



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:09 PM UTC

PDB ID : 1KGN / pdb_00001kgn
Title : R2F from Corynebacterium Ammoniagenes in its oxidised, Fe containing, form
Authors : Hogbom, M.; Huque, Y.; Sjoberg, B.M.; Nordlund, P.
Deposited on : 2001-11-28
Resolution : 1.85 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

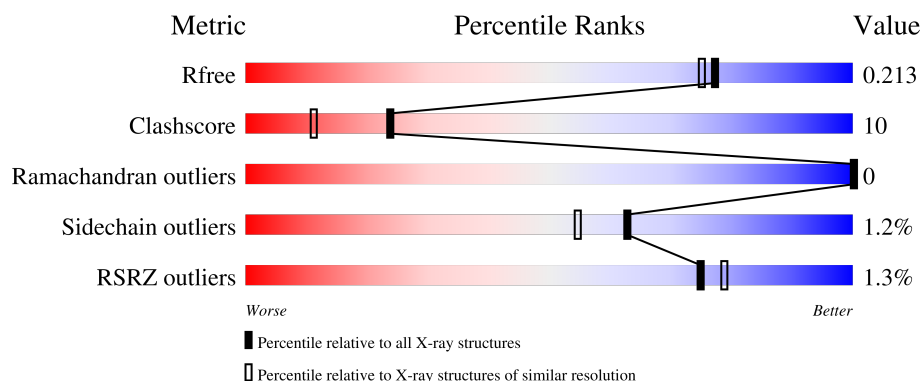
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	329	2% 72% 16% 10%
1	B	329	72% 17% 10%
1	C	329	% 76% 14% 10%
1	D	329	% 74% 14% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11215 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 protein 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	296	Total	C	N	O	S	0	0	0
			2419	1550	383	478	8			
1	D	296	Total	C	N	O	S	0	0	0
			2419	1550	383	478	8			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

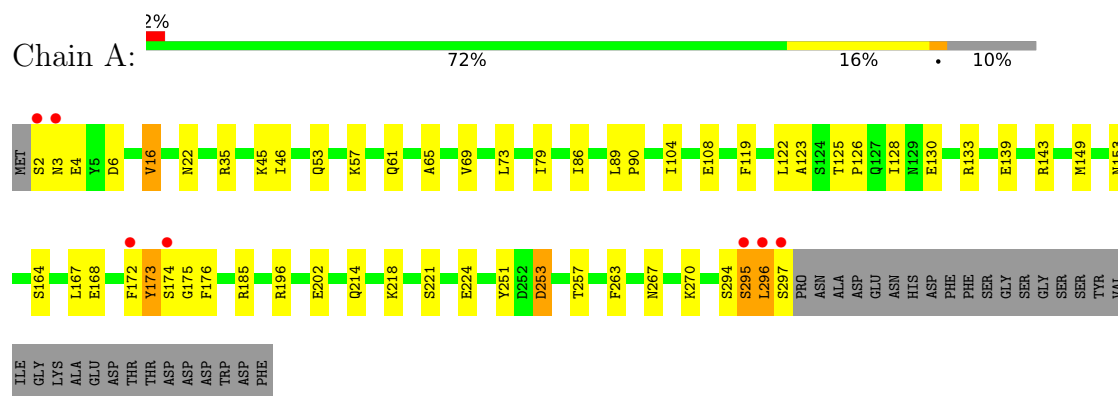
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	426	Total	O	0	0
			426	426		
3	B	362	Total	O	0	0
			362	362		
3	C	401	Total	O	0	0
			401	401		
3	D	342	Total	O	0	0
			342	342		

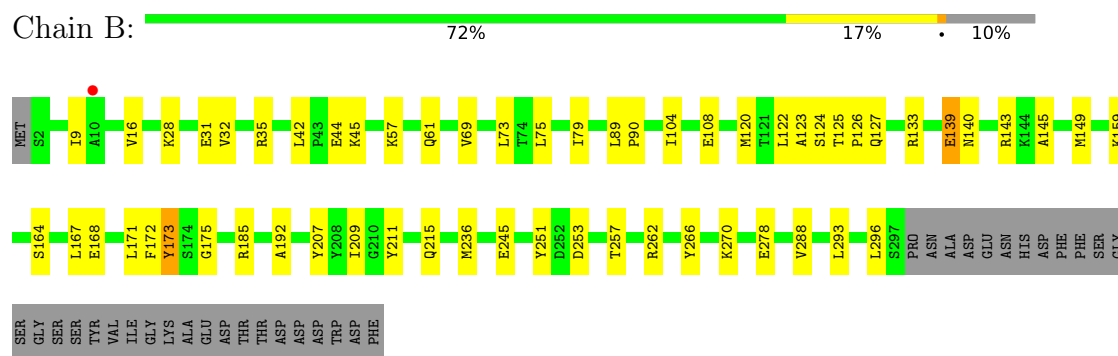
3 Residue-property plots [i](#)

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.

