



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:41 PM UTC

PDB ID : 8FFC / pdb_00008ffc
Title : Crystal structure of iron bound Dps protein (PA0962) from *Pseudomonas aeruginosa* (cubic form)
Authors : Lovell, S.; Kashipathy, M.M.; Battaile, K.P.; Rivera, M.
Deposited on : 2022-12-08
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
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

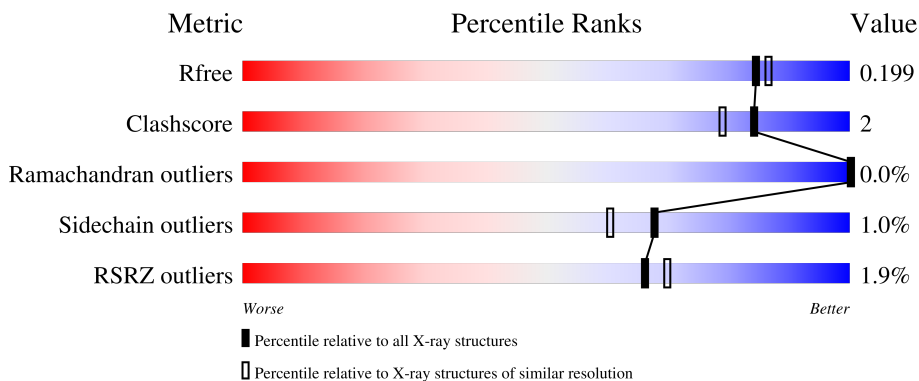
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	156	 90% 8% ..
1	B	156	 95% ..
1	C	156	 94% 6% .
1	D	156	 95% ..
1	E	156	 92% 8% .

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Mol	Chain	Length	Quality of chain
1	F	156	 3% 92% 7%
1	G	156	 % 95%
1	H	156	 % 96%
1	I	156	 % 93% 6%
1	J	156	 3% 90% 10%
1	K	156	 3% 94% 6%
1	L	156	 2% 92% 8%
1	M	156	 % 94% 5%
1	N	156	 2% 94% 5%
1	O	156	 5% 92% 8%
1	P	156	 2% 93% 6%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21761 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.

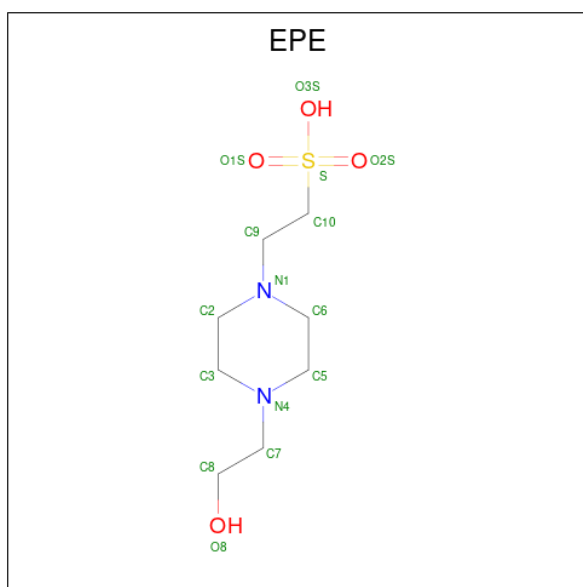
- Molecule 1 is a protein called Probable dna-binding stress protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	155	1215	774	206	229	6	0	3	0
1	B	155	1231	784	210	231	6	0	4	0
1	C	155	1220	777	208	229	6	0	3	0
1	D	155	1225	780	209	230	6	0	4	0
1	E	155	1218	776	208	228	6	0	4	0
1	F	155	1215	774	208	227	6	0	3	0
1	G	155	1221	776	209	230	6	0	3	0
1	H	155	1225	780	209	230	6	0	4	0
1	I	155	1226	781	209	230	6	0	4	0
1	J	155	1222	778	208	230	6	0	4	0
1	K	155	1215	774	207	228	6	0	3	0
1	L	155	1207	771	204	226	6	0	3	0
1	M	155	1230	783	209	232	6	0	4	0
1	N	155	1212	773	207	226	6	0	3	0
1	O	155	1221	777	208	230	6	0	4	0
1	P	155	1212	772	205	229	6	0	3	0

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Fe 4 4	0	0
2	B	8	Total Fe 8 8	0	0
2	C	4	Total Fe 4 4	0	0
2	D	4	Total Fe 4 4	0	0
2	E	5	Total Fe 5 5	0	0
2	F	3	Total Fe 3 3	0	0
2	G	4	Total Fe 4 4	0	0
2	H	4	Total Fe 4 4	0	0
2	I	4	Total Fe 4 4	0	0
2	J	2	Total Fe 2 2	0	0
2	K	3	Total Fe 3 3	0	0
2	L	2	Total Fe 2 2	0	0
2	M	6	Total Fe 6 6	0	0
2	N	2	Total Fe 2 2	0	0
2	O	6	Total Fe 6 6	0	0
2	P	2	Total Fe 2 2	0	0

