



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:09 AM UTC

PDB ID : 3EQQ / pdb_00003eqq
Title : Apo Toluene 2,3-Dioxygenase
Authors : Friemann, R.; Lee, K.; Brown, E.N.; Gibson, D.T.; Eklund, H.; Ramaswamy, S.
Deposited on : 2008-10-01
Resolution : 3.20 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
Mogul : 2022.3.0, CSD as543be (2022)
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

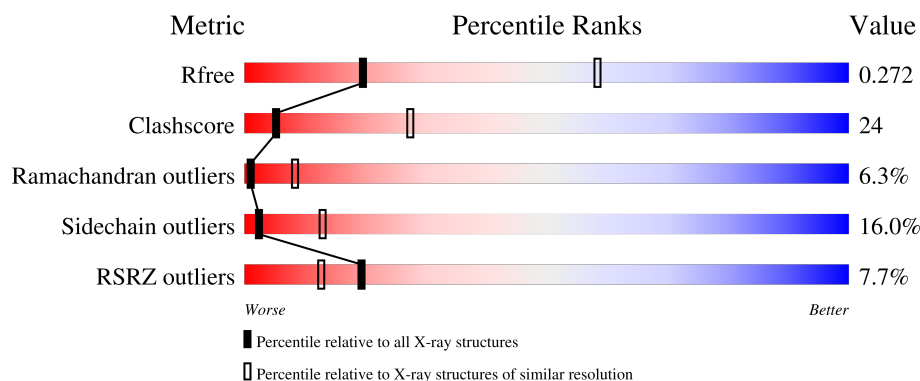
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	450	
2	B	187	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	A	451	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4826 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.

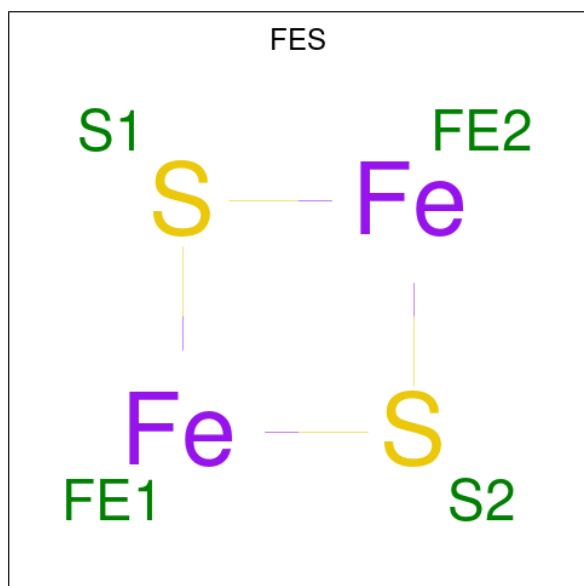
- Molecule 1 is a protein called Benzene 1,2-dioxygenase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3322	2100	576	626	20			

- Molecule 2 is a protein called Benzene 1,2-dioxygenase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	180	Total	C	N	O	S	0	0	0
			1499	947	267	280	5			

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		

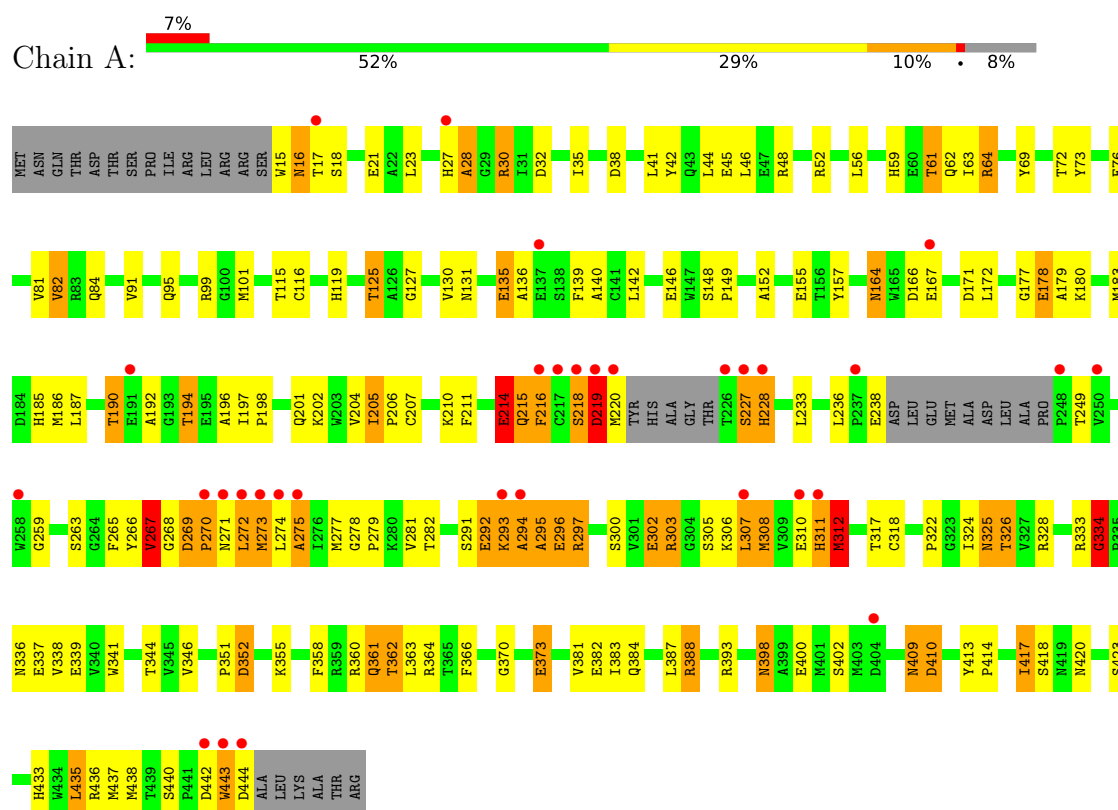
- Molecule 4 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Fe	0	0
			1	1		