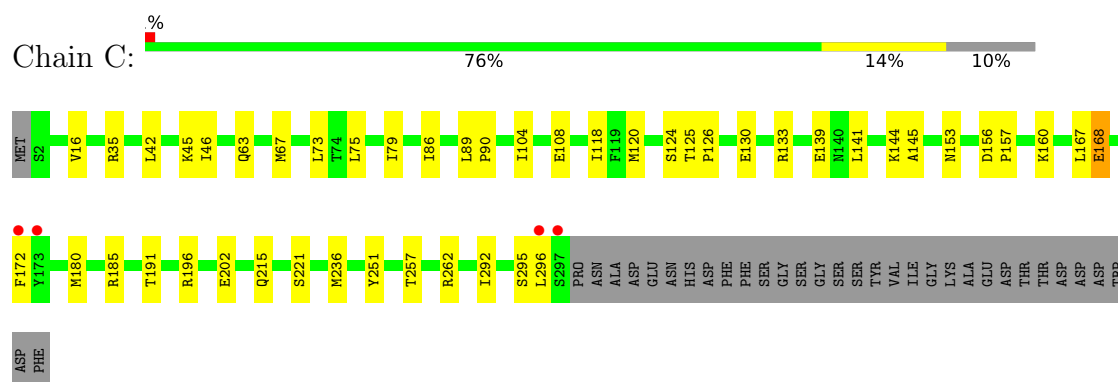
• Molecule 1: Ribonucleotide reductase protein R2F



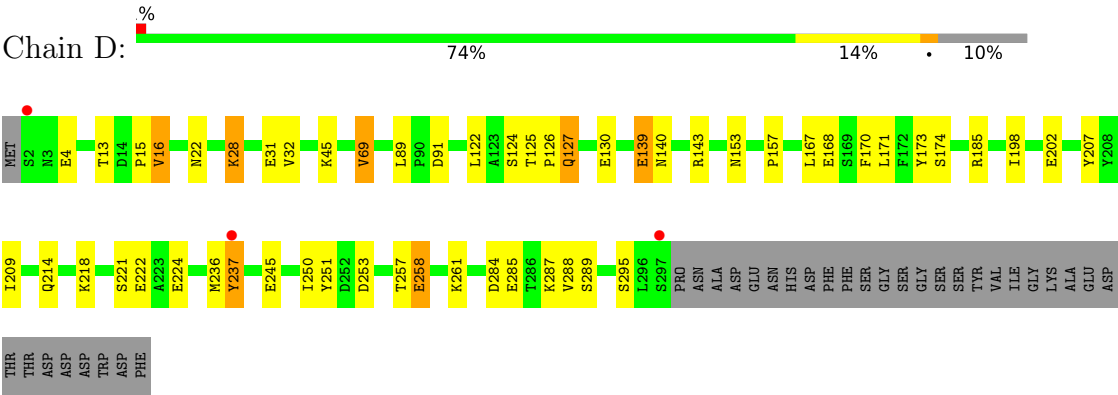
• Molecule 1: Ribonucleotide reductase protein R2F