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	Total 12	C 6	N 2	O 3	S 1	0	0
3	C	1	Total 12	C 6	N 2	O 3	S 1	0	0
3	E	1	Total 12	C 6	N 2	O 3	S 1	0	0
3	F	1	Total 12	C 6	N 2	O 3	S 1	0	0
3	M	1	Total 12	C 6	N 2	O 3	S 1	0	0
3	O	1	Total 12	C 6	N 2	O 3	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	113	Total 113	O 113	0	0
4	B	163	Total 163	O 163	0	0
4	C	114	Total 114	O 114	0	0
4	D	130	Total 130	O 130	0	0
4	E	131	Total 131	O 131	0	0
4	F	121	Total 121	O 121	0	0

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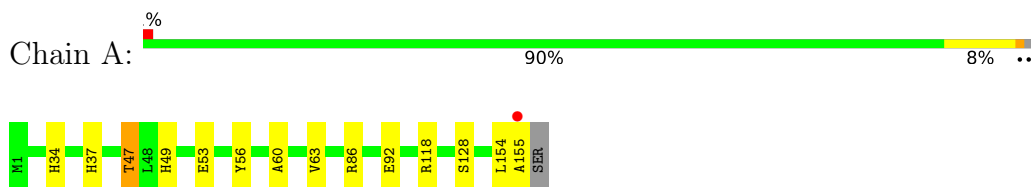
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	127	Total 127	O 127	0	0
4	H	162	Total 162	O 162	0	0
4	I	161	Total 161	O 161	0	0
4	J	110	Total 110	O 110	0	0
4	K	131	Total 131	O 131	0	0
4	L	131	Total 131	O 131	0	0
4	M	168	Total 168	O 168	0	0
4	N	128	Total 128	O 128	0	0
4	O	104	Total 104	O 104	0	0
4	P	117	Total 117	O 117	0	0

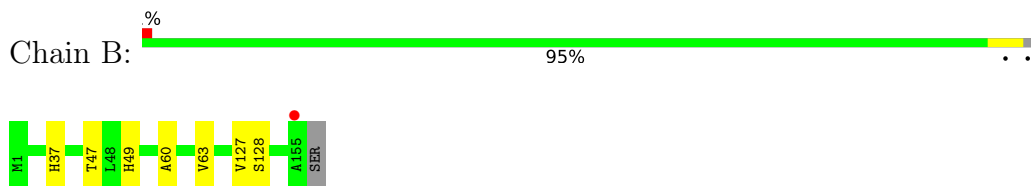
3 Residue-property plots [i](#)

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.

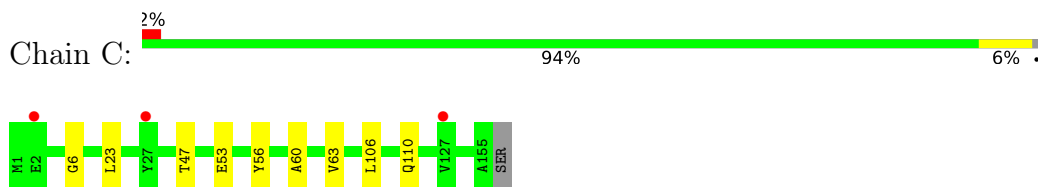
- Molecule 1: Probable dna-binding stress protein



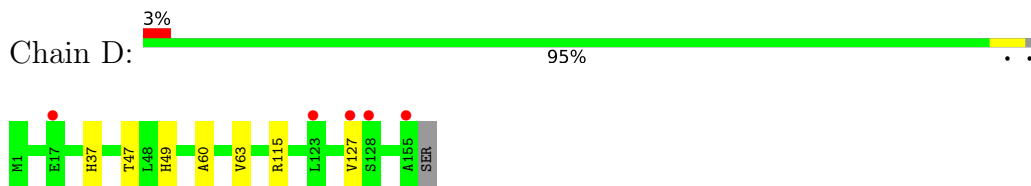
- Molecule 1: Probable dna-binding stress protein



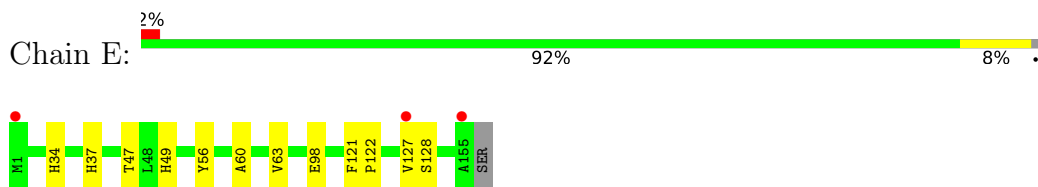
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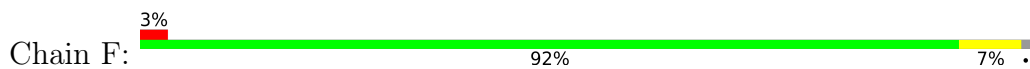
- Molecule 1: Probable dna-binding stress protein



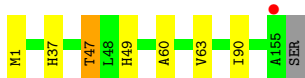
- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



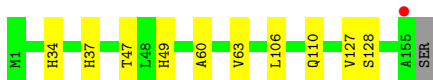
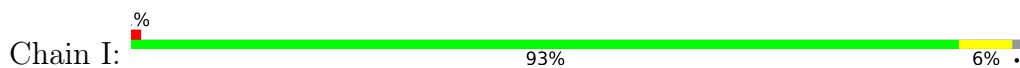
- Molecule 1: Probable dna-binding stress protein



