Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 01:07 PM EST

PDB ID	:	1OQU
Title	:	A protein coordinated tri-nuclear Fe complex formed during soaking of crystals of the ribonucleotide reductase R2F protein from Corynebacterium Ammoniagenes
Authors	:	Hogbom, M.; Nordlund, P.
Deposited on	:	2003-03-11
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

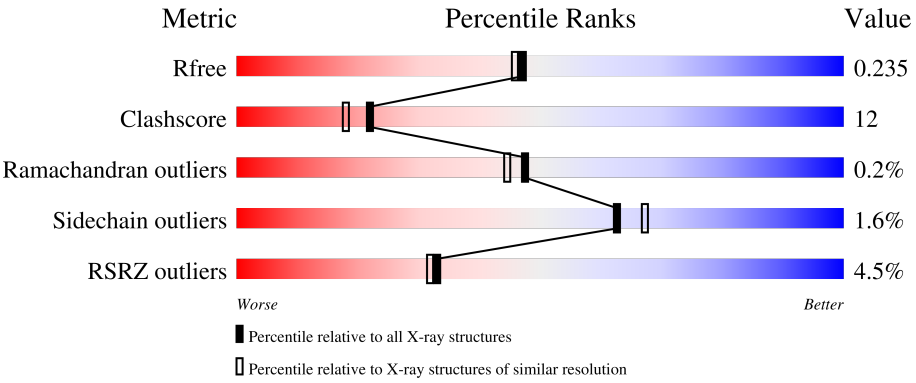
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	329	2% 73% 17% 10%
1	B	329	7% 66% 23% • 10%
1	C	329	3% 73% 18% • 8%
1	D	329	4% 73% 16% • 10%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10489 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.

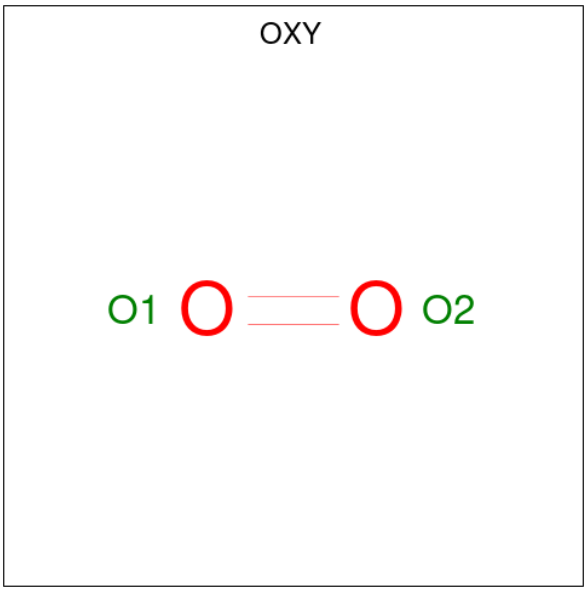
- Molecule 1 is a protein called ribonucleotide reductase subunit R2F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2419	1550	383	478	8			
1	B	296	Total	C	N	O	S	0	0	0
			2419	1550	383	478	8			
1	C	302	Total	C	N	O	S	0	0	0
			2477	1586	390	493	8			
1	D	296	Total	C	N	O	S	0	0	0
			2419	1550	383	478	8			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

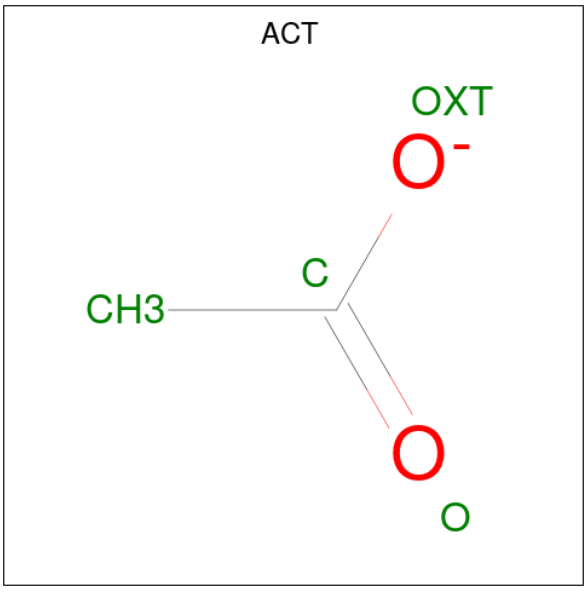
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Fe	0	0
			5	5		
2	B	5	Total	Fe	0	0
			5	5		
2	C	5	Total	Fe	0	0
			5	5		
2	D	5	Total	Fe	0	0
			5	5		