• Molecule 1: Ribonucleotide reductase protein R2F



● Molecule 1: Ribonucleotide reductase protein R2F



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.81Å 90.70Å 136.81Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-1.85) 95.9 (30.00-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 1.85Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.158 , 0.213 0.158 , 0.213	Depositor DCC
R_{free} test set	5064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.64 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3157e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.76	0/2477	0.96	8/3365 (0.2%)
1	B	0.76	2/2477 (0.1%)	0.94	6/3365 (0.2%)
1	C	0.78	1/2477 (0.0%)	0.95	7/3365 (0.2%)
1	D	0.73	0/2477	0.95	7/3365 (0.2%)
All	All	0.76	3/9908 (0.0%)	0.95	28/13460 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	MET	SD-CE	-7.30	1.61	1.79
1	B	236	MET	SD-CE	-6.15	1.64	1.79
1	B	192	ALA	CA-CB	5.37	1.62	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	TYR	N-CA-C	8.77	123.28	112.23
1	D	173	TYR	N-CA-C	7.91	122.19	112.54
1	D	16	VAL	N-CA-C	-7.20	99.38	108.89
1	A	257	THR	N-CA-C	7.15	119.69	111.11
1	B	173	TYR	N-CA-C	6.59	119.47	111.82
1	A	122	LEU	N-CA-C	6.53	121.53	112.45
1	A	296	LEU	N-CA-C	-6.49	103.83	111.03
1	C	257	THR	N-CA-C	6.41	118.81	111.11
1	A	251	TYR	N-CA-C	6.34	121.18	113.38
1	B	251	TYR	N-CA-C	6.34	121.79	113.30
1	D	251	TYR	N-CA-C	6.33	121.95	113.72
1	C	139	GLU	N-CA-C	6.21	118.05	111.28
1	D	122	LEU	N-CA-C	6.17	120.84	113.12
1	A	16	VAL	N-CA-C	-6.03	101.01	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	ALA	N-CA-C	5.99	119.39	110.52
1	D	171	LEU	N-CA-C	5.99	118.59	111.71
1	D	258	GLU	N-CA-C	5.91	117.73	111.28
1	A	174	SER	N-CA-C	-5.83	105.88	112.87
1	B	171	LEU	N-CA-C	5.74	119.38	112.38
1	B	257	THR	N-CA-C	5.73	120.82	111.37
1	A	123	ALA	N-CA-C	5.55	118.74	110.52
1	B	122	LEU	N-CA-C	5.50	119.99	113.12
1	D	174	SER	N-CA-C	-5.39	105.81	112.38
1	C	16	VAL	N-CA-C	-5.37	101.80	108.89
1	C	168	GLU	N-CA-C	5.23	117.78	111.40
1	C	156	ASP	CA-C-N	5.09	124.27	118.97
1	C	156	ASP	C-N-CA	5.09	124.27	118.97
1	C	251	TYR	N-CA-C	5.08	120.32	113.72

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	66	0
1	B	2419	0	2331	54	0
1	C	2419	0	2331	40	0
1	D	2419	0	2331	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	426	0	0	27	0
3	B	362	0	0	16	0
3	C	401	0	0	11	0
3	D	342	0	0	16	0
All	All	11215	0	9324	191	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 10.

