



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2025 – 10:38 AM EDT

PDB ID : 1OQU / pdb_00001oqu
Title : A protein coordinated tri-nuclear Fe complex formed during soaking of crystals of the ribonucleotide reductase R2F protein from *Corynebacterium Ammonigenes*
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 ⓘ 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

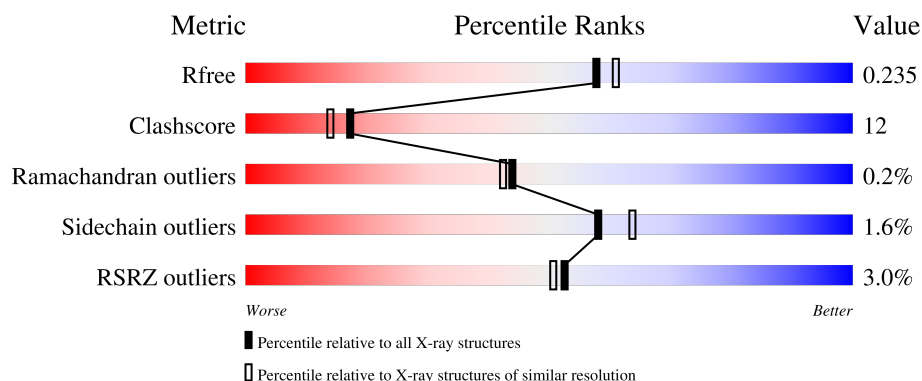
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 $\leq 5\%$. 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	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>18%</div> <div>10%</div> </div> </div>
1	B	329	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>25%</div> <div>10%</div> </div> </div>
1	C	329	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>20%</div> <div>8%</div> </div> </div>
1	D	329	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>19%</div> <div>10%</div> </div> </div>

2 Entry composition

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.

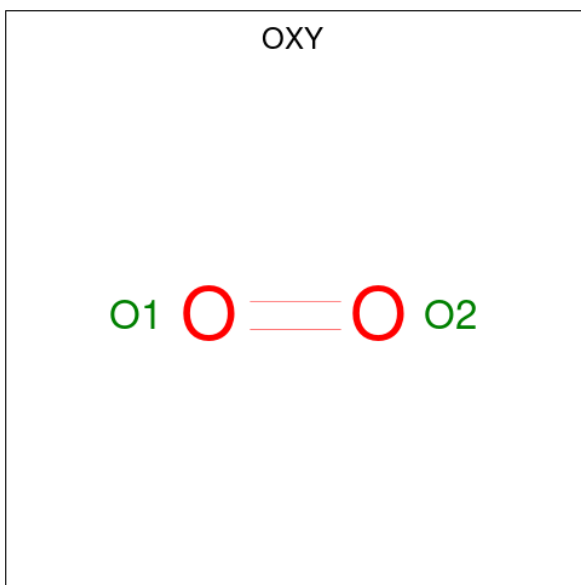
- Molecule 1 is a protein called ribonucleotide reductase subunit R2F.

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 (CCD ID: FE) (formula: Fe).

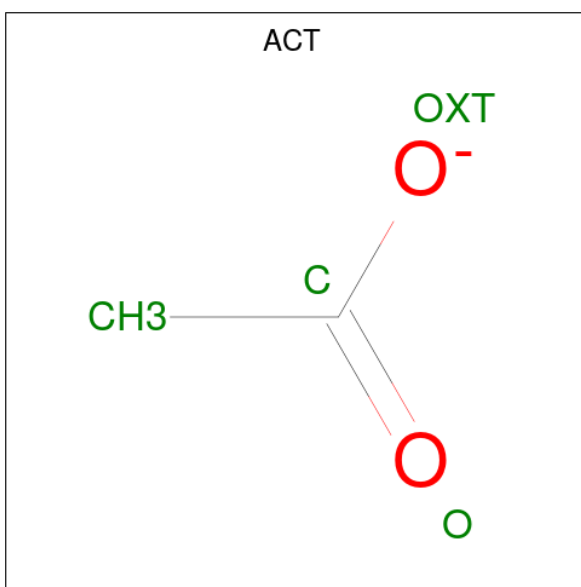
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Fe	0	0
			5	5		
2	B	5	Total	Fe	0	0
			5	5		
2	C	5	Total	Fe	0	0
			5	5		
2	D	5	Total	Fe	0	0
			5	5		