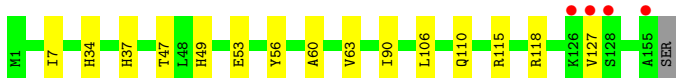
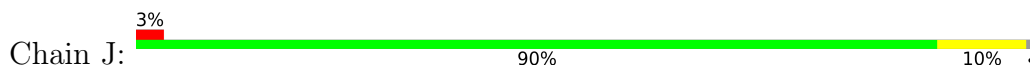
- Molecule 1: Probable dna-binding stress protein



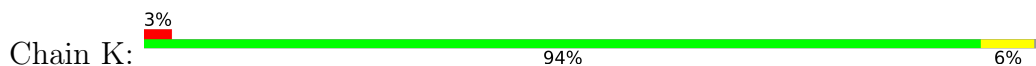
- Molecule 1: Probable dna-binding stress protein



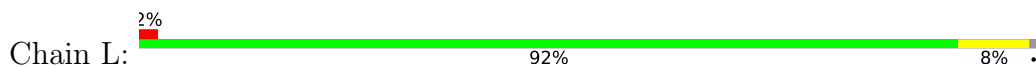
- Molecule 1: Probable dna-binding stress protein



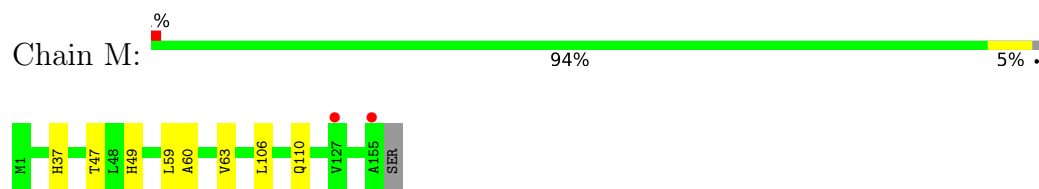
- Molecule 1: Probable dna-binding stress protein



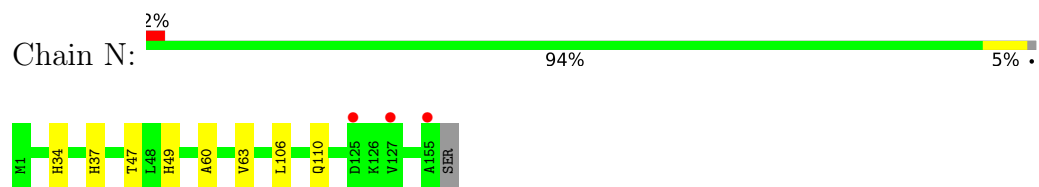
- Molecule 1: Probable dna-binding stress protein



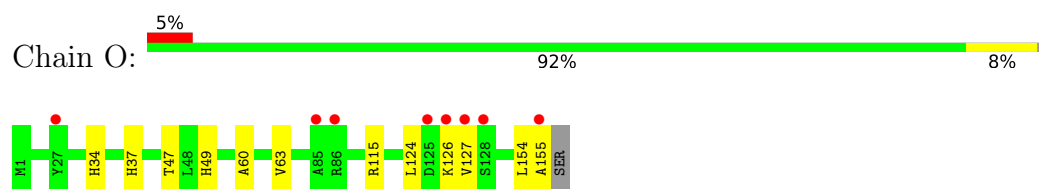
- Molecule 1: Probable dna-binding stress protein



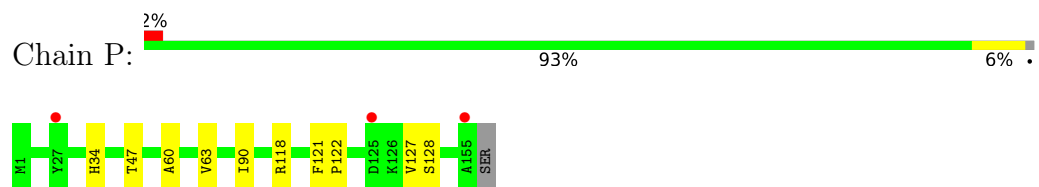
- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



- Molecule 1: Probable dna-binding stress protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	223.90Å 223.90Å 223.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.91 – 1.85 43.91 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (43.91-1.85) 100.0 (43.91-1.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.86Å)	Xtrriage
Refinement program	PHENIX 1.19rc5_4043	Depositor
R, R_{free}	0.162 , 0.192 0.171 , 0.199	Depositor DCC
R_{free} test set	15618 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21761	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.38% 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, EPE