- Molecule 3 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

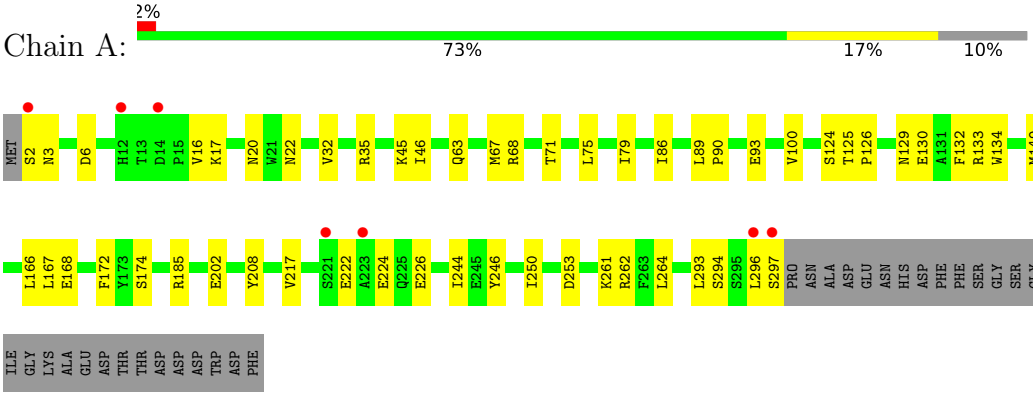
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	197	Total O 197 197	0	0
5	B	117	Total O 117 117	0	0
5	C	234	Total O 234 234	0	0
5	D	180	Total O 180 180	0	0

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.

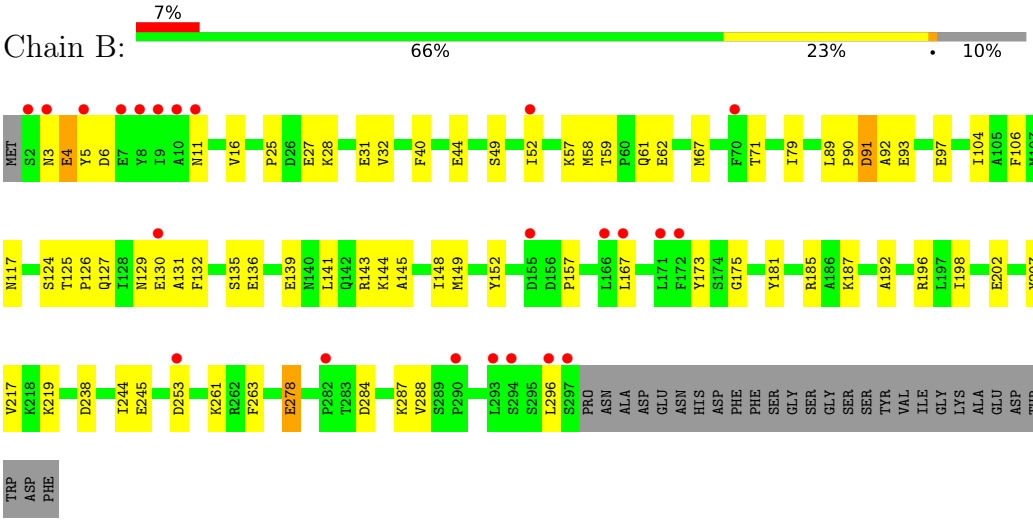
• Molecule 1: ribonucleotide reductase subunit R2F

Chain A:



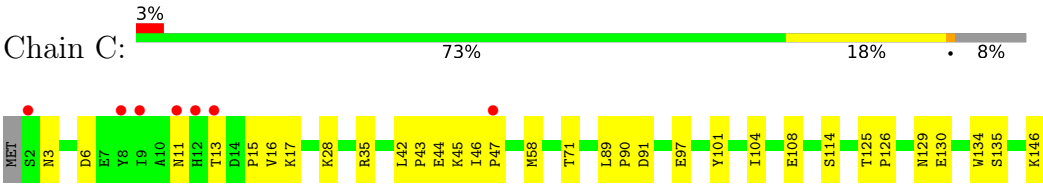
• Molecule 1: ribonucleotide reductase subunit R2F

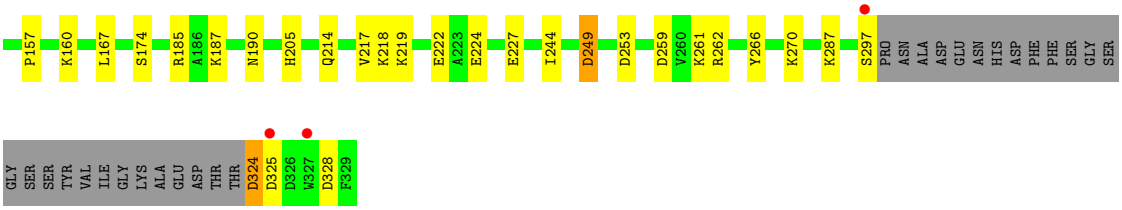
Chain B:



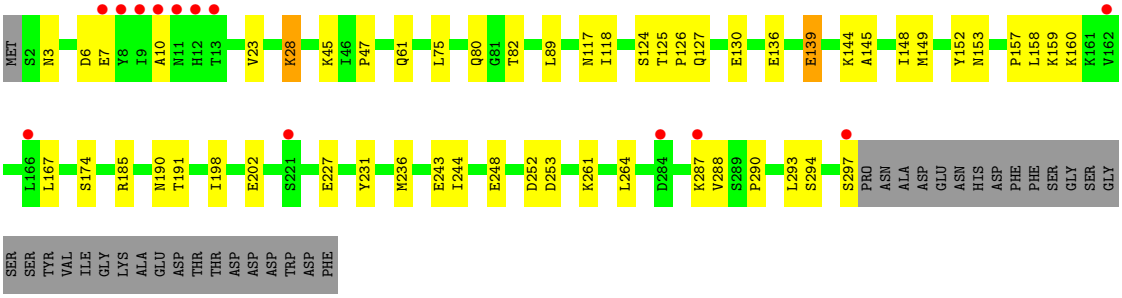
• Molecule 1: ribonucleotide reductase subunit R2F

Chain C:





• Molecule 1: ribonucleotide reductase subunit R2F



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	49.32Å 91.24Å 136.96Å 90.00° 91.46° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 24.37 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 98.3 (24.37-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.28 (at 1.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.239 0.177 , 0.235	Depositor DCC
R_{free} test set	4043 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 71.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10489	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 9.47% 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, OXY, ACT

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	0.66	0/2477	0.73	0/3365
1	B	0.55	0/2477	0.66	0/3365
1	C	0.72	0/2537	0.74	0/3445
1	D	0.64	0/2477	0.71	0/3365
All	All	0.65	0/9968	0.71	0/13540

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2419	0	2331	52	0
1	B	2419	0	2331	79	0
1	C	2477	0	2365	61	0
1	D	2419	0	2331	43	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	C	4	0	3	0	0
5	A	197	0	0	12	0
5	B	117	0	0	13	0
5	C	234	0	0	27	1
5	D	180	0	0	10	1
All	All	10489	0	9361	226	1

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 12.