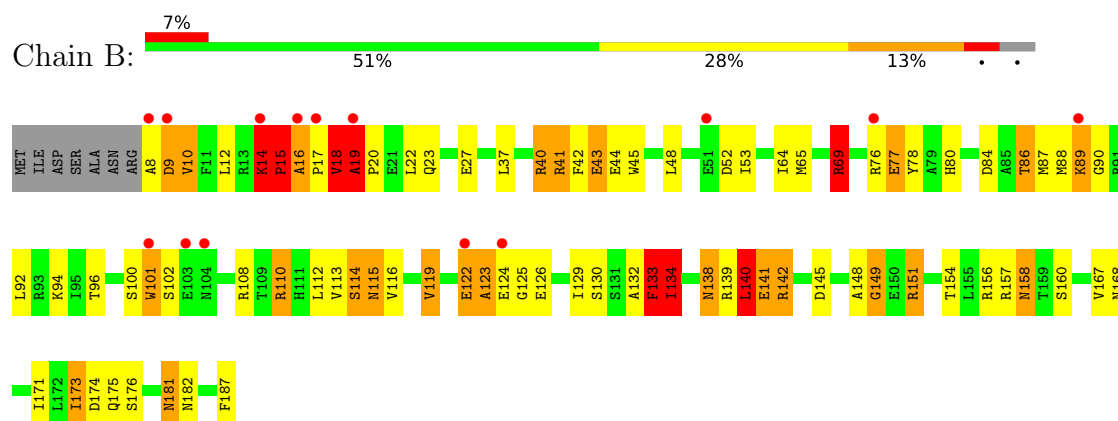
3 Residue-property plots

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: Benzene 1,2-dioxygenase subunit alpha



- Molecule 2: Benzene 1,2-dioxygenase subunit beta



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	235.87Å 235.87Å 235.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20 48.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.17-3.20) 95.7 (48.17-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 3.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.245 , 0.279 0.236 , 0.272	Depositor DCC
R_{free} test set	1805 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	83.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4826	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.85% 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: FE2, FES

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	0.93	1/3413 (0.0%)	1.14	16/4634 (0.3%)
2	B	0.94	1/1532 (0.1%)	1.25	16/2067 (0.8%)
All	All	0.94	2/4945 (0.0%)	1.17	32/6701 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
2	B	0	3
All	All	0	7