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	0.40	0/1247	0.54	0/1696
1	B	0.47	0/1266	0.59	0/1719
1	C	0.40	0/1252	0.52	0/1702
1	D	0.43	0/1260	0.58	0/1712
1	E	0.43	0/1253	0.59	0/1704
1	F	0.42	0/1247	0.57	0/1696
1	G	0.44	0/1253	0.55	0/1704
1	H	0.45	0/1260	0.59	0/1712
1	I	0.45	0/1261	0.58	0/1713
1	J	0.40	0/1257	0.54	0/1709
1	K	0.44	0/1247	0.57	0/1696
1	L	0.46	0/1239	0.59	0/1686
1	M	0.46	0/1265	0.61	0/1718
1	N	0.43	0/1244	0.59	0/1692
1	O	0.41	0/1256	0.55	0/1708
1	P	0.39	0/1244	0.54	0/1693
All	All	0.43	0/20051	0.57	0/27260

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	H	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	118	ARG	Sidechain

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	1215	0	1203	8	0
1	B	1231	0	1234	6	0
1	C	1220	0	1212	8	0
1	D	1225	0	1224	6	0
1	E	1218	0	1211	8	0
1	F	1215	0	1206	8	0
1	G	1221	0	1212	5	0
1	H	1225	0	1224	6	0
1	I	1226	0	1226	7	0
1	J	1222	0	1215	9	0
1	K	1215	0	1205	6	0
1	L	1207	0	1193	10	0
1	M	1230	0	1230	4	0
1	N	1212	0	1202	3	0
1	O	1221	0	1213	6	0
1	P	1212	0	1197	6	0
2	A	4	0	0	0	0
2	B	8	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	5	0	0	0	0
2	F	3	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	0
2	J	2	0	0	0	0
2	K	3	0	0	0	0
2	L	2	0	0	0	0
2	M	6	0	0	0	0
2	N	2	0	0	0	0
2	O	6	0	0	0	0
2	P	2	0	0	0	0
3	A	12	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	12	0	0
3	E	12	0	12	0	0
3	F	12	0	12	0	0
3	M	12	0	12	1	0
3	O	12	0	12	0	0
4	A	113	0	0	2	0
4	B	163	0	0	0	0
4	C	114	0	0	0	0
4	D	130	0	0	2	0
4	E	131	0	0	0	0
4	F	121	0	0	1	0
4	G	127	0	0	1	0
4	H	162	0	0	1	0
4	I	161	0	0	0	0
4	J	110	0	0	1	0
4	K	131	0	0	1	0
4	L	131	0	0	2	0
4	M	168	0	0	0	0
4	N	128	0	0	0	0
4	O	104	0	0	1	0
4	P	117	0	0	2	0
All	All	21761	0	19479	90	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 2.