All (191) 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:173:TYR:HA	3:A:2123:HOH:O	1.62	0.98
1:D:168:GLU:HG3	3:D:1202:HOH:O	1.64	0.97
1:C:215:GLN:HG2	3:C:3256:HOH:O	1.68	0.90
1:A:22:ASN:HB2	3:B:2085:HOH:O	1.75	0.85
1:B:140:ASN:HD21	1:B:245:GLU:HG2	1.40	0.84
1:B:28:LYS:HE2	1:B:207:TYR:HE2	1.44	0.83
1:D:139:GLU:H	1:D:139:GLU:CD	1.89	0.80
1:C:153:ASN:HB3	3:C:3373:HOH:O	1.81	0.80
1:B:35:ARG:HH11	1:B:35:ARG:HG3	1.46	0.80
1:A:45:LYS:HG3	3:A:2172:HOH:O	1.82	0.79
1:B:140:ASN:ND2	1:B:245:GLU:HG2	1.97	0.78
1:A:139:GLU:HB3	3:A:2276:HOH:O	1.84	0.77
1:B:139:GLU:H	1:B:139:GLU:CD	1.92	0.76
1:A:176:PHE:HB2	3:A:2123:HOH:O	1.87	0.74
1:A:35:ARG:HH11	1:A:35:ARG:HG2	1.52	0.73
1:C:196:ARG:HH21	1:C:295:SER:HB2	1.54	0.71
1:A:16:VAL:HG11	1:B:79:ILE:HD11	1.73	0.70
1:A:167:LEU:C	1:A:167:LEU:HD23	2.15	0.70
1:C:126:PRO:O	1:C:130:GLU:HG3	1.93	0.69
1:B:44:GLU:OE1	3:B:2041:HOH:O	2.10	0.69
1:B:124:SER:H	1:B:127:GLN:HE21	1.40	0.69
1:A:53:GLN:HB3	3:A:2395:HOH:O	1.93	0.68
1:C:167:LEU:HD21	1:C:172:PHE:CE2	2.29	0.67
1:B:211:TYR:CZ	1:B:215:GLN:NE2	2.63	0.66
1:B:28:LYS:HE2	1:B:207:TYR:CE2	2.29	0.66
1:D:13:THR:HG23	3:D:1282:HOH:O	1.96	0.66
1:A:73:LEU:HD22	1:A:172:PHE:HD1	1.61	0.65
1:D:91:ASP:OD2	3:D:1173:HOH:O	2.15	0.65
1:B:28:LYS:HE3	1:B:32:VAL:HG23	1.79	0.65
1:C:221:SER:HA	3:C:3292:HOH:O	1.97	0.65
1:A:79:ILE:HD11	1:B:16:VAL:HG11	1.79	0.64
1:D:285:GLU:HG2	3:D:1339:HOH:O	1.97	0.64
1:D:153:ASN:HB3	3:D:1299:HOH:O	1.97	0.64
1:B:35:ARG:HG3	1:B:35:ARG:NH1	2.09	0.63
1:C:45:LYS:HG2	1:C:46:ILE:HD12	1.81	0.63
1:D:28:LYS:HE3	1:D:28:LYS:HA	1.81	0.63
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.64	0.62
1:C:133:ARG:HD2	3:C:3358:HOH:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HD2	3:C:3177:HOH:O	2.00	0.61
1:D:209:ILE:HD12	3:D:1202:HOH:O	1.99	0.60
1:B:143:ARG:HD3	3:B:2196:HOH:O	2.02	0.60
1:A:214:GLN:HB3	1:A:218:LYS:HE2	1.84	0.60
1:B:120:MET:HG3	3:B:2085:HOH:O	2.01	0.60
1:C:120:MET:SD	3:C:3222:HOH:O	2.56	0.59
1:A:221:SER:OG	1:A:224:GLU:HG3	2.02	0.58
1:A:16:VAL:CG1	1:B:79:ILE:HD11	2.32	0.58
1:A:35:ARG:HG2	1:A:35:ARG:NH1	2.19	0.57
1:D:45:LYS:O	1:D:45:LYS:HG2	2.04	0.57
1:B:120:MET:SD	3:B:2085:HOH:O	2.57	0.57
1:C:120:MET:HG2	1:D:22:ASN:OD1	2.03	0.57
1:B:133:ARG:NH2	3:B:2161:HOH:O	2.36	0.57
1:D:185:ARG:HD3	3:D:1221:HOH:O	2.04	0.57
1:C:180:MET:HG3	1:C:296:LEU:HD13	1.85	0.57
1:B:42:LEU:O	1:B:45:LYS:HG2	2.05	0.56
1:C:79:ILE:HD11	1:D:16:VAL:HG11	1.88	0.56
1:D:28:LYS:HD3	1:D:207:TYR:OH	2.06	0.56
1:D:237:TYR:C	1:D:237:TYR:CD1	2.83	0.56
1:A:185:ARG:NE	3:A:2185:HOH:O	2.39	0.56
1:A:104:ILE:O	1:A:108:GLU:HG2	2.05	0.55
1:C:35:ARG:HD2	3:C:3109:HOH:O	2.06	0.55
1:A:79:ILE:HD11	1:B:16:VAL:CG1	2.36	0.55
1:A:57:LYS:HE2	3:D:1296:HOH:O	2.06	0.55
1:B:173:TYR:HB2	3:B:2263:HOH:O	2.06	0.55
1:B:164:SER:O	1:B:168:GLU:HG3	2.06	0.55
1:A:173:TYR:HB2	3:A:2074:HOH:O	2.06	0.55
1:A:143:ARG:CZ	3:A:2276:HOH:O	2.55	0.55
1:B:28:LYS:HD2	1:B:31:GLU:OE1	2.07	0.54