All (226) 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:244:ILE:HG23	1:A:261:LYS:HE2	1.37	1.06
1:B:57:LYS:HB2	5:B:1099:HOH:O	1.56	1.02
1:C:45:LYS:HG2	1:C:46:ILE:HD12	1.46	0.97
1:D:130:GLU:HB3	5:D:1157:HOH:O	1.64	0.97
1:B:284:ASP:HA	1:B:287:LYS:HE2	1.55	0.89
1:B:278:GLU:HG3	5:B:1019:HOH:O	1.73	0.88
1:B:28:LYS:HA	1:B:31:GLU:OE1	1.76	0.85
1:A:16:VAL:HG11	1:B:79:ILE:HD11	1.58	0.85
1:B:192:ALA:HB1	1:B:196:ARG:HH12	1.41	0.84
3:D:1015:OXY:O1	5:D:1033:HOH:O	1.95	0.83
1:B:145:ALA:O	1:B:149:MET:HG3	1.78	0.83
1:A:16:VAL:CG1	1:B:79:ILE:HD11	2.10	0.81
1:D:244:ILE:HG23	1:D:261:LYS:HE2	1.61	0.80
1:D:287:LYS:HG2	5:D:1134:HOH:O	1.83	0.79
1:A:45:LYS:HG3	5:A:2177:HOH:O	1.82	0.78
1:A:79:ILE:HD11	1:B:16:VAL:HG11	1.67	0.76
1:A:297:SER:HB2	5:A:2036:HOH:O	1.86	0.76
1:A:93:GLU:HG3	5:A:2051:HOH:O	1.85	0.76
1:C:287:LYS:HD2	5:C:1116:HOH:O	1.86	0.75
1:A:174:SER:HB3	1:A:264:LEU:HD21	1.70	0.74
1:B:61:GLN:HG2	1:B:253:ASP:OD1	1.89	0.73
1:C:222:GLU:OE2	5:C:1037:HOH:O	2.06	0.72
1:B:58:MET:HG2	1:B:187:LYS:HD3	1.71	0.72
1:B:93:GLU:HG3	1:B:215:GLN:OE1	1.91	0.71
1:A:172:PHE:CE2	1:A:202:GLU:OE1	2.44	0.71
1:D:227:GLU:OE1	5:D:1056:HOH:O	2.09	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LYS:O	5:C:1115:HOH:O	2.09	0.70
1:C:262:ARG:CZ	5:C:1132:HOH:O	2.38	0.70
1:B:263:PHE:HA	1:B:288:VAL:HG21	1.72	0.70
1:B:117:ASN:OD1	5:B:1114:HOH:O	2.09	0.70
1:A:17:LYS:HE3	5:A:2102:HOH:O	1.91	0.70
1:C:249:ASP:CG	5:C:1061:HOH:O	2.31	0.69
1:C:42:LEU:O	1:C:45:LYS:HB3	1.93	0.69
1:C:47:PRO:HG2	1:C:190:ASN:ND2	2.09	0.68
1:C:287:LYS:HE3	5:C:1233:HOH:O	1.93	0.67
1:D:145:ALA:O	1:D:149:MET:HG3	1.96	0.66
1:B:196:ARG:HD2	5:B:1051:HOH:O	1.96	0.66
1:C:227:GLU:OE1	5:C:1049:HOH:O	2.13	0.65
1:A:75:LEU:HD11	1:B:16:VAL:HG12	1.77	0.65
1:C:227:GLU:OE2	5:C:1014:HOH:O	2.15	0.65
1:C:45:LYS:HG2	1:C:46:ILE:CD1	2.25	0.63
1:D:139:GLU:H	1:D:139:GLU:CD	2.01	0.63
1:C:214:GLN:O	1:C:218:LYS:HG2	1.98	0.63
1:C:224:GLU:HG2	5:C:1100:HOH:O	1.98	0.63
1:D:227:GLU:OE2	5:D:1044:HOH:O	2.15	0.62
1:A:3:ASN:HA	1:A:6:ASP:OD2	2.00	0.62
1:A:35:ARG:HH11	1:A:35:ARG:HG2	1.64	0.61
1:B:57:LYS:O	1:B:57:LYS:HG2	1.99	0.61
1:C:174:SER:OG	5:C:1081:HOH:O	2.16	0.61
1:B:192:ALA:CB	1:B:196:ARG:HH12	2.13	0.61
5:C:1202:HOH:O	1:D:82:THR:HG21	2.01	0.61
1:B:28:LYS:HD2	1:B:31:GLU:OE1	2.01	0.61
1:C:3:ASN:HB2	1:C:6:ASP:OD2	2.01	0.61
1:B:215:GLN:HB3	5:B:1077:HOH:O	2.00	0.60
1:B:71:THR:HG21	1:B:135:SER:HB3	1.84	0.60
1:C:185:ARG:HH11	1:C:185:ARG:HG3	1.67	0.60