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	18	VAL	N-CA	6.04	1.53	1.46
1	A	63	ILE	CA-CB	5.04	1.61	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	278	GLY	CA-C-N	9.56	131.79	119.84
1	A	278	GLY	C-N-CA	9.56	131.79	119.84
2	B	124	GLU	N-CA-C	8.45	121.33	111.02
1	A	214	GLU	N-CA-C	8.39	124.39	111.56
2	B	133	PHE	N-CA-C	7.84	127.50	110.80
2	B	14	LYS	CA-C-N	7.69	129.45	119.84
2	B	14	LYS	C-N-CA	7.69	129.45	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	19	ALA	N-CA-C	-7.46	93.31	109.81
2	B	114	SER	N-CA-C	7.10	125.92	110.80
1	A	197	ILE	CB-CA-C	-6.33	103.40	110.68
2	B	16	ALA	N-CA-C	-6.25	93.50	111.00
2	B	134	ILE	N-CA-C	5.99	121.79	109.34
1	A	334	GLY	CA-C-N	-5.95	113.51	120.12
1	A	334	GLY	C-N-CA	-5.95	113.51	120.12
1	A	148	SER	CA-C-N	-5.87	113.64	119.92
1	A	148	SER	C-N-CA	-5.87	113.64	119.92
1	A	370	GLY	N-CA-C	5.79	118.59	111.93
2	B	113	VAL	CA-C-N	-5.62	110.80	121.54
2	B	113	VAL	C-N-CA	-5.62	110.80	121.54
1	A	131	ASN	N-CA-C	5.56	118.53	108.69
2	B	149	GLY	N-CA-C	5.51	117.44	110.38
1	A	135	GLU	N-CA-C	-5.44	106.60	113.18
2	B	12	LEU	N-CA-C	-5.32	105.64	111.82
1	A	82	VAL	N-CA-C	5.31	115.76	108.12
1	A	205	ILE	N-CA-CB	-5.25	103.87	111.21
1	A	297	ARG	N-CA-C	-5.23	105.76	111.82
2	B	65	MET	N-CA-C	5.14	117.55	111.33
2	B	15	PRO	CA-C-N	5.12	130.91	121.70
2	B	15	PRO	C-N-CA	5.12	130.91	121.70
1	A	440	SER	CA-C-N	-5.08	115.15	120.94
1	A	440	SER	C-N-CA	-5.08	115.15	120.94
2	B	125	GLY	N-CA-C	-5.07	98.60	113.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	GLU	Peptide
1	A	219	ASP	Peptide
1	A	227	SER	Peptide
1	A	334	GLY	Peptide
2	B	123	ALA	Peptide
2	B	132	ALA	Peptide
2	B	18	VAL	Peptide

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	3322	0	3149	155	0
2	B	1499	0	1451	84	0
3	A	4	0	0	3	0
4	B	1	0	0	0	0
All	All	4826	0	4600	230	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 24.