1:A:53:GLN:HG3	3:A:2095:HOH:O	2.08	0.54
1:A:61:GLN:NE2	1:A:253:ASP:OD2	2.41	0.54
1:B:278:GLU:HG3	3:B:2016:HOH:O	2.06	0.54
1:D:28:LYS:HE3	1:D:31:GLU:HB2	1.89	0.54
1:B:262:ARG:CZ	3:B:2333:HOH:O	2.57	0.53
1:A:173:TYR:C	1:A:175:GLY:H	2.16	0.53
1:A:61:GLN:HG3	3:A:2106:HOH:O	2.08	0.53
1:C:46:ILE:HD12	1:C:46:ILE:N	2.23	0.53
1:D:198:ILE:O	1:D:202:GLU:HG2	2.09	0.52
1:A:173:TYR:C	1:A:175:GLY:N	2.61	0.52
1:A:46:ILE:HD12	1:A:46:ILE:N	2.25	0.52
1:B:139:GLU:CD	1:B:139:GLU:N	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:LEU:O	1:A:297:SER:C	2.52	0.52
1:A:143:ARG:NH1	3:A:2276:HOH:O	2.42	0.52
1:A:86:ILE:HA	1:A:89:LEU:HD23	1.92	0.51
1:B:278:GLU:CG	3:B:2016:HOH:O	2.57	0.51
1:A:175:GLY:N	3:A:2130:HOH:O	2.44	0.51
1:B:9:ILE:HD12	3:B:2267:HOH:O	2.11	0.51
1:C:168:GLU:CD	1:C:202:GLU:OE1	2.54	0.51
1:B:266:TYR:O	1:B:270:LYS:HG2	2.11	0.51
1:A:172:PHE:CE2	1:A:202:GLU:OE2	2.63	0.50
1:B:61:GLN:HG2	1:B:253:ASP:OD1	2.11	0.50
1:A:125:THR:HB	1:A:126:PRO:HD3	1.94	0.50
1:A:2:SER:N	3:A:2422:HOH:O	2.45	0.49
1:A:143:ARG:NH2	3:A:2276:HOH:O	2.44	0.49
1:A:89:LEU:HB2	1:A:90:PRO:HD3	1.95	0.49
1:B:69:VAL:HG13	1:B:175:GLY:HA2	1.93	0.49
1:C:262:ARG:CZ	3:C:3155:HOH:O	2.61	0.49
1:A:173:TYR:CA	3:A:2123:HOH:O	2.38	0.48
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.28	0.48
1:A:153:ASN:HB3	3:A:2252:HOH:O	2.12	0.48
1:A:294:SER:O	1:A:297:SER:HB2	2.15	0.47
1:C:73:LEU:HD22	1:C:172:PHE:HD1	1.78	0.47
1:A:61:GLN:NE2	3:A:2297:HOH:O	2.45	0.47
1:D:140:ASN:ND2	1:D:245:GLU:HG2	2.29	0.47
1:D:218:LYS:HE3	3:D:1337:HOH:O	2.13	0.47
1:A:45:LYS:CG	3:A:2172:HOH:O	2.52	0.47
1:D:284:ASP:HA	1:D:287:LYS:HE3	1.96	0.47
1:D:124:SER:H	1:D:127:GLN:HE21	1.61	0.47
1:A:185:ARG:NH1	3:A:2188:HOH:O	2.48	0.47
1:C:125:THR:N	1:C:126:PRO:CD	2.78	0.47
1:A:65:ALA:O	1:A:69:VAL:HG22	2.15	0.47
1:C:167:LEU:C	1:C:167:LEU:HD23	2.40	0.47
1:B:125:THR:HB	1:B:126:PRO:HD3	1.96	0.46
1:A:172:PHE:CD2	1:A:202:GLU:OE2	2.68	0.46
1:D:126:PRO:O	1:D:130:GLU:HG3	2.16	0.46
1:A:3:ASN:HA	1:A:6:ASP:OD2	2.15	0.46
1:C:75:LEU:HD11	1:D:16:VAL:HG12	1.96	0.46
1:A:45:LYS:HE2	3:A:2172:HOH:O	2.14	0.46
1:A:173:TYR:CG	3:A:2123:HOH:O	2.69	0.46
1:C:104:ILE:O	1:C:108:GLU:HG2	2.15	0.46
1:D:140:ASN:HD21	1:D:245:GLU:HG2	1.80	0.46
1:C:89:LEU:HB2	1:C:90:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:GLN:HG3	3:A:2349:HOH:O	2.15	0.46
1:B:104:ILE:O	1:B:108:GLU:HG2	2.15	0.46
1:A:79:ILE:HD12	1:A:149:MET:SD	2.56	0.46
1:B:45:LYS:HB3	3:B:2358:HOH:O	2.15	0.46
1:A:173:TYR:HB3	1:A:267:ASN:ND2	2.32	0.45
1:B:293:LEU:HA	1:B:296:LEU:HD12	1.98	0.45
1:B:28:LYS:HE3	1:B:32:VAL:CG2	2.44	0.45
1:B:28:LYS:HD2	1:B:28:LYS:HA	1.74	0.45
1:C:79:ILE:HD11	1:C:145:ALA:HB1	1.99	0.45
1:A:143:ARG:HD2	3:A:2383:HOH:O	2.17	0.45
1:C:86:ILE:HA	1:C:89:LEU:HD23	1.98	0.45
1:A:57:LYS:CD	3:D:1296:HOH:O	2.65	0.45
1:B:69:VAL:CG1	1:B:175:GLY:HA2	2.47	0.45
1:B:145:ALA:O	1:B:149:MET:HG3	2.17	0.45
1:C:172:PHE:CD2	1:C:202:GLU:OE2	2.70	0.45