All (90) 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:G:47[A]:THR:HG22	4:G:404:HOH:O	1.81	0.80
1:D:47[A]:THR:HG22	4:D:405:HOH:O	1.85	0.74
1:P:47[A]:THR:HG22	4:P:393:HOH:O	1.92	0.69
1:F:47[A]:THR:HG23	1:L:47[A]:THR:HG21	1.76	0.66
1:B:47[A]:THR:HG21	1:K:47[A]:THR:HG23	1.75	0.66
1:B:47[A]:THR:HG23	1:E:47[A]:THR:HG21	1.79	0.64
1:D:47[A]:THR:HG23	1:J:47[A]:THR:HG21	1.83	0.61
1:G:47[A]:THR:HG23	1:H:47[A]:THR:HG21	1.85	0.59
1:P:118:ARG:NH1	4:P:304:HOH:O	2.33	0.58
1:I:47[A]:THR:HG21	1:L:47[A]:THR:HG23	1.86	0.57
1:H:60:ALA:O	1:H:63[A]:VAL:HG22	2.04	0.56
1:C:47[A]:THR:HG21	1:H:47[A]:THR:HG23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:ALA:O	1:J:63[A]:VAL:HG22	2.06	0.56
1:L:128:SER:O	1:L:128:SER:OG	2.25	0.54
1:E:47[A]:THR:HG23	1:K:47[A]:THR:HG21	1.90	0.54
1:G:60:ALA:O	1:G:63[A]:VAL:HG22	2.07	0.54
1:M:60:ALA:O	1:M:63[A]:VAL:HG22	2.06	0.53
1:C:47[A]:THR:CG2	1:H:47[A]:THR:HG23	2.39	0.53
1:F:37:HIS:CE1	1:F:49:HIS:CE1	2.97	0.53
1:K:86:ARG:NH2	4:K:304:HOH:O	2.41	0.52
1:B:47[A]:THR:HG23	1:E:47[A]:THR:CG2	2.39	0.52
1:K:60:ALA:O	1:K:63[A]:VAL:HG22	2.10	0.52
1:D:115:ARG:NH2	4:D:301:HOH:O	2.26	0.51
1:A:47[A]:THR:CG2	1:J:47[A]:THR:HG23	2.40	0.51
1:O:37:HIS:CE1	1:O:49:HIS:CE1	2.99	0.51
1:A:86:ARG:NH2	4:A:304:HOH:O	2.40	0.51
1:I:47[A]:THR:CG2	1:L:47[A]:THR:HG23	2.41	0.51
1:O:60:ALA:O	1:O:63[A]:VAL:HG22	2.11	0.51
1:P:60:ALA:O	1:P:63[A]:VAL:HG22	2.12	0.50
1:I:60:ALA:O	1:I:63[A]:VAL:HG22	2.12	0.49
1:O:115:ARG:NH2	4:O:301:HOH:O	2.37	0.49
1:A:60:ALA:O	1:A:63[A]:VAL:HG22	2.13	0.49
1:A:37:HIS:CE1	1:A:49:HIS:CE1	3.00	0.49
1:F:60:ALA:O	1:F:63[A]:VAL:HG22	2.13	0.49
1:F:47[A]:THR:HG21	1:I:47[A]:THR:HG23	1.95	0.48
1:C:60:ALA:O	1:C:63[A]:VAL:HG22	2.14	0.48
1:D:60:ALA:O	1:D:63[A]:VAL:HG22	2.13	0.48
1:C:47[A]:THR:HG23	1:G:47[A]:THR:HG21	1.96	0.47
1:B:60:ALA:O	1:B:63[A]:VAL:HG22	2.15	0.47
1:A:53:GLU:HA	1:A:56:TYR:CE2	2.50	0.47
1:I:37:HIS:CE1	1:I:49:HIS:CE1	3.03	0.47
1:E:60:ALA:O	1:E:63[A]:VAL:HG22	2.15	0.46
1:N:106:LEU:O	1:N:110:GLN:HG2	2.15	0.46
1:O:154:LEU:O	1:O:155:ALA:C	2.59	0.46
1:L:106:LEU:O	1:L:110:GLN:HG2	2.15	0.46
1:K:37:HIS:CE1	1:K:49:HIS:CE1	3.04	0.46
1:N:37:HIS:CE1	1:N:49:HIS:CE1	3.03	0.46
1:O:124:LEU:C	1:O:126:LYS:H	2.23	0.46
1:N:60:ALA:O	1:N:63[A]:VAL:HG22	2.15	0.45
1:J:106:LEU:O	1:J:110:GLN:HG2	2.16	0.45
1:J:115:ARG:NH2	4:J:303:HOH:O	2.43	0.45
1:H:118:ARG:HD2	4:H:418:HOH:O	2.16	0.45
1:B:127:VAL:O	1:B:128:SER:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:LEU:O	1:I:110:GLN:HG2	2.16	0.45
1:A:154:LEU:O	1:A:155:ALA:C	2.60	0.44
1:G:37:HIS:CE1	1:G:49:HIS:CE1	3.05	0.44
1:D:37:HIS:CE1	1:D:49:HIS:CE1	3.05	0.44
1:J:7:ILE:HG23	1:J:127:VAL:HG11	2.00	0.44
1:J:53:GLU:HA	1:J:56:TYR:CE2	2.52	0.44
1:J:37:HIS:CE1	1:J:49:HIS:CE1	3.05	0.44
1:P:127:VAL:O	1:P:128:SER:HB3	2.18	0.44
1:E:121:PHE:N	1:E:122:PRO:CD	2.81	0.44
1:M:37:HIS:CE1	1:M:49:HIS:CE1	3.06	0.44
3:M:207:EPE:O1S	1:P:47[A]:THR:HG21	2.17	0.44
1:A:118:ARG:NE	1:C:6:GLY:HA3	2.33	0.43
1:O:127:VAL:O	1:O:127:VAL:HG22	2.17	0.43
1:K:106:LEU:O	1:K:110:GLN:HG2	2.19	0.43
1:F:92:GLU:OE1	4:F:301:HOH:O	2.21	0.43
1:C:23:LEU:HD11	1:C:63[B]:VAL:HG13	2.00	0.43
1:L:60:ALA:O	1:L:63[A]:VAL:HG22	2.19	0.43
1:B:37:HIS:CE1	1:B:49:HIS:CE1	3.07	0.42
1:A:92:GLU:OE1	4:A:301:HOH:O	2.22	0.42
1:E:127:VAL:O	1:E:128:SER:HB3	2.20	0.42
1:E:37:HIS:CE1	1:E:49:HIS:CE1	3.08	0.42
1:L:46:ASN:OD1	4:L:301:HOH:O	2.21	0.42
1:F:5:ILE:O	1:J:118:ARG:NH2	2.52	0.42
1:L:56:TYR:C	1:L:56:TYR:CD1	2.98	0.41
1:M:59:LEU:O	1:M:63[A]:VAL:HG13	2.21	0.41
1:C:106:LEU:O	1:C:110:GLN:HG2	2.21	0.41
1:E:56:TYR:CD1	1:E:56:TYR:C	2.98	0.41
1:M:106:LEU:O	1:M:110:GLN:HG2	2.21	0.41
1:F:56:TYR:C	1:F:56:TYR:CD1	2.99	0.41
1:F:154:LEU:O	1:F:155:ALA:C	2.63	0.41
1:D:127:VAL:O	1:D:127:VAL:HG12	2.21	0.41
1:H:127:VAL:O	1:H:128:SER:HB3	2.21	0.41
1:I:127:VAL:O	1:I:128:SER:HB3	2.21	0.40
1:L:125:ASP:CB	4:L:401:HOH:O	2.69	0.40
1:C:53:GLU:HA	1:C:56:TYR:CE2	2.57	0.40
1:L:37:HIS:CE1	1:L:49:HIS:CE1	3.10	0.40
1:P:121:PHE:N	1:P:122:PRO:CD	2.85	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	156/156 (100%)	152 (97%)	3 (2%)	1 (1%)	21	10
1	B	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	C	156/156 (100%)	152 (97%)	4 (3%)	0	100	100
1	D	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	E	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	F	156/156 (100%)	154 (99%)	2 (1%)	0	100	100
1	G	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	H	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	I	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	J	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	K	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	L	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	M	157/156 (101%)	153 (98%)	4 (2%)	0	100	100
1	N	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
1	O	157/156 (101%)	151 (96%)	6 (4%)	0	100	100
1	P	156/156 (100%)	153 (98%)	3 (2%)	0	100	100
All	All	2504/2496 (100%)	2445 (98%)	58 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	SER