All (230) 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:207:CYS:HA	1:A:384:GLN:HG3	1.18	1.16
1:A:269:ASP:HB2	1:A:270:PRO:HD2	1.18	1.14
2:B:19:ALA:HB3	2:B:20:PRO:HA	1.31	1.06
2:B:14:LYS:H	2:B:14:LYS:HD2	1.21	1.02
1:A:116:CYS:HG	3:A:451:FES:FE2	0.74	0.97
1:A:291:SER:O	1:A:295:ALA:HB3	1.62	0.96
1:A:216:PHE:HD1	1:A:216:PHE:H	1.02	0.95
1:A:296:GLU:OE2	1:A:296:GLU:HA	1.67	0.92
2:B:19:ALA:HB3	2:B:20:PRO:CA	2.00	0.92
2:B:108:ARG:HE	2:B:138:ASN:ND2	1.67	0.91
2:B:84:ASP:H	2:B:87:MET:HE3	1.37	0.90
1:A:344:THR:OG1	1:A:362:THR:HG21	1.72	0.90
2:B:139:ARG:NH2	2:B:181:ASN:HD21	1.73	0.85
1:A:216:PHE:HD1	1:A:216:PHE:N	1.76	0.84
1:A:269:ASP:HB2	1:A:270:PRO:CD	2.06	0.83
2:B:158:ASN:HD22	2:B:160:SER:H	1.24	0.82
1:A:164:ASN:ND2	1:A:166:ASP:H	1.77	0.82
1:A:205:ILE:HG23	1:A:205:ILE:O	1.78	0.82
1:A:205:ILE:CG2	1:A:338:VAL:HG12	2.09	0.81
2:B:15:PRO:HB2	2:B:16:ALA:HA	1.62	0.81
2:B:14:LYS:H	2:B:14:LYS:CD	1.94	0.80
2:B:139:ARG:HH22	2:B:181:ASN:ND2	1.81	0.79
1:A:227:SER:O	1:A:228:HIS:HB2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:CB	1:A:270:PRO:HD2	2.07	0.77
2:B:15:PRO:HB2	2:B:16:ALA:CA	2.14	0.77
1:A:207:CYS:CA	1:A:384:GLN:HG3	2.06	0.77
1:A:201:GLN:HE21	2:B:80:HIS:HD2	1.32	0.77
1:A:294:ALA:O	1:A:297:ARG:HG3	1.86	0.75
1:A:164:ASN:HD22	1:A:166:ASP:H	1.32	0.73
1:A:186:MET:HB2	1:A:322:PRO:HB3	1.70	0.72
1:A:328:ARG:NH1	1:A:373:GLU:OE2	2.22	0.72
2:B:108:ARG:HE	2:B:138:ASN:HD22	1.38	0.72
2:B:139:ARG:NH2	2:B:181:ASN:ND2	2.36	0.71
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.55	0.71
1:A:84:GLN:OE1	1:A:125:THR:HG22	1.90	0.71
1:A:277:MET:HA	1:A:361:GLN:HG2	1.72	0.71
2:B:19:ALA:HB1	2:B:22:LEU:HB3	1.72	0.70
2:B:133:PHE:HD2	2:B:148:ALA:C	1.99	0.70
1:A:119:HIS:HB2	3:A:451:FES:S1	2.31	0.70
1:A:205:ILE:HG22	1:A:338:VAL:O	1.92	0.70
1:A:205:ILE:O	1:A:205:ILE:CG2	2.39	0.70
1:A:310:GLU:HB3	1:A:322:PRO:HG2	1.73	0.70
2:B:14:LYS:HD2	2:B:14:LYS:N	2.03	0.69
1:A:266:TYR:O	1:A:267:VAL:HG13	1.92	0.69
1:A:302:GLU:HA	1:A:306:LYS:HB2	1.73	0.69
1:A:205:ILE:HG23	1:A:338:VAL:HG12	1.76	0.67
1:A:211:PHE:O	1:A:215:GLN:HB2	1.95	0.66
2:B:10:VAL:HG13	2:B:119:VAL:HG21	1.78	0.66
1:A:21:GLU:HA	1:A:435:LEU:HD21	1.77	0.66
1:A:15:TRP:O	1:A:16:ASN:CB	2.43	0.66
1:A:302:GLU:HG3	1:A:303:ARG:N	2.11	0.66
2:B:154:THR:HB	2:B:168:ASN:HB2	1.78	0.66
2:B:9:ASP:O	2:B:10:VAL:HB	1.96	0.65
1:A:202:LYS:HD3	1:A:341:TRP:CE2	2.31	0.65
2:B:133:PHE:HB2	2:B:149:GLY:O	1.97	0.65
2:B:149:GLY:HA2	2:B:174:ASP:OD2	1.97	0.64
2:B:19:ALA:CB	2:B:23:GLN:H	2.11	0.64
1:A:442:ASP:O	1:A:443:TRP:HB2	1.97	0.64