1:A:263:PHE:CE1	1:A:296:LEU:HD21	2.52	0.45
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.66	0.44
1:C:45:LYS:C	1:C:46:ILE:HD12	2.43	0.44
1:C:292:ILE:O	1:C:296:LEU:HB2	2.16	0.44
3:C:3126:HOH:O	1:D:4:GLU:CD	2.60	0.44
1:D:287:LYS:HE3	3:D:1297:HOH:O	2.17	0.44
1:B:168:GLU:OE1	1:B:209:ILE:HD12	2.18	0.44
1:C:35:ARG:HG2	1:C:35:ARG:HH11	1.81	0.44
1:B:270:LYS:NZ	3:B:2176:HOH:O	2.50	0.44
1:C:42:LEU:O	1:C:45:LYS:HB3	2.17	0.44
1:A:175:GLY:CA	3:A:2130:HOH:O	2.65	0.44
1:B:57:LYS:NZ	3:B:2261:HOH:O	2.51	0.44
1:B:293:LEU:HD23	1:B:296:LEU:HD12	1.99	0.44
1:B:73:LEU:HD22	1:B:172:PHE:HD1	1.83	0.44
1:B:167:LEU:C	1:B:167:LEU:HD23	2.42	0.44
1:D:214:GLN:O	1:D:218:LYS:HG3	2.18	0.44
1:B:253:ASP:OD1	1:B:253:ASP:C	2.61	0.43
1:D:125:THR:N	1:D:126:PRO:CD	2.81	0.43
1:A:119:PHE:HB3	1:A:128:ILE:HG12	1.99	0.43
1:A:167:LEU:C	1:A:167:LEU:CD2	2.88	0.43
1:D:167:LEU:C	1:D:167:LEU:HD23	2.43	0.43
1:A:133:ARG:HD2	3:A:2363:HOH:O	2.18	0.43
1:D:157:PRO:HB2	3:D:1174:HOH:O	2.18	0.43
1:A:126:PRO:O	1:A:130:GLU:HG3	2.19	0.43
1:C:168:GLU:CG	1:C:202:GLU:OE1	2.67	0.43
1:C:130:GLU:HG3	3:C:3229:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:LEU:HA	1:C:144:LYS:HE3	2.01	0.43
1:C:160:LYS:NZ	3:C:3103:HOH:O	2.39	0.43
1:B:120:MET:CG	3:B:2085:HOH:O	2.64	0.42
1:C:63:GLN:O	1:C:67:MET:HG2	2.19	0.42
1:C:124:SER:HB2	1:C:126:PRO:HD2	2.01	0.42
1:D:257:THR:HG22	1:D:261:LYS:HE3	2.01	0.42
1:C:35:ARG:HG2	1:C:35:ARG:NH1	2.33	0.42
1:D:170:PHE:CD2	1:D:236:MET:HE1	2.54	0.42
1:A:4:GLU:OE2	1:B:159:LYS:NZ	2.51	0.42
1:A:196:ARG:HH21	1:A:295:SER:HB3	1.84	0.42
1:D:221:SER:OG	1:D:224:GLU:HG3	2.20	0.42
1:A:16:VAL:HG12	1:B:75:LEU:HD11	2.01	0.42
1:C:118:ILE:HD13	1:C:191:THR:HG23	2.01	0.42
1:D:15:PRO:HG3	3:D:1256:HOH:O	2.20	0.41
1:D:143:ARG:HD3	3:D:1236:HOH:O	2.21	0.41
1:B:44:GLU:CD	3:B:2041:HOH:O	2.59	0.41
1:B:69:VAL:HG13	1:B:175:GLY:CA	2.50	0.41
1:A:35:ARG:NH1	1:A:35:ARG:CG	2.84	0.41
1:D:222:GLU:HG2	3:D:1175:HOH:O	2.19	0.41
1:A:164:SER:O	1:A:168:GLU:HG3	2.20	0.41
1:D:253:ASP:HB2	3:D:1091:HOH:O	2.19	0.41
1:B:89:LEU:HB2	1:B:90:PRO:HD3	2.03	0.41
1:D:69:VAL:HG23	1:D:250:ILE:HG21	2.01	0.41
1:C:124:SER:CB	1:C:126:PRO:HD2	2.50	0.41
1:C:185:ARG:HH11	1:C:185:ARG:HG3	1.86	0.41
1:D:28:LYS:HE2	1:D:32:VAL:HG23	2.03	0.41
1:A:143:ARG:HD3	3:A:2413:HOH:O	2.19	0.40
1:A:173:TYR:CB	3:A:2074:HOH:O	2.69	0.40
1:D:139:GLU:CD	1:D:139:GLU:N	2.68	0.40
1:D:288:VAL:O	1:D:289:SER:C	2.61	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	294/329 (89%)	291 (99%)	3 (1%)	0	100	100
1	B	294/329 (89%)	290 (99%)	4 (1%)	0	100	100
1	C	294/329 (89%)	291 (99%)	3 (1%)	0	100	100
1	D	294/329 (89%)	288 (98%)	6 (2%)	0	100	100
All	All	1176/1316 (89%)	1160 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	265/293 (90%)	262 (99%)	3 (1%)	65	57
1	B	265/293 (90%)	263 (99%)	2 (1%)	73	67
1	C	265/293 (90%)	265 (100%)	0	100	100
1	D	265/293 (90%)	257 (97%)	8 (3%)	36	21
All	All	1060/1172 (90%)	1047 (99%)	13 (1%)	63	55