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	125/129 (97%)	122 (98%)	3 (2%)	43	28
1	B	129/129 (100%)	129 (100%)	0	100	100
1	C	126/129 (98%)	126 (100%)	0	100	100
1	D	128/129 (99%)	128 (100%)	0	100	100
1	E	126/129 (98%)	124 (98%)	2 (2%)	55	44
1	F	125/129 (97%)	124 (99%)	1 (1%)	73	67
1	G	127/129 (98%)	123 (97%)	4 (3%)	35	20
1	H	128/129 (99%)	128 (100%)	0	100	100
1	I	128/129 (99%)	127 (99%)	1 (1%)	73	67
1	J	127/129 (98%)	125 (98%)	2 (2%)	55	44
1	K	125/129 (97%)	124 (99%)	1 (1%)	73	67
1	L	123/129 (95%)	122 (99%)	1 (1%)	73	67
1	M	129/129 (100%)	127 (98%)	2 (2%)	55	44
1	N	124/129 (96%)	121 (98%)	3 (2%)	43	28
1	O	127/129 (98%)	124 (98%)	3 (2%)	43	28
1	P	125/129 (97%)	123 (98%)	2 (2%)	55	44
All	All	2022/2064 (98%)	1997 (99%)	25 (1%)	68	55

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	47[A]	THR
1	A	47[B]	THR
1	E	34	HIS
1	E	98	GLU
1	F	34	HIS
1	G	1	MET
1	G	47[A]	THR
1	G	47[B]	THR
1	G	90	ILE
1	I	34	HIS
1	J	34	HIS

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Mol	Chain	Res	Type
1	J	90	ILE
1	K	34	HIS
1	L	34	HIS
1	M	47[A]	THR
1	M	47[B]	THR
1	N	34	HIS
1	N	47[A]	THR
1	N	47[B]	THR
1	O	34	HIS
1	O	47[A]	THR
1	O	47[B]	THR
1	P	34	HIS
1	P	90	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	4	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 69 ligands modelled in this entry, 63 are monoatomic - leaving 6 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	EPE	E	206	-	12,12,15	1.20	1 (8%)	15,16,20	2.41	3 (20%)
3	EPE	O	207	-	12,12,15	1.09	1 (8%)	15,16,20	1.32	2 (13%)
3	EPE	A	205	-	12,12,15	1.17	1 (8%)	15,16,20	1.43	3 (20%)
3	EPE	C	205	-	12,12,15	1.02	1 (8%)	15,16,20	2.23	3 (20%)
3	EPE	F	204	-	12,12,15	0.99	1 (8%)	15,16,20	1.95	2 (13%)
3	EPE	M	207	-	12,12,15	1.10	1 (8%)	15,16,20	1.66	3 (20%)

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	EPE	E	206	-	-	3/6/14/19	0/1/1/1
3	EPE	O	207	-	-	3/6/14/19	0/1/1/1
3	EPE	A	205	-	-	0/6/14/19	0/1/1/1
3	EPE	C	205	-	-	5/6/14/19	0/1/1/1
3	EPE	F	204	-	-	5/6/14/19	0/1/1/1
3	EPE	M	207	-	-	2/6/14/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	205	EPE	C10-S	3.73	1.82	1.77
3	E	206	EPE	C10-S	3.72	1.82	1.77
3	M	207	EPE	C10-S	3.43	1.82	1.77
3	O	207	EPE	C10-S	3.40	1.82	1.77
3	F	204	EPE	C10-S	3.14	1.82	1.77
3	C	205	EPE	C10-S	3.07	1.81	1.77

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	205	EPE	O2S-S-C10	7.24	117.67	106.73
3	E	206	EPE	O2S-S-C10	6.84	117.06	106.73
3	F	204	EPE	O3S-S-C10	5.67	117.10	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	206	EPE	O1S-S-C10	-5.20	98.87	106.73
3	M	207	EPE	O2S-S-C10	4.47	113.49	106.73
3	A	205	EPE	O2S-S-C10	3.39	111.86	106.73
3	F	204	EPE	O2S-S-C10	-3.18	101.93	106.73
3	O	207	EPE	C5-N4-C3	3.15	119.31	110.40
3	O	207	EPE	O2S-S-C10	2.83	111.00	106.73
3	M	207	EPE	O3S-S-C10	2.72	111.32	106.00
3	A	205	EPE	C5-N4-C3	2.68	117.99	110.40
3	C	205	EPE	O2S-S-O1S	-2.57	105.48	113.82
3	E	206	EPE	C5-N4-C3	2.23	116.71	110.40
3	M	207	EPE	C5-N4-C3	2.14	116.44	110.40
3	A	205	EPE	O1S-S-C10	2.04	109.82	106.73
3	C	205	EPE	C5-N4-C3	2.01	116.09	110.40