2:B:84:ASP:HB3	2:B:86:THR:H	1.62	0.63
1:A:205:ILE:CG2	1:A:338:VAL:CG1	2.76	0.63
1:A:311:HIS:O	1:A:312:MET:HB2	1.99	0.63
1:A:417:ILE:N	1:A:417:ILE:HD12	2.14	0.62
2:B:69:ARG:NH1	2:B:69:ARG:HB3	2.13	0.62
1:A:101:MET:HE2	1:A:101:MET:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:LEU:O	2:B:96:THR:HG23	1.99	0.62
2:B:69:ARG:H	2:B:69:ARG:HD2	1.65	0.61
1:A:358:PHE:O	1:A:362:THR:HB	2.02	0.60
1:A:324:ILE:O	1:A:325:ASN:HB2	1.99	0.60
1:A:387:LEU:O	1:A:393:ARG:HD2	2.01	0.60
1:A:185:HIS:NE2	1:A:303:ARG:HD3	2.16	0.60
1:A:362:THR:HG22	2:B:78:TYR:HE1	1.67	0.59
1:A:274:LEU:O	1:A:275:ALA:HB3	2.03	0.59
2:B:19:ALA:CB	2:B:20:PRO:CA	2.79	0.59
1:A:61:THR:HG21	1:A:196:ALA:O	2.03	0.58
1:A:334:GLY:C	1:A:336:ASN:H	2.11	0.58
1:A:269:ASP:H	1:A:308:MET:HE2	1.67	0.58
2:B:19:ALA:CB	2:B:22:LEU:HB3	2.33	0.58
1:A:216:PHE:N	1:A:216:PHE:CD1	2.48	0.58
1:A:81:VAL:HG22	1:A:91:VAL:HG22	1.86	0.57
2:B:9:ASP:O	2:B:10:VAL:CB	2.52	0.57
1:A:116:CYS:SG	3:A:451:FES:FE2	1.86	0.57
1:A:272:LEU:HD23	1:A:308:MET:HA	1.85	0.57
1:A:190:THR:HG23	1:A:192:ALA:H	1.70	0.57
1:A:291:SER:O	1:A:295:ALA:CB	2.47	0.56
1:A:44:LEU:HD13	1:A:48:ARG:HH21	1.68	0.56
1:A:202:LYS:HD3	1:A:341:TRP:CD2	2.41	0.56
1:A:206:PRO:HA	1:A:337:GLU:HA	1.87	0.56
2:B:41:ARG:HD2	2:B:44:GLU:OE1	2.05	0.55
2:B:88:MET:O	2:B:89:LYS:C	2.50	0.55
1:A:273:MET:O	1:A:274:LEU:C	2.49	0.55
1:A:177:GLY:O	1:A:180:LYS:HE2	2.07	0.55
1:A:164:ASN:HD22	1:A:166:ASP:N	2.02	0.55
2:B:181:ASN:H	2:B:181:ASN:HD22	1.55	0.54
2:B:17:PRO:O	2:B:18:VAL:HG22	2.06	0.54
1:A:30:ARG:NH2	1:A:400:GLU:OE2	2.41	0.54
1:A:273:MET:HA	1:A:282:THR:OG1	2.08	0.54
2:B:140:LEU:O	2:B:141:GLU:HB2	2.07	0.54
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.22	0.54
1:A:219:ASP:OD1	1:A:219:ASP:N	2.40	0.54
1:A:263:SER:HB2	1:A:312:MET:HG2	1.90	0.53
2:B:122:GLU:O	2:B:123:ALA:HB3	2.08	0.53
1:A:211:PHE:O	1:A:215:GLN:CB	2.56	0.53
1:A:16:ASN:HD21	1:A:18:SER:HB3	1.74	0.53
1:A:204:VAL:O	2:B:181:ASN:HA	2.08	0.52
1:A:346:VAL:HG21	1:A:355:LYS:HG2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:SER:HB2	2:B:101:TRP:HD1	1.74	0.52
1:A:270:PRO:HB3	1:A:274:LEU:HD12	1.92	0.52
1:A:293:LYS:O	1:A:295:ALA:N	2.42	0.52
2:B:133:PHE:CE1	2:B:151:ARG:HD2	2.44	0.51
2:B:171:ILE:HD13	2:B:187:PHE:HB2	1.92	0.51
2:B:115:ASN:N	2:B:115:ASN:ND2	2.58	0.51
2:B:27:GLU:HG2	2:B:116:VAL:HG21	1.93	0.51
1:A:157:TYR:OH	1:A:180:LYS:HB3	2.11	0.51
1:A:387:LEU:O	1:A:393:ARG:CD	2.59	0.51
2:B:158:ASN:ND2	2:B:160:SER:H	2.02	0.51
2:B:84:ASP:HB3	2:B:86:THR:N	2.26	0.50
1:A:32:ASP:OD1	1:A:32:ASP:C	2.53	0.50