1:B:3:ASN:HB2	1:B:6:ASP:OD2	2.02	0.60
1:A:2:SER:HA	1:B:238:ASP:OD2	2.01	0.59
1:C:44:GLU:OE1	5:C:1021:HOH:O	2.16	0.59
1:B:28:LYS:HE2	1:B:207:TYR:CE2	2.38	0.59
1:C:244:ILE:HD12	1:C:261:LYS:HE3	1.85	0.59
1:B:143:ARG:HD3	5:B:1066:HOH:O	2.02	0.58
1:A:126:PRO:O	1:A:130:GLU:HG3	2.03	0.58
1:B:11:ASN:N	1:B:11:ASN:HD22	2.02	0.58
1:B:139:GLU:H	1:B:139:GLU:CD	2.08	0.57
1:D:117:ASN:ND2	5:D:1162:HOH:O	2.37	0.57
1:A:167:LEU:C	1:A:167:LEU:HD23	2.25	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD11	1:B:16:VAL:CG1	2.35	0.57
1:C:134:TRP:CZ2	5:C:1240:HOH:O	2.58	0.57
1:B:89:LEU:HB2	1:B:90:PRO:HD3	1.87	0.56
1:B:148:ILE:HG21	1:B:167:LEU:HD12	1.88	0.56
1:C:58:MET:CG	1:C:187:LYS:HE3	2.35	0.56
1:C:130:GLU:HG3	5:C:1089:HOH:O	2.06	0.56
1:B:198:ILE:O	1:B:202:GLU:HG2	2.05	0.55
1:D:23:VAL:HG13	5:D:1068:HOH:O	2.06	0.55
1:C:58:MET:HG2	1:C:187:LYS:HE3	1.89	0.54
1:D:248:GLU:HB3	1:D:252:ASP:OD2	2.08	0.54
1:A:185:ARG:NE	5:A:2190:HOH:O	2.40	0.54
1:A:86:ILE:HA	1:A:89:LEU:HD23	1.89	0.54
1:B:124:SER:OG	1:B:126:PRO:HD2	2.08	0.54
1:B:3:ASN:N	1:B:6:ASP:OD2	2.41	0.54
1:C:16:VAL:HG12	1:D:75:LEU:HD11	1.89	0.54
1:C:134:TRP:NE1	5:C:1240:HOH:O	2.33	0.53
1:B:192:ALA:HB1	1:B:196:ARG:NH1	2.18	0.53
1:C:89:LEU:HB2	1:C:90:PRO:HD3	1.89	0.53
1:A:68:ARG:HG2	1:A:134:TRP:CD2	2.43	0.53
1:B:104:ILE:O	1:B:108:GLU:HG2	2.09	0.53
1:A:35:ARG:HG2	1:A:35:ARG:NH1	2.23	0.53
1:A:261:LYS:CD	5:A:2183:HOH:O	2.57	0.53
1:B:244:ILE:HG23	1:B:261:LYS:HE2	1.92	0.52
1:C:297:SER:HB2	5:C:1155:HOH:O	2.09	0.52
1:D:61:GLN:HG2	1:D:253:ASP:OD2	2.10	0.52
1:D:28:LYS:HE3	1:D:28:LYS:HA	1.92	0.52
1:A:262:ARG:NE	5:A:2117:HOH:O	2.42	0.52
1:B:173:TYR:C	1:B:175:GLY:N	2.58	0.52
1:D:7:GLU:O	1:D:10:ALA:HB3	2.10	0.52
1:B:89:LEU:CB	1:B:90:PRO:HD3	2.40	0.51
1:B:124:SER:OG	1:B:127:GLN:HG3	2.11	0.51
1:D:236:MET:O	1:D:236:MET:HE2	2.11	0.51
1:A:125:THR:N	1:A:126:PRO:CD	2.74	0.51
1:B:181:TYR:CZ	1:B:185:ARG:CZ	2.92	0.51
1:D:144:LYS:HZ3	1:D:243:GLU:CD	2.14	0.51
1:D:159:LYS:HG2	1:D:231:TYR:CE2	2.46	0.51
1:B:25:PRO:HD2	5:B:1016:HOH:O	2.11	0.51
1:B:71:THR:CG2	1:B:135:SER:HB3	2.41	0.51
1:D:244:ILE:CD1	1:D:261:LYS:HG2	2.41	0.51
1:C:125:THR:HB	1:C:126:PRO:HD3	1.94	0.50
1:C:146:LYS:NZ	5:C:1196:HOH:O	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:OE1	1:A:202:GLU:OE1	2.30	0.50
1:B:215:GLN:CB	5:B:1077:HOH:O	2.60	0.49
1:B:263:PHE:HA	1:B:288:VAL:CG2	2.39	0.49
1:A:46:ILE:HD12	1:A:46:ILE:N	2.27	0.49
1:A:222:GLU:O	1:A:226:GLU:HG2	2.12	0.49