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	206	EPE	C9-C10-S-O1S
3	F	204	EPE	C9-C10-S-O1S
3	F	204	EPE	C9-C10-S-O3S
3	O	207	EPE	C9-C10-S-O3S
3	C	205	EPE	C9-C10-S-O3S
3	E	206	EPE	C9-C10-S-O3S
3	F	204	EPE	C10-C9-N1-C2
3	F	204	EPE	C10-C9-N1-C6
3	C	205	EPE	C9-C10-S-O1S
3	C	205	EPE	C9-C10-S-O2S
3	E	206	EPE	C9-C10-S-O2S
3	F	204	EPE	C9-C10-S-O2S
3	O	207	EPE	C9-C10-S-O1S
3	O	207	EPE	C9-C10-S-O2S
3	C	205	EPE	C10-C9-N1-C2
3	C	205	EPE	C10-C9-N1-C6
3	M	207	EPE	C10-C9-N1-C2
3	M	207	EPE	C10-C9-N1-C6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	M	207	EPE	1	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 [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	155/156 (99%)	0.09	1 (0%) 85 88	16, 29, 46, 68	3 (1%)
1	B	155/156 (99%)	-0.29	1 (0%) 85 88	12, 22, 34, 48	4 (2%)
1	C	155/156 (99%)	0.12	3 (1%) 66 70	16, 29, 48, 60	3 (1%)
1	D	155/156 (99%)	0.13	5 (3%) 50 54	14, 27, 45, 68	4 (2%)
1	E	155/156 (99%)	0.12	3 (1%) 66 70	16, 28, 45, 54	4 (2%)
1	F	155/156 (99%)	0.07	4 (2%) 57 61	16, 27, 44, 58	3 (1%)
1	G	155/156 (99%)	-0.03	1 (0%) 85 88	14, 26, 44, 60	3 (1%)
1	H	155/156 (99%)	-0.29	1 (0%) 85 88	12, 22, 35, 47	4 (2%)
1	I	155/156 (99%)	-0.26	1 (0%) 85 88	12, 23, 35, 47	4 (2%)
1	J	155/156 (99%)	0.28	4 (2%) 57 61	16, 29, 46, 64	4 (2%)
1	K	155/156 (99%)	-0.10	5 (3%) 50 54	13, 25, 44, 59	3 (1%)
1	L	155/156 (99%)	-0.07	3 (1%) 66 70	14, 25, 42, 58	3 (1%)
1	M	155/156 (99%)	-0.32	2 (1%) 75 79	13, 22, 36, 45	4 (2%)
1	N	155/156 (99%)	-0.14	3 (1%) 66 70	15, 25, 42, 57	3 (1%)
1	O	155/156 (99%)	0.09	8 (5%) 33 35	16, 28, 46, 71	4 (2%)
1	P	155/156 (99%)	0.02	3 (1%) 66 70	16, 28, 44, 53	3 (1%)
All	All	2480/2496 (99%)	-0.04	48 (1%) 66 70	12, 26, 44, 71	56 (2%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	155	ALA	4.5
1	K	155	ALA	4.0
1	N	155	ALA	3.7
1	P	155	ALA	3.7
1	F	155	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	127	VAL	3.6
1	H	155	ALA	3.4
1	M	155	ALA	3.2
1	G	155	ALA	3.1
1	K	125	ASP	3.0
1	O	128	SER	3.0
1	A	155	ALA	3.0
1	O	127	VAL	3.0
1	F	27	TYR	2.8
1	J	126	LYS	2.8
1	O	125	ASP	2.8
1	J	155	ALA	2.7
1	E	155	ALA	2.6
1	D	123	LEU	2.6
1	L	127	VAL	2.5
1	J	128	SER	2.5
1	D	17	GLU	2.5
1	D	155	ALA	2.5
1	D	128	SER	2.4
1	D	127	VAL	2.4
1	L	27	TYR	2.3
1	L	155	ALA	2.3
1	N	127	VAL	2.3
1	O	27	TYR	2.3
1	O	126	LYS	2.3
1	C	27	TYR	2.2
1	I	155	ALA	2.2
1	C	2	GLU	2.2
1	K	127	VAL	2.2
1	K	123	LEU	2.2
1	O	85	ALA	2.2
1	P	27	TYR	2.2
1	F	125	ASP	2.2
1	B	155	ALA	2.2
1	N	125	ASP	2.1
1	K	128	SER	2.1
1	E	1	MET	2.1
1	F	127	VAL	2.1
1	O	86	ARG	2.1
1	C	127	VAL	2.1
1	P	125	ASP	2.1
1	E	127	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	M	127	VAL	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
2	FE2	B	204	1/1	0.62	0.16	99,99,99,99	1
2	FE2	O	206	1/1	0.67	0.19	77,77,77,77	1
2	FE2	G	204	1/1	0.72	0.16	110,110,110,110	0
2	FE2	L	202	1/1	0.75	0.13	67,67,67,67	1