2:B:8:ALA:O	2:B:9:ASP:HB2	2.11	0.50
1:A:164:ASN:HD22	1:A:164:ASN:C	2.19	0.50
1:A:333:ARG:NH1	1:A:339:GLU:OE2	2.45	0.50
1:A:351:PRO:O	1:A:352:ASP:C	2.54	0.50
1:A:265:PHE:HB3	1:A:310:GLU:HG3	1.94	0.50
1:A:56:LEU:HD22	1:A:318:CYS:SG	2.51	0.50
1:A:201:GLN:HE21	2:B:80:HIS:CD2	2.21	0.50
2:B:15:PRO:HB2	2:B:16:ALA:CB	2.41	0.49
2:B:116:VAL:HG23	2:B:116:VAL:O	2.12	0.49
1:A:139:PHE:HB3	1:A:142:LEU:HB2	1.94	0.49
2:B:108:ARG:HE	2:B:138:ASN:HD21	1.52	0.49
1:A:42:TYR:HA	1:A:45:GLU:HG3	1.95	0.49
1:A:127:GLY:O	1:A:149:PRO:HD2	2.13	0.48
1:A:211:PHE:HE1	1:A:384:GLN:HE21	1.61	0.48
1:A:91:VAL:HG12	1:A:152:ALA:HB3	1.96	0.48
1:A:402:SER:HB2	1:A:423:SER:HB2	1.96	0.48
2:B:15:PRO:CB	2:B:16:ALA:CA	2.90	0.48
2:B:151:ARG:NH1	2:B:187:PHE:OXT	2.44	0.48
1:A:268:GLY:O	1:A:269:ASP:CG	2.57	0.48
1:A:417:ILE:HD12	1:A:417:ILE:H	1.79	0.48
1:A:373:GLU:HG3	1:A:373:GLU:O	2.14	0.48
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.78	0.48
1:A:409:ASN:O	1:A:410:ASP:C	2.57	0.48
1:A:388:ARG:HG3	1:A:388:ARG:NH1	2.29	0.48
2:B:182:ASN:OD1	2:B:182:ASN:C	2.57	0.48
1:A:300:SER:HB3	1:A:303:ARG:HB2	1.95	0.47
2:B:158:ASN:ND2	2:B:160:SER:OG	2.48	0.47
2:B:45:TRP:O	2:B:48:LEU:HB2	2.15	0.47
1:A:185:HIS:NE2	1:A:303:ARG:CD	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:A:220:MET:N	2.48	0.47
1:A:398:ASN:C	1:A:398:ASN:HD22	2.23	0.47
1:A:292:GLU:C	1:A:293:LYS:O	2.58	0.47
1:A:268:GLY:O	1:A:269:ASP:CB	2.63	0.47
1:A:35:ILE:HA	1:A:41:LEU:HD23	1.97	0.46
1:A:398:ASN:ND2	1:A:400:GLU:H	2.12	0.46
2:B:10:VAL:HG13	2:B:119:VAL:CG2	2.43	0.46
1:A:272:LEU:HG	1:A:282:THR:HG23	1.97	0.46
1:A:179:ALA:O	1:A:183:MET:HG3	2.15	0.46
2:B:110:ARG:HA	2:B:110:ARG:HD3	1.52	0.46
1:A:328:ARG:NH2	1:A:366:PHE:O	2.48	0.46
1:A:274:LEU:O	1:A:275:ALA:CB	2.64	0.46
1:A:155:GLU:OE2	1:A:172:LEU:HB3	2.16	0.46
1:A:294:ALA:O	1:A:296:GLU:N	2.49	0.46
1:A:326:THR:HG21	1:A:328:ARG:HH21	1.79	0.46
2:B:157:ARG:NH1	2:B:157:ARG:HG2	2.31	0.46
2:B:171:ILE:CD1	2:B:187:PHE:HB2	2.46	0.46
1:A:15:TRP:O	1:A:16:ASN:HB3	2.16	0.46
1:A:72:THR:OG1	1:A:73:TYR:N	2.49	0.46
1:A:259:GLY:HA2	1:A:433:HIS:CE1	2.50	0.46
1:A:398:ASN:C	1:A:398:ASN:ND2	2.74	0.45
1:A:442:ASP:O	1:A:443:TRP:CB	2.64	0.45
1:A:300:SER:CB	1:A:303:ARG:HB2	2.45	0.45
2:B:18:VAL:HG23	2:B:19:ALA:HB2	1.99	0.45
1:A:300:SER:OG	1:A:303:ARG:HB2	2.15	0.45
1:A:362:THR:HG22	1:A:363:LEU:N	2.31	0.45
2:B:126:GLU:OE1	2:B:156:ARG:HD3	2.17	0.44
2:B:173:ILE:HA	2:B:173:ILE:HD12	1.74	0.44
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.75	0.44