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	253	ASP
1	A	270	LYS
1	A	295	SER
1	B	139	GLU
1	B	288	VAL
1	D	28	LYS
1	D	69	VAL
1	D	89	LEU
1	D	127	GLN
1	D	139	GLU

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Mol	Chain	Res	Type
1	D	237	TYR
1	D	258	GLU
1	D	295	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	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	140	ASN
1	B	190	ASN
1	B	215	GLN
1	B	273	ASN
1	C	11	ASN
1	C	153	ASN
1	C	215	GLN
1	C	225	GLN
1	D	39	ASN
1	D	127	GLN
1	D	140	ASN
1	D	273	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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 [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	296/329 (89%)	-0.52	7 (2%) 59 63	9, 16, 32, 59	0
1	B	296/329 (89%)	-0.44	1 (0%) 90 92	10, 17, 34, 57	0
1	C	296/329 (89%)	-0.50	4 (1%) 73 77	10, 16, 33, 56	0
1	D	296/329 (89%)	-0.27	3 (1%) 79 83	9, 20, 37, 54	0
All	All	1184/1316 (89%)	-0.43	15 (1%) 75 79	9, 17, 34, 59	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	4.3
1	A	174	SER	4.3
1	D	237	TYR	3.9
1	A	296	LEU	3.7
1	C	297	SER	3.1
1	A	172	PHE	3.1
1	D	2	SER	2.9
1	C	172	PHE	2.7
1	C	173	TYR	2.5
1	A	297	SER	2.4
1	C	296	LEU	2.3
1	B	10	ALA	2.2
1	A	295	SER	2.2
1	A	3	ASN	2.1
1	D	297	SER	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	D	1003	1/1	0.98	0.05	20,20,20,20	1
2	FE	B	1002	1/1	0.99	0.02	19,19,19,19	1
2	FE	C	3001	1/1	0.99	0.03	16,16,16,16	1
2	FE	A	1001	1/1	0.99	0.06	15,15,15,15	1
2	FE	A	2001	1/1	1.00	0.04	16,16,16,16	0
2	FE	C	3002	1/1	1.00	0.01	16,16,16,16	1
2	FE	B	2002	1/1	1.00	0.03	15,15,15,15	1
2	FE	D	1004	1/1	1.00	0.02	17,17,17,17	1

6.5 Other polymers [i](#)

There are no such residues in this entry.