	C	114	SER
1	A	90	PRO
1	C	90	PRO
1	G	90	PRO
1	E	90	PRO
1	C	92	GLY
1	A	92	GLY
1	E	92	GLY
1	G	92	GLY
2	F	148	GLY

5.3.2 Protein sidechains (i)

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	163/172 (95%)	155 (95%)	8 (5%)	25	38
1	C	163/172 (95%)	154 (94%)	9 (6%)	21	33
1	E	163/172 (95%)	152 (93%)	11 (7%)	16	25
1	G	163/172 (95%)	159 (98%)	4 (2%)	47	66
2	B	173/173 (100%)	168 (97%)	5 (3%)	42	60
2	D	173/173 (100%)	167 (96%)	6 (4%)	36	52
2	F	173/173 (100%)	166 (96%)	7 (4%)	31	47
2	H	173/173 (100%)	166 (96%)	7 (4%)	31	47
All	All	1344/1380 (97%)	1287 (96%)	57 (4%)	30	45

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	73	LEU
1	A	116	THR
1	A	126	THR
1	A	163	THR
1	A	164	THR
1	A	180	GLU
1	A	206	THR
2	B	31	GLU
2	B	46	GLU
2	B	84	MET
2	B	103	PHE
2	B	194	THR
1	C	26	LEU
1	C	46	LYS
1	C	51	ASP
1	C	73	LEU
1	C	104	LEU
1	C	116	THR
1	C	142	ARG
1	C	164	THR
1	C	180	GLU
2	D	31	GLU
2	D	46	GLU
2	D	84	MET
2	D	103	PHE
2	D	112	GLU
2	D	194	THR
1	E	21	ASP
1	E	26	LEU
1	E	42	GLU
1	E	51	ASP
1	E	72	GLN
1	E	116	THR
1	E	132	GLU
1	E	164	THR
1	E	180	GLU
1	E	189	GLU
1	E	199	VAL
2	F	19	THR
2	F	31	GLU
2	F	46	GLU
2	F	84	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	103	PHE
2	F	112	GLU
2	F	194	THR
1	G	51	ASP
1	G	79	THR
1	G	104	LEU
1	G	126	THR
2	H	31	GLU
2	H	46	GLU
2	H	84	MET
2	H	97	SER
2	H	103	PHE
2	H	121	THR
2	H	194	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	C	91	GLN
1	C	203	GLN
1	E	72	GLN
1	E	91	GLN
2	F	18	HIS
2	F	29	HIS
1	G	91	GLN
2	H	29	HIS

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

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, 95^{th} 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	198/207 (95%)	-0.13	7 (3%)	44	40	2, 20, 50, 77	0
1	C	198/207 (95%)	0.07	8 (4%)	38	34	5, 26, 55, 73	0
1	E	198/207 (95%)	0.09	5 (2%)	57	53	12, 29, 55, 74	0
1	G	198/207 (95%)	-0.18	8 (4%)	38	34	2, 20, 45, 77	0
2	B	212/212 (100%)	-0.30	2 (0%)	84	83	2, 21, 41, 73	0
2	D	212/212 (100%)	-0.36	1 (0%)	91	91	3, 20, 43, 70	0
2	F	212/212 (100%)	-0.30	4 (1%)	66	63	3, 22, 45, 69	0
2	H	212/212 (100%)	-0.32	4 (1%)	66	63	3, 20, 42, 69	0
All	All	1640/1676 (97%)	-0.18	39 (2%)	59	54	2, 22, 49, 77	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	207	VAL	9.1
1	G	207	VAL	7.6
1	E	207	VAL	7.1
1	A	205	PRO	6.9
2	B	212	ALA	5.7
1	A	207	VAL	5.5
2	F	212	ALA	4.9
1	A	206	THR	4.6
1	C	205	PRO	4.6
1	A	12	ALA	4.3
1	C	177	ALA	4.0
1	E	12	ALA	3.9
1	C	206	THR	3.8
2	F	120	THR	3.6
2	H	212	ALA	3.6
2	H	119	GLU	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	205	PRO	3.5
2	D	212	ALA	3.3
1	A	180	GLU	3.1
1	G	206	THR	3.0
1	G	12	ALA	3.0
1	E	177	ALA	3.0
1	G	180	GLU	2.7
1	G	10	GLU	2.7
2	B	120	THR	2.7
1	C	13	ALA	2.6
1	G	11	ASN	2.6
1	C	178	GLY	2.6
2	F	173	ASP	2.6
2	F	19	THR	2.5
1	E	155	ASP	2.4
1	C	69	GLU	2.4
1	A	10	GLU	2.4
1	A	11	ASN	2.3
1	C	12	ALA	2.3
2	H	120	THR	2.2
1	G	113	CYS	2.2
2	H	112	GLU	2.1
1	G	205	PRO	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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, 95^{th} 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE	G	208	1/1	0.94	0.20	19,19,19,19	0
3	FE	A	208	1/1	0.96	0.17	19,19,19,19	0
3	FE	C	208	1/1	0.97	0.15	19,19,19,19	0
3	FE	E	208	1/1	0.98	0.11	19,19,19,19	0

6.5 Other polymers (i)

There are no such residues in this entry.