1:D:80:GLN:HA	1:D:80:GLN:OE1	2.13	0.49
1:C:45:LYS:HE3	5:C:1205:HOH:O	2.13	0.49
1:C:259:ASP:OD2	5:C:1147:HOH:O	2.20	0.49
1:A:293:LEU:O	1:A:296:LEU:HB3	2.12	0.48
1:A:35:ARG:HD2	5:A:2154:HOH:O	2.14	0.48
1:C:47:PRO:HG2	1:C:190:ASN:HD22	1.79	0.48
1:D:290:PRO:O	1:D:294:SER:HB2	2.13	0.48
1:D:153:ASN:ND2	5:D:1054:HOH:O	2.47	0.48
1:D:124:SER:OG	1:D:126:PRO:HD2	2.13	0.47
1:B:79:ILE:HD12	1:B:149:MET:SD	2.54	0.47
1:D:144:LYS:NZ	1:D:243:GLU:OE2	2.47	0.47
1:A:294:SER:C	1:A:296:LEU:H	2.17	0.47
1:C:43:PRO:HB3	1:C:114:SER:HB2	1.95	0.47
1:A:75:LEU:O	1:A:79:ILE:HG12	2.13	0.47
1:C:47:PRO:O	1:C:190:ASN:ND2	2.47	0.47
1:C:148:ILE:HG22	1:C:152:TYR:CE2	2.49	0.47
1:C:253:ASP:HB2	5:C:1086:HOH:O	2.13	0.47
1:B:27:GLU:O	1:B:31:GLU:HG3	2.15	0.47
1:C:160:LYS:NZ	5:C:1203:HOH:O	2.26	0.47
1:A:63:GLN:O	1:A:67:MET:HG2	2.14	0.47
1:B:28:LYS:HE2	1:B:207:TYR:HE2	1.79	0.47
1:B:148:ILE:HG22	1:B:152:TYR:CE2	2.49	0.47
1:C:262:ARG:NE	5:C:1090:HOH:O	2.44	0.47
1:A:86:ILE:O	1:A:89:LEU:HD23	2.15	0.47
1:B:132:PHE:O	1:B:136:GLU:HG3	2.14	0.47
1:D:125:THR:N	1:D:126:PRO:CD	2.78	0.47
1:C:134:TRP:CE2	5:C:1240:HOH:O	2.68	0.46
1:A:224:GLU:OE2	5:A:2078:HOH:O	2.20	0.46
1:B:126:PRO:O	1:B:130:GLU:HG3	2.15	0.46
1:B:141:LEU:HD12	1:B:144:LYS:HE3	1.98	0.46
1:C:15:PRO:HD2	5:C:1232:HOH:O	2.15	0.46
1:D:174:SER:HB3	1:D:264:LEU:HD21	1.98	0.46
1:C:35:ARG:HG2	1:C:35:ARG:HH11	1.81	0.46
1:D:47:PRO:HG2	1:D:190:ASN:OD1	2.16	0.46
1:A:246:TYR:CZ	1:A:250:ILE:HD11	2.51	0.46
1:C:266:TYR:CZ	1:C:270:LYS:HE2	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:GLU:HG2	1:C:101:TYR:CE2	2.51	0.46
1:B:278:GLU:N	1:B:278:GLU:OE1	2.48	0.45
1:C:324:ASP:HB2	1:C:325:ASP:H	1.53	0.45
1:A:185:ARG:NH1	5:A:2092:HOH:O	2.50	0.45
1:C:17:LYS:HA	5:C:1176:HOH:O	2.16	0.45
1:D:244:ILE:O	1:D:248:GLU:HG3	2.16	0.45
1:D:198:ILE:O	1:D:202:GLU:HG2	2.17	0.45
1:C:11:ASN:HD22	1:C:11:ASN:N	2.15	0.45
1:A:261:LYS:HD3	5:A:2183:HOH:O	2.16	0.45
1:D:118:ILE:HD13	1:D:191:THR:HG23	1.98	0.45
1:B:3:ASN:C	1:B:5:TYR:H	2.20	0.45
1:B:32:VAL:HG21	1:B:208:TYR:CD1	2.52	0.45
1:C:266:TYR:CE2	1:C:270:LYS:HE2	2.51	0.45
1:D:23:VAL:HG13	1:D:23:VAL:O	2.17	0.45
1:A:20:ASN:OD1	1:A:22:ASN:HB3	2.17	0.44
1:B:58:MET:CG	1:B:187:LYS:HD3	2.43	0.44
1:B:216:GLY:O	1:B:219:LYS:HB2	2.17	0.44
1:B:125:THR:CG2	1:B:129:ASN:HD22	2.30	0.44
1:D:124:SER:CB	1:D:126:PRO:HD2	2.47	0.44
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.82	0.44
1:D:3:ASN:N	1:D:6:ASP:OD2	2.50	0.44
1:A:294:SER:C	1:A:296:LEU:N	2.71	0.43