1:A:69:TYR:CD1	1:A:69:TYR:C	2.94	0.44
2:B:84:ASP:O	2:B:88:MET:HG2	2.18	0.44
1:A:177:GLY:C	1:A:179:ALA:H	2.25	0.44
2:B:133:PHE:CD2	2:B:149:GLY:N	2.85	0.44
2:B:157:ARG:HG2	2:B:157:ARG:HH11	1.83	0.44
1:A:44:LEU:HB2	1:A:438:MET:HE1	1.99	0.44
1:A:307:LEU:HD23	1:A:307:LEU:HA	1.66	0.44
1:A:84:GLN:CD	1:A:125:THR:HG22	2.43	0.43
1:A:269:ASP:O	1:A:308:MET:HE2	2.17	0.43
1:A:362:THR:CG2	2:B:78:TYR:HE1	2.28	0.43
1:A:409:ASN:O	1:A:410:ASP:O	2.36	0.43
2:B:133:PHE:HD2	2:B:149:GLY:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PHE:O	1:A:215:GLN:HG3	2.18	0.43
1:A:15:TRP:O	1:A:16:ASN:HB2	2.17	0.43
2:B:115:ASN:N	2:B:115:ASN:HD22	2.15	0.43
1:A:44:LEU:O	1:A:45:GLU:C	2.61	0.43
1:A:334:GLY:CA	1:A:336:ASN:H	2.32	0.43
1:A:164:ASN:ND2	1:A:166:ASP:N	2.57	0.43
2:B:114:SER:O	2:B:116:VAL:N	2.52	0.43
1:A:59:HIS:H	1:A:62:GLN:NE2	2.17	0.43
2:B:88:MET:C	2:B:90:GLY:N	2.77	0.43
1:A:187:LEU:HD23	1:A:194:THR:HG21	2.01	0.43
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.80	0.43
1:A:334:GLY:HA3	1:A:336:ASN:H	1.83	0.43
2:B:52:ASP:O	2:B:53:ILE:C	2.62	0.43
1:A:388:ARG:HA	1:A:388:ARG:HD2	1.70	0.42
1:A:409:ASN:HD22	1:A:409:ASN:C	2.27	0.42
2:B:129:ILE:CG2	2:B:130:SER:N	2.81	0.42
1:A:334:GLY:C	1:A:336:ASN:N	2.69	0.42
2:B:52:ASP:OD1	2:B:52:ASP:N	2.53	0.42
1:A:23:LEU:HD13	1:A:35:ILE:HG22	2.01	0.42
1:A:360:ARG:HE	2:B:87:MET:HE1	1.85	0.42
1:A:382:GLU:O	1:A:383:ILE:C	2.62	0.42
2:B:40:ARG:HE	2:B:40:ARG:HB2	1.73	0.42
2:B:53:ILE:O	2:B:53:ILE:HG23	2.20	0.42
1:A:413:TYR:HA	1:A:414:PRO:HD3	1.94	0.42
1:A:27:HIS:O	1:A:28:ALA:CB	2.68	0.42
1:A:269:ASP:N	1:A:308:MET:HE2	2.34	0.42
1:A:52:ARG:HG2	1:A:166:ASP:OD1	2.20	0.41
1:A:402:SER:CB	1:A:423:SER:HB2	2.49	0.41
1:A:215:GLN:HB3	1:A:216:PHE:HA	2.02	0.41
1:A:360:ARG:NE	2:B:87:MET:HE1	2.35	0.41
2:B:19:ALA:HB1	2:B:23:GLN:H	1.84	0.41
1:A:38:ASP:HB3	1:A:41:LEU:HB2	2.02	0.41
2:B:42:PHE:O	2:B:43:GLU:C	2.64	0.41
2:B:133:PHE:HE1	2:B:151:ARG:HD2	1.84	0.41
2:B:101:TRP:N	2:B:101:TRP:CD1	2.89	0.41
1:A:198:PRO:HG2	2:B:77:GLU:HB3	2.01	0.40
1:A:206:PRO:HG2	1:A:381:VAL:HG13	2.03	0.40
1:A:99:ARG:HD3	1:A:99:ARG:HA	1.94	0.40
1:A:273:MET:C	1:A:274:LEU:O	2.64	0.40
1:A:333:ARG:HD2	1:A:339:GLU:OE2	2.22	0.40
1:A:364:ARG:HD3	2:B:87:MET:HG2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:THR:HB	1:A:328:ARG:HE	1.87	0.40
2:B:141:GLU:C	2:B:142:ARG:HG2	2.47	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	410/450 (91%)	336 (82%)	47 (12%)	27 (7%)	1	7
2	B	178/187 (95%)	150 (84%)	18 (10%)	10 (6%)	1	11
All	All	588/637 (92%)	486 (83%)	65 (11%)	37 (6%)	1	8