- Molecule 3 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

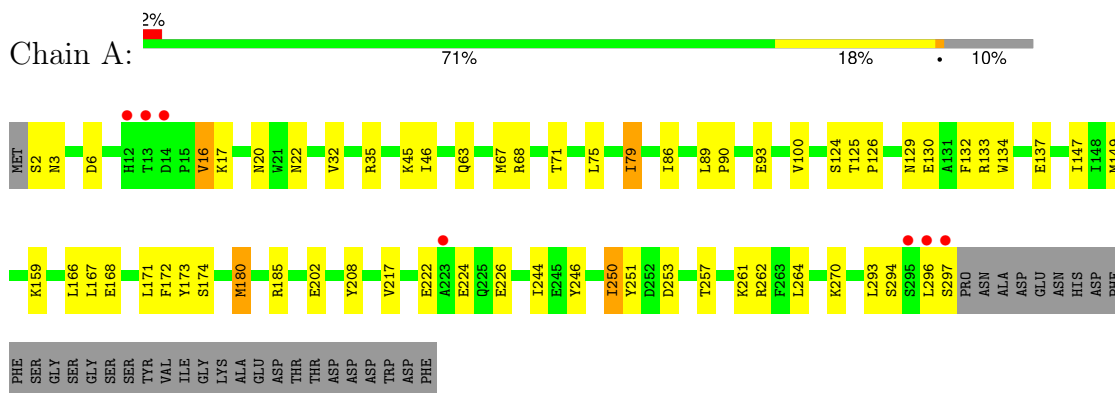
- Molecule 5 is water.

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

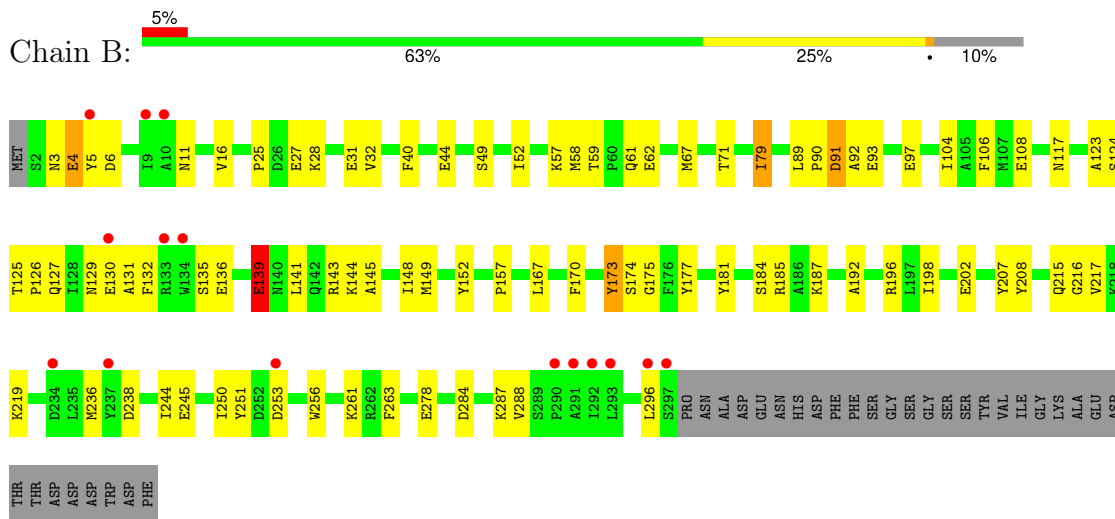
3 Residue-property plots [i](#)

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.

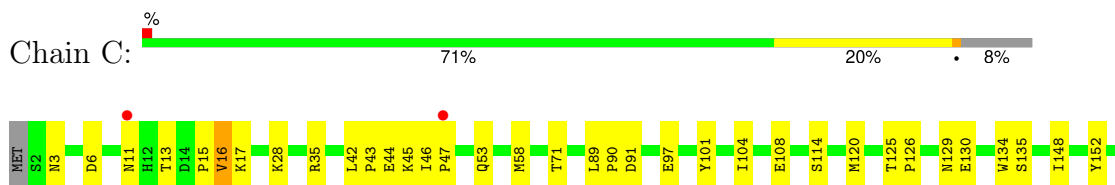
• Molecule 1: ribonucleotide reductase subunit R2F