2	FE2	O	205	1/1	0.76	0.18	63,63,63,63	1
2	FE2	E	205	1/1	0.77	0.13	83,83,83,83	1
2	FE2	O	204	1/1	0.78	0.13	78,78,78,78	1
2	FE2	A	204	1/1	0.78	0.13	87,87,87,87	1
2	FE2	M	204	1/1	0.78	0.13	86,86,86,86	1
2	FE2	C	204	1/1	0.81	0.13	66,66,66,66	1
2	FE2	E	203	1/1	0.82	0.17	66,66,66,66	1
2	FE2	F	203	1/1	0.82	0.18	76,76,76,76	1
2	FE2	F	202	1/1	0.83	0.14	66,66,66,66	1
2	FE2	E	204	1/1	0.83	0.20	97,97,97,97	1
2	FE2	M	206	1/1	0.85	0.15	66,66,66,66	1
2	FE2	B	206	1/1	0.85	0.20	58,58,58,58	1
2	FE2	B	207	1/1	0.86	0.13	65,65,65,65	1
2	FE2	D	204	1/1	0.86	0.12	63,63,63,63	1
2	FE2	B	202	1/1	0.88	0.12	42,42,42,42	1
2	FE2	B	205	1/1	0.88	0.10	45,45,45,45	1
2	FE2	I	204	1/1	0.88	0.12	49,49,49,49	1
2	FE2	I	203	1/1	0.89	0.12	60,60,60,60	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	N	202	1/1	0.89	0.10	47,47,47,47	1
2	FE2	M	202	1/1	0.89	0.12	44,44,44,44	1
2	FE2	M	203	1/1	0.89	0.21	64,64,64,64	1
2	FE2	C	202	1/1	0.89	0.10	45,45,45,45	1
2	FE2	M	205	1/1	0.90	0.08	36,36,36,36	1
2	FE2	I	202	1/1	0.90	0.09	42,42,42,42	1
2	FE2	H	204	1/1	0.91	0.09	48,48,48,48	1
2	FE2	G	203	1/1	0.91	0.12	44,44,44,44	1
2	FE2	G	202	1/1	0.91	0.10	46,46,46,46	1
2	FE2	H	202	1/1	0.91	0.11	48,48,48,48	1
2	FE2	K	202	1/1	0.91	0.10	44,44,44,44	1
2	FE2	B	208	1/1	0.92	0.11	42,42,42,42	1
2	FE2	O	203	1/1	0.92	0.07	40,40,40,40	1
2	FE2	D	202	1/1	0.92	0.09	47,47,47,47	1
2	FE2	D	203	1/1	0.92	0.12	51,51,51,51	1
2	FE2	B	203	1/1	0.92	0.11	47,47,47,47	1
2	FE2	A	202	1/1	0.93	0.09	41,41,41,41	1
2	FE2	J	202	1/1	0.93	0.10	43,43,43,43	1
2	FE2	P	202	1/1	0.93	0.09	45,45,45,45	1
2	FE2	E	202	1/1	0.94	0.08	46,46,46,46	1
2	FE2	C	203	1/1	0.94	0.07	41,41,41,41	1
3	EPE	A	205	12/15	0.94	0.14	38,48,59,65	0
2	FE2	H	203	1/1	0.95	0.10	54,54,54,54	1
2	FE2	A	203	1/1	0.95	0.07	47,47,47,47	1
3	EPE	E	206	12/15	0.95	0.14	31,46,59,61	0
3	EPE	O	207	12/15	0.95	0.12	33,38,39,40	12
2	FE2	K	203	1/1	0.96	0.06	46,46,46,46	1
3	EPE	M	207	12/15	0.96	0.12	32,45,52,63	0
2	FE2	O	202	1/1	0.96	0.08	44,44,44,44	1
3	EPE	C	205	12/15	0.97	0.11	31,41,55,60	0
3	EPE	F	204	12/15	0.97	0.10	32,42,51,54	0
2	FE2	B	201	1/1	0.98	0.04	23,23,23,23	1
2	FE2	C	201	1/1	0.99	0.03	28,28,28,28	1
2	FE2	A	201	1/1	0.99	0.03	26,26,26,26	1
2	FE2	L	201	1/1	0.99	0.03	24,24,24,24	1
2	FE2	G	201	1/1	0.99	0.03	24,24,24,24	1
2	FE2	M	201	1/1	0.99	0.03	24,24,24,24	1
2	FE2	P	201	1/1	0.99	0.03	26,26,26,26	1
2	FE2	I	201	1/1	0.99	0.02	23,23,23,23	1
2	FE2	D	201	1/1	0.99	0.04	27,27,27,27	1
2	FE2	E	201	1/1	0.99	0.04	27,27,27,27	1
2	FE2	F	201	1/1	0.99	0.03	28,28,28,28	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FE2	J	201	1/1	0.99	0.05	29,29,29,29	0
2	FE2	N	201	1/1	0.99	0.02	24,24,24,24	1
2	FE2	H	201	1/1	0.99	0.05	23,23,23,23	0
2	FE2	O	201	1/1	1.00	0.04	26,26,26,26	1
2	FE2	K	201	1/1	1.00	0.03	23,23,23,23	1

6.5 Other polymers [i](#)

There are no such residues in this entry.