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	171	ASP
1	A	269	ASP
1	A	270	PRO
1	A	271	ASN
1	A	273	MET
1	A	275	ALA
1	A	293	LYS
1	A	294	ALA
2	B	10	VAL
2	B	15	PRO
2	B	19	ALA
2	B	69	ARG
2	B	134	ILE
1	A	17	THR
1	A	28	ALA

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Mol	Chain	Res	Type
1	A	136	ALA
1	A	215	GLN
1	A	219	ASP
1	A	267	VAL
1	A	295	ALA
1	A	352	ASP
2	B	18	VAL
1	A	125	THR
1	A	292	GLU
1	A	311	HIS
1	A	443	TRP
2	B	9	ASP
1	A	140	ALA
2	B	141	GLU
2	B	176	SER
1	A	279	PRO
1	A	312	MET
1	A	325	ASN
1	A	410	ASP
2	B	140	LEU
1	A	178	GLU

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	348/376 (93%)	298 (86%)	50 (14%)	3	16
2	B	159/165 (96%)	128 (80%)	31 (20%)	1	8
All	All	507/541 (94%)	426 (84%)	81 (16%)	2	13

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	61	THR

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Mol	Chain	Res	Type
1	A	64	ARG
1	A	76	GLU
1	A	82	VAL
1	A	95	GLN
1	A	115	THR
1	A	130	VAL
1	A	135	GLU
1	A	146	GLU
1	A	164	ASN
1	A	167	GLU
1	A	178	GLU
1	A	190	THR
1	A	194	THR
1	A	210	LYS
1	A	214	GLU
1	A	216	PHE
1	A	218	SER
1	A	219	ASP
1	A	228	HIS
1	A	233	LEU
1	A	236	LEU
1	A	238	GLU
1	A	249	THR
1	A	267	VAL
1	A	272	LEU
1	A	281	VAL
1	A	296	GLU
1	A	302	GLU
1	A	303	ARG
1	A	305	SER
1	A	307	LEU
1	A	308	MET
1	A	312	MET
1	A	317	THR
1	A	326	THR
1	A	361	GLN
1	A	362	THR
1	A	373	GLU
1	A	388	ARG
1	A	398	ASN
1	A	409	ASN
1	A	417	ILE

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Mol	Chain	Res	Type
1	A	418	SER
1	A	420	ASN
1	A	435	LEU
1	A	436	ARG
1	A	437	MET
1	A	444	ASP
2	B	14	LYS
2	B	37	LEU
2	B	40	ARG
2	B	41	ARG
2	B	43	GLU
2	B	64	ILE
2	B	69	ARG
2	B	76	ARG
2	B	77	GLU
2	B	86	THR
2	B	89	LYS
2	B	94	LYS
2	B	101	TRP
2	B	102	SER
2	B	110	ARG
2	B	112	LEU
2	B	115	ASN
2	B	119	VAL
2	B	122	GLU
2	B	133	PHE
2	B	134	ILE
2	B	138	ASN
2	B	140	LEU
2	B	142	ARG
2	B	145	ASP
2	B	151	ARG
2	B	158	ASN
2	B	167	VAL
2	B	173	ILE
2	B	175	GLN
2	B	181	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN

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Mol	Chain	Res	Type
1	A	27	HIS
1	A	62	GLN
1	A	164	ASN
1	A	398	ASN
1	A	409	ASN
1	A	420	ASN
2	B	38	ASN
2	B	80	HIS
2	B	115	ASN
2	B	138	ASN
2	B	143	GLN
2	B	158	ASN
2	B	168	ASN
2	B	181	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 2 ligands modelled in this entry, 1 is monoatomic - 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
3	FES	A	451	1	0,4,4	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FES	A	451	1	-	-	0/1/1/1

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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	451	FES	3	0

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	416/450 (92%)	0.37	32 (7%) 19 13	55, 72, 102, 115	0
2	B	180/187 (96%)	0.30	14 (7%) 19 12	57, 71, 91, 101	0
All	All	596/637 (93%)	0.35	46 (7%) 19 13	55, 72, 100, 115	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	7.8
1	A	444	ASP	6.9
1	A	273	MET	6.3
1	A	248	PRO	6.2
1	A	226	THR	5.7
2	B	8	ALA	5.2
1	A	217	CYS	5.1
1	A	294	ALA	4.6
1	A	218	SER	4.0
2	B	101	TRP	4.0
1	A	220	MET	3.9
1	A	307	LEU	3.6
1	A	293	LYS	3.5
1	A	219	ASP	3.4
1	A	271	ASN	3.4
1	A	270	PRO	3.2
1	A	191	GLU	3.2
2	B	124	GLU	3.1
2	B	51	GLU	3.1
1	A	443	TRP	3.0
1	A	442	ASP	3.0
1	A	27	HIS	3.0
2	B	19	ALA	2.9
1	A	237	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	228	HIS	2.8
1	A	258	TRP	2.8
2	B	17	PRO	2.8
1	A	227	SER	2.8
1	A	311	HIS	2.7
1	A	137	GLU	2.7
1	A	272	LEU	2.5
2	B	16	ALA	2.4
2	B	104	ASN	2.4
1	A	250	VAL	2.4
1	A	17	THR	2.4
1	A	404	ASP	2.4
2	B	103	GLU	2.3
2	B	89	LYS	2.2
2	B	14	LYS	2.2
1	A	216	PHE	2.2
2	B	76	ARG	2.2
2	B	122	GLU	2.2
1	A	275	ALA	2.1
2	B	9	ASP	2.1
1	A	167	GLU	2.1
1	A	310	GLU	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 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(Å ²)	Q<0.9
4	FE2	B	188	1/1	0.98	0.11	94,94,94,94	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FES	A	451	4/4	1.00	0.02	66,67,68,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.