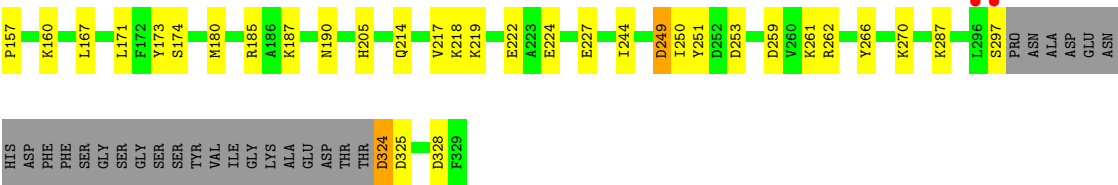


• Molecule 1: ribonucleotide reductase subunit R2F

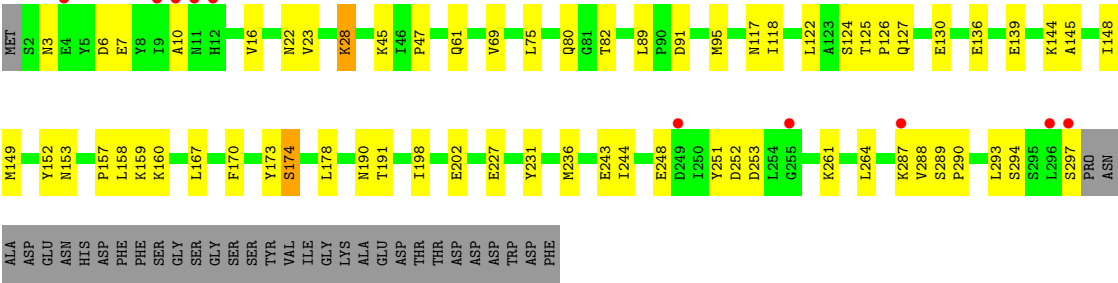


• Molecule 1: ribonucleotide reductase subunit R2F





● Molecule 1: ribonucleotide reductase subunit R2F



4 Data and refinement statistics

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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 98.4 (20.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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	4038 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)	0.40 , 70.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: ACT, OXY, 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	0.80	1/2477 (0.0%)	1.04	8/3365 (0.2%)
1	B	0.67	0/2477	0.98	9/3365 (0.3%)
1	C	0.87	0/2537	1.02	4/3445 (0.1%)
1	D	0.81	1/2477 (0.0%)	1.04	7/3365 (0.2%)
All	All	0.79	2/9968 (0.0%)	1.02	28/13540 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	95	MET	SD-CE	-7.45	1.60	1.79
1	A	180	MET	SD-CE	5.04	1.92	1.79

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	TYR	N-CA-C	9.43	124.04	112.54
1	B	174	SER	N-CA-C	-8.36	102.18	112.38
1	A	173	TYR	N-CA-C	8.15	121.27	111.82
1	D	251	TYR	N-CA-C	7.41	122.50	113.38
1	B	173	TYR	N-CA-C	7.16	121.77	112.89
1	A	79	ILE	CB-CA-C	-6.80	103.26	111.97
1	D	174	SER	N-CA-C	-6.49	104.62	112.54
1	C	171	LEU	N-CA-C	6.32	118.98	111.71
1	C	251	TYR	N-CA-C	6.28	121.71	113.30
1	C	173	TYR	N-CA-C	6.18	120.55	112.89
1	A	251	TYR	N-CA-C	6.13	120.92	113.38
1	A	257	THR	N-CA-C	6.00	118.31	111.11
1	D	122	LEU	N-CA-C	5.97	120.58	113.12
1	B	251	TYR	N-CA-C	5.93	120.67	113.38
1	A	171	LEU	N-CA-C	5.87	118.46	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	16	VAL	N-CA-C	-5.83	101.28	109.21
1	D	289	SER	CA-C-N	5.80	125.66	119.28
1	D	289	SER	C-N-CA	5.80	125.66	119.28
1	A	16	VAL	N-CA-C	-5.70	101.36	108.89
1	B	123	ALA	N-CA-C	5.70	119.19	110.36
1	A	250	ILE	N-CA-C	5.45	116.94	111.00
1	B	256	TRP	N-CA-C	-5.37	106.77	113.38
1	B	184	SER	N-CA-C	-5.33	106.29	112.89
1	B	79	ILE	CB-CA-C	-5.26	105.13	112.02
1	A	147	ILE	N-CA-C	-5.16	105.50	110.72
1	B	139	GLU	N-CA-C	5.13	116.87	111.28
1	B	250	ILE	CB-CA-C	-5.04	105.59	111.94
1	D	16	VAL	N-CA-C	-5.02	101.36	108.58