1:C:17:LYS:HE2	1:D:136:GLU:OE1	2.18	0.43
1:C:185:ARG:HG3	1:C:185:ARG:NH1	2.31	0.43
1:D:167:LEU:C	1:D:167:LEU:HD23	2.39	0.43
1:A:75:LEU:HD11	1:B:16:VAL:CG1	2.45	0.43
1:A:79:ILE:HD12	1:A:149:MET:SD	2.59	0.43
1:C:91:ASP:CG	1:C:157:PRO:HB3	2.39	0.43
1:A:124:SER:HB2	1:A:126:PRO:HD2	2.00	0.43
1:D:288:VAL:HG13	1:D:293:LEU:HG	1.99	0.43
1:A:125:THR:HG22	1:A:129:ASN:ND2	2.33	0.43
1:C:35:ARG:HD2	5:C:1092:HOH:O	2.18	0.43
1:A:32:VAL:HG21	1:A:208:TYR:CD1	2.53	0.43
1:C:44:GLU:CD	5:C:1021:HOH:O	2.57	0.43
1:D:126:PRO:O	1:D:130:GLU:HG3	2.19	0.43
1:A:159:LYS:NZ	1:B:4:GLU:OE2	2.52	0.43
1:B:173:TYR:C	1:B:175:GLY:H	2.21	0.43
1:B:181:TYR:CE1	1:B:185:ARG:HD2	2.54	0.42
1:A:89:LEU:N	1:A:90:PRO:HD2	2.33	0.42
1:A:100:VAL:HG11	1:A:208:TYR:CE2	2.54	0.42
1:B:113:LYS:NZ	5:B:1114:HOH:O	2.42	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:THR:N	1:B:126:PRO:CD	2.82	0.42
1:B:284:ASP:O	1:B:287:LYS:HG2	2.19	0.42
1:C:125:THR:HG22	1:C:129:ASN:ND2	2.34	0.42
1:C:244:ILE:HG21	1:C:328:ASP:HB3	2.01	0.42
1:A:71:THR:HG21	1:A:132:PHE:HA	2.01	0.42
1:B:92:ALA:HA	1:B:97:GLU:OE2	2.20	0.42
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.34	0.42
1:D:124:SER:H	1:D:127:GLN:HE21	1.67	0.42
1:B:67:MET:HB3	1:B:131:ALA:HB2	2.01	0.42
1:C:104:ILE:O	1:C:108:GLU:HG2	2.20	0.42
1:B:167:LEU:C	1:B:167:LEU:HD23	2.40	0.42
1:C:104:ILE:HG12	1:C:205:HIS:CD2	2.54	0.42
1:D:45:LYS:HG3	1:D:45:LYS:O	2.19	0.42
1:D:148:ILE:HG22	1:D:152:TYR:CE2	2.54	0.42
1:B:91:ASP:OD2	1:B:157:PRO:HG3	2.20	0.41
1:B:196:ARG:CZ	5:B:1051:HOH:O	2.68	0.41
1:B:196:ARG:NH1	5:B:1051:HOH:O	2.52	0.41
1:B:11:ASN:N	1:B:11:ASN:ND2	2.68	0.41
1:B:40:PHE:HE1	1:B:106:PHE:HE2	1.69	0.41
1:D:157:PRO:HB3	5:D:1172:HOH:O	2.20	0.41
1:D:158:LEU:HA	1:D:158:LEU:HD23	1.83	0.41
1:D:160:LYS:NZ	5:D:1193:HOH:O	2.53	0.41
1:A:166:LEU:HD23	1:A:166:LEU:HA	1.80	0.41
1:B:44:GLU:CD	5:B:1017:HOH:O	2.58	0.41
1:B:278:GLU:HG3	5:B:1055:HOH:O	2.19	0.41
1:C:71:THR:CG2	1:C:135:SER:HB3	2.51	0.41
1:B:49:SER:O	1:B:52:ILE:HG13	2.21	0.41
1:A:45:LYS:HE3	5:A:2177:HOH:O	2.20	0.41
1:A:172:PHE:HE2	1:A:202:GLU:OE1	1.96	0.41
1:C:91:ASP:CB	1:C:157:PRO:HB3	2.51	0.41
1:C:167:LEU:HD23	1:C:167:LEU:C	2.41	0.41
1:A:296:LEU:O	1:A:297:SER:CB	2.69	0.40
1:C:91:ASP:HB3	1:C:157:PRO:HB3	2.02	0.40
1:C:28:LYS:HE2	1:C:28:LYS:HB2	1.73	0.40
1:B:59:THR:OG1	1:B:62:GLU:HG3	2.21	0.40
1:B:28:LYS:HA	1:B:28:LYS:HD2	1.81	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:1037:HOH:O	5:D:1189:HOH:O[2_546]	2.13	0.07