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	55	0
1	B	2419	0	2331	83	0
1	C	2477	0	2365	62	0
1	D	2419	0	2331	47	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
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	12	0
5	C	234	0	0	25	1
5	D	180	0	0	10	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10489	0	9361	237	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 (237) 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:249:ASP:CG	5:C:1061:HOH:O	2.31	0.72
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
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:42:LEU:O	1:C:45:LYS:HB3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLU:CD	1:D:139:GLU:H	2.01	0.68
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:D:236:MET:HE3	1:D:236:MET:O	1.98	0.64
1:C:45:LYS:HG2	1:C:46:ILE:CD1	2.25	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:B:139:GLU:CD	1:B:139:GLU:H	2.08	0.62
1:A:35:ARG:HG2	1:A:35:ARG:HH11	1.64	0.61
1:B:57:LYS:O	1:B:57:LYS:HG2	1.99	0.61
1:A:167:LEU:C	1:A:167:LEU:HD23	2.25	0.61
1:B:236:MET:HE3	1:B:236:MET:O	1.99	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:HG3	1:C:185:ARG:HH11	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:174:SER:OG	5:C:1081:HOH:O	2.16	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:C:134:TRP:NE1	5:C:1240:HOH:O	2.33	0.58
1:D:117:ASN:ND2	5:D:1162:HOH:O	2.37	0.57
1:A:79:ILE:HD11	1:B:16:VAL:CG1	2.35	0.57
1:B:173:TYR:C	1:B:175:GLY:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:144:LYS:HZ3	1:D:243:GLU:CD	2.17	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:A:294:SER:C	1:A:296:LEU:H	2.17	0.52
1:A:180:MET:HA	1:A:180:MET:HE2	1.92	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: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: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: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:3:ASN:C	1:B:5:TYR:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:GLN:OE1	1:D:80:GLN:HA	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:91:ASP:CG	1:C:157:PRO:HB3	2.39	0.48
1:D:167:LEU:HD23	1:D:167:LEU:C	2.39	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:A:294:SER:C	1:A:296:LEU:N	2.71	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: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:B:173:TYR:C	1:B:175:GLY:H	2.21	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:B:167:LEU:HD23	1:B:167:LEU:C	2.40	0.46
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:HH11	1:C:35:ARG:HG2	1.81	0.46
1:D:47:PRO:HG2	1:D:190:ASN:OD1	2.16	0.46
1:B:44:GLU:CD	5:B:1017:HOH:O	2.58	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

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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:C:167:LEU:C	1:C:167:LEU:HD23	2.41	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:N	1:C:11:ASN:HD22	2.15	0.45
1:A:261:LYS:HD3	5:A:2183:HOH:O	2.16	0.45
1:C:44:GLU:CD	5:C:1021:HOH:O	2.57	0.45
1:D:118:ILE:HD13	1:D:191:THR:HG23	1.98	0.45
1:B:32:VAL:HG21	1:B:208:TYR:CD1	2.52	0.45
1:B:170:PHE:CD2	1:B:236:MET:HE1	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:61:GLN:HG2	1:B:253:ASP:CG	2.43	0.44
1:D:91:ASP:CG	1:D:157:PRO:HB3	2.43	0.44
1:C:120:MET:HE3	1:D:22:ASN:HA	2.00	0.44
1:D:170:PHE:CD2	1:D:236:MET:HE1	2.52	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: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: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:B:177:TYR:CD1	1:B:177:TYR:C	2.96	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:VAL:HG11	1:A:208:TYR:CE2	2.54	0.42
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:A:133:ARG:HE	1:A:137:GLU:CD	2.28	0.42
1:C:104:ILE:HG12	1:C:205:HIS:CD2	2.54	0.42
1:D:45:LYS:O	1:D:45:LYS:HG3	2.19	0.42
1:D:148:ILE:HG22	1:D:152:TYR:CE2	2.54	0.42
1:D:178:LEU:C	1:D:178:LEU:HD23	2.45	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: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:A:167:LEU:C	1:A:167:LEU:CD2	2.93	0.41
1:B:3:ASN:C	1:B:5:TYR:N	2.77	0.41
1:C:3:ASN:HB2	1:C:6:ASP:CG	2.46	0.41
1:C:91:ASP:CB	1:C:157:PRO:HB3	2.51	0.41
1:C:180:MET:HA	1:C:180:MET:HE2	2.03	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 sym-

metry 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%)	19	14
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%)	44	42

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%)	70	76
1	B	265/293 (90%)	261 (98%)	4 (2%)	60	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	271/293 (92%)	265 (98%)	6 (2%)	47	51
1	D	265/293 (90%)	261 (98%)	4 (2%)	60	66
All	All	1066/1172 (91%)	1049 (98%)	17 (2%)	58	64

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

Mol	Chain	Res	Type
1	A	217	VAL
1	A	253	ASP
1	A	270	LYS
1	B	91	ASP
1	B	139	GLU
1	B	217	VAL
1	B	245	GLU
1	C	13	THR
1	C	53	GLN
1	C	217	VAL
1	C	249	ASP
1	C	250	ILE
1	C	324	ASP
1	D	28	LYS
1	D	69	VAL
1	D	89	LEU
1	D	297	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	50	ASN
1	A	153	ASN
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	129	ASN
1	B	153	ASN
1	B	215	GLN

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Mol	Chain	Res	Type
1	B	273	ASN
1	C	11	ASN
1	C	129	ASN
1	C	140	ASN
1	C	190	ASN
1	C	225	GLN
1	D	11	ASN
1	D	39	ASN
1	D	127	GLN
1	D	140	ASN
1	D	153	ASN
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 oligosaccharides 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	1.16	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, 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%)	-0.24	7 (2%) 59 58	13, 26, 62, 92	0
1	B	296/329 (89%)	0.32	15 (5%) 34 32	17, 38, 74, 106	0
1	C	302/329 (91%)	-0.42	4 (1%) 74 73	11, 23, 51, 75	0
1	D	296/329 (89%)	-0.15	10 (3%) 48 46	12, 28, 68, 93	0
All	All	1190/1316 (90%)	-0.12	36 (3%) 52 51	11, 29, 68, 106	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	10	ALA	4.5
1	A	297	SER	4.5
1	C	11	ASN	4.0
1	B	253	ASP	3.6
1	B	297	SER	3.6
1	B	234	ASP	3.5
1	A	296	LEU	3.4
1	B	293	LEU	3.0
1	D	11	ASN	3.0
1	C	297	SER	2.8
1	D	12	HIS	2.8
1	B	10	ALA	2.7
1	A	12	HIS	2.7
1	D	249	ASP	2.7
1	D	296	LEU	2.6
1	B	291	ALA	2.6
1	A	13	THR	2.6
1	B	9	ILE	2.5
1	B	134	TRP	2.5
1	B	296	LEU	2.5
1	B	290	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	255	GLY	2.4
1	A	14	ASP	2.4
1	B	292	ILE	2.4
1	D	9	ILE	2.4
1	A	223	ALA	2.3
1	C	296	LEU	2.3
1	D	287	LYS	2.2
1	D	297	SER	2.2
1	B	133	ARG	2.2
1	B	5	TYR	2.2
1	A	295	SER	2.2
1	B	130	GLU	2.2
1	D	4	GLU	2.1
1	B	237	TYR	2.0
1	C	47	PRO	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, 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(\AA^2)	Q<0.9
2	FE	B	1007	1/1	0.87	0.28	32,32,32,32	1
2	FE	B	1005	1/1	0.89	0.20	26,26,26,26	1
2	FE	B	1006	1/1	0.92	0.21	36,36,36,36	1
2	FE	D	1013	1/1	0.92	0.14	45,45,45,45	1
2	FE	D	1014	1/1	0.94	0.06	34,34,34,34	1
3	OXY	A	2004	1/2	0.94	0.07	26,26,26,26	0
4	ACT	C	1011	4/4	0.94	0.13	28,30,31,41	0
3	OXY	D	1015	1/2	0.95	0.15	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE	D	1012	1/1	0.95	0.09	31,31,31,31	1
2	FE	A	2002	1/1	0.96	0.05	28,28,28,28	1
2	FE	A	2003	1/1	0.98	0.04	30,30,30,30	1
2	FE	A	2001	1/1	0.98	0.06	26,26,26,26	1
2	FE	C	1010	1/1	0.99	0.07	25,25,25,25	0
2	FE	D	1004	1/1	0.99	0.01	16,16,16,16	0
2	FE	B	1004	1/1	0.99	0.03	22,22,22,22	0
2	FE	A	1002	1/1	0.99	0.05	26,26,26,26	0
2	FE	A	1001	1/1	0.99	0.05	31,31,31,31	0
2	FE	B	1003	1/1	0.99	0.03	27,27,27,27	0
3	OXY	C	1012	1/2	0.99	0.10	18,18,18,18	0
2	FE	C	1001	1/1	0.99	0.05	31,31,31,31	1
2	FE	C	1002	1/1	0.99	0.08	23,23,23,23	1
2	FE	D	1003	1/1	1.00	0.04	19,19,19,19	0
2	FE	C	1009	1/1	1.00	0.06	26,26,26,26	0
2	FE	C	1008	1/1	1.00	0.04	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.