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	294/329 (89%)	286 (97%)	8 (3%)	0	100 100
1	B	294/329 (89%)	286 (97%)	6 (2%)	2 (1%)	22 16
1	C	298/329 (91%)	296 (99%)	2 (1%)	0	100 100
1	D	294/329 (89%)	287 (98%)	7 (2%)	0	100 100
All	All	1180/1316 (90%)	1155 (98%)	23 (2%)	2 (0%)	47 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	4	GLU
1	B	296	LEU

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	265/293 (90%)	262 (99%)	3 (1%)	73 78
1	B	265/293 (90%)	260 (98%)	5 (2%)	57 61
1	C	271/293 (92%)	267 (98%)	4 (2%)	65 69

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	265/293 (90%)	260 (98%)	5 (2%)	57 61
All	All	1066/1172 (91%)	1049 (98%)	17 (2%)	62 67

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	ARG
1	A	217	VAL
1	A	253	ASP
1	B	91	ASP
1	B	215	GLN
1	B	217	VAL
1	B	245	GLU
1	B	278	GLU
1	C	13	THR
1	C	217	VAL
1	C	249	ASP
1	C	324	ASP
1	D	28	LYS
1	D	89	LEU
1	D	139	GLU
1	D	185	ARG
1	D	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	53	GLN
1	A	190	ASN
1	A	215	GLN
1	A	225	GLN
1	B	11	ASN
1	B	39	ASN
1	B	50	ASN
1	B	127	GLN
1	B	129	ASN
1	B	153	ASN
1	C	11	ASN
1	C	50	ASN
1	C	140	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	190	ASN
1	C	225	GLN
1	D	11	ASN
1	D	39	ASN
1	D	127	GLN
1	D	215	GLN
1	D	273	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 20 are monoatomic and 3 are modelled with single atom - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACT	C	1011	2	3,3,3	1.09	0	3,3,3	0.62	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	296/329 (89%)	-0.10	8 (2%)	54	53	13, 26, 62, 92	0
1	B	296/329 (89%)	0.30	23 (7%)	13	12	17, 38, 74, 106	0
1	C	302/329 (91%)	-0.22	10 (3%)	46	45	11, 23, 51, 75	0
1	D	296/329 (89%)	0.05	13 (4%)	34	33	12, 28, 68, 93	0
All	All	1190/1316 (90%)	0.01	54 (4%)	33	32	11, 29, 68, 106	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	SER	6.4
1	B	2	SER	6.4
1	D	10	ALA	5.5
1	B	297	SER	5.4
1	B	11	ASN	5.1
1	D	12	HIS	4.6
1	D	7	GLU	4.5
1	B	7	GLU	4.2
1	D	11	ASN	4.0
1	B	8	TYR	4.0
1	D	297	SER	3.8
1	C	327	TRP	3.7
1	A	221	SER	3.7
1	B	9	ILE	3.3
1	D	9	ILE	3.3
1	D	8	TYR	3.2
1	C	11	ASN	3.1
1	A	223	ALA	3.1
1	C	297	SER	3.1
1	C	13	THR	3.1
1	C	12	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	10	ALA	3.0
1	D	13	THR	3.0
1	D	284	ASP	2.9
1	A	2	SER	2.9
1	A	12	HIS	2.9
1	B	155	ASP	2.9
1	B	296	LEU	2.8
1	A	296	LEU	2.6
1	B	290	PRO	2.6
1	D	221	SER	2.6
1	B	70	PHE	2.6
1	C	8	TYR	2.5
1	B	167	LEU	2.5
1	C	2	SER	2.5
1	B	166	LEU	2.4
1	B	253	ASP	2.4
1	C	9	ILE	2.4
1	A	155	ASP	2.4
1	A	14	ASP	2.4
1	B	3	ASN	2.3
1	D	162	VAL	2.3
1	B	172	PHE	2.3
1	B	282	PRO	2.3
1	B	5	TYR	2.3
1	B	171	LEU	2.3
1	B	293	LEU	2.3
1	D	287	LYS	2.3
1	B	130	GLU	2.2
1	C	47	PRO	2.1
1	C	325	ASP	2.1
1	B	294	SER	2.1
1	D	166	LEU	2.0
1	B	52	ILE	2.0

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FE	B	1005	1/1	0.92	0.11	26,26,26,26	1
2	FE	B	1007	1/1	0.92	0.14	32,32,32,32	1
2	FE	B	1006	1/1	0.93	0.10	36,36,36,36	1
2	FE	D	1012	1/1	0.96	0.05	31,31,31,31	1
4	ACT	C	1011	4/4	0.96	0.31	28,30,31,41	0
2	FE	A	2003	1/1	0.97	0.04	30,30,30,30	1
2	FE	A	2001	1/1	0.97	0.05	26,26,26,26	1
2	FE	D	1013	1/1	0.97	0.07	45,45,45,45	1
3	OXY	D	1015	1/2	0.97	0.07	26,26,26,26	0
2	FE	A	2002	1/1	0.97	0.04	28,28,28,28	1
2	FE	D	1014	1/1	0.98	0.03	34,34,34,34	1
2	FE	C	1008	1/1	0.99	0.04	26,26,26,26	0
2	FE	C	1009	1/1	0.99	0.06	26,26,26,26	0
2	FE	A	1002	1/1	0.99	0.03	26,26,26,26	0
2	FE	B	1003	1/1	0.99	0.04	27,27,27,27	0
2	FE	B	1004	1/1	0.99	0.04	22,22,22,22	0
3	OXY	A	2004	1/2	0.99	0.08	26,26,26,26	0
2	FE	C	1001	1/1	0.99	0.03	31,31,31,31	1
2	FE	C	1002	1/1	0.99	0.02	23,23,23,23	1
2	FE	D	1003	1/1	1.00	0.04	19,19,19,19	0
2	FE	D	1004	1/1	1.00	0.05	16,16,16,16	0
3	OXY	C	1012	1/2	1.00	0.20	18,18,18,18	0
2	FE	A	1001	1/1	1.00	0.02	31,31,31,31	0
2	FE	C	1010	1/1	1.00	0.08	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.