



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 07:29 AM EDT

PDB ID : 3JYI
Title : Structural and biochemical evidence that a TEM-1 {beta}-lactamase Asn170Gly active site mutant acts via substrate-assisted catalysis
Authors : Brown, N.G.; Palzkill, T.G.; Prasad, B.V.V.; Shanker, S.
Deposited on : 2009-09-21
Resolution : 2.70 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

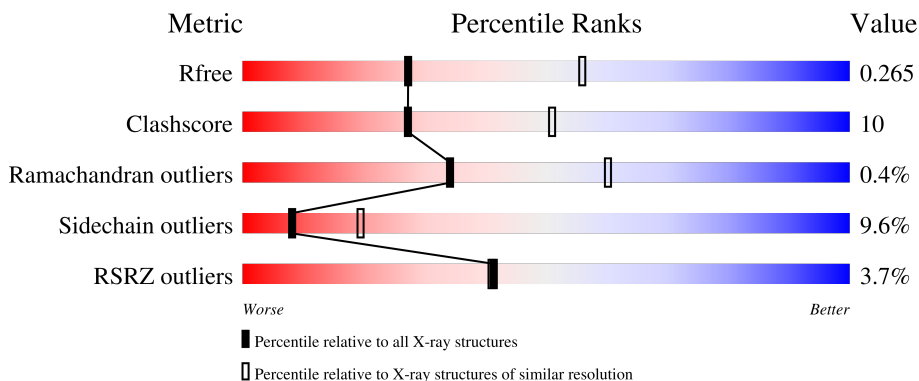
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



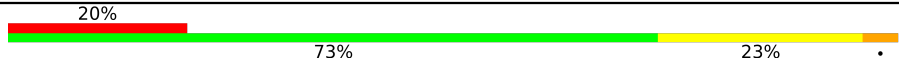
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	263	77% 20% .
1	B	263	75% 22% .
1	C	263	74% 22% .
1	D	263	76% 20% .
1	E	263	2% 75% 22% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	263	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '20%', a green segment in the middle labeled '73%', and a yellow/orange segment on the right labeled '23%'. A small black dot is visible at the far right end of the bar.</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12416 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 Beta-lactamase TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2022	1263	359	389	11	12	0	0
1	B	263	2022	1263	359	389	11	12	0	0
1	C	263	2022	1263	359	389	11	12	0	0
1	D	263	2022	1263	359	389	11	12	0	0
1	E	263	2022	1263	359	389	11	12	0	0
1	F	263	2022	1263	359	389	11	12	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	ASN	engineered mutation	UNP P62593
B	170	GLY	ASN	engineered mutation	UNP P62593
C	170	GLY	ASN	engineered mutation	UNP P62593
D	170	GLY	ASN	engineered mutation	UNP P62593
E	170	GLY	ASN	engineered mutation	UNP P62593
F	170	GLY	ASN	engineered mutation	UNP P62593

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total 15	8	2	4	1	0	0
2	B	1	Total 15	8	2	4	1	10	0
2	C	1	Total 15	8	2	4	1	9	0
2	D	1	Total 15	8	2	4	1	9	0
2	E	1	Total 15	8	2	4	1	10	0
2	F	1	Total 15	8	2	4	1	11	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

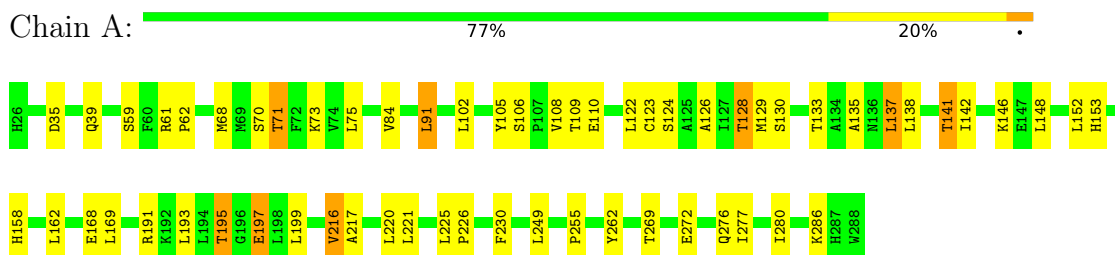
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	33	Total	O	0	0
			33	33		
4	C	47	Total	O	0	0
			47	47		
4	D	31	Total	O	0	0
			31	31		
4	E	20	Total	O	0	0
			20	20		
4	F	4	Total	O	0	0
			4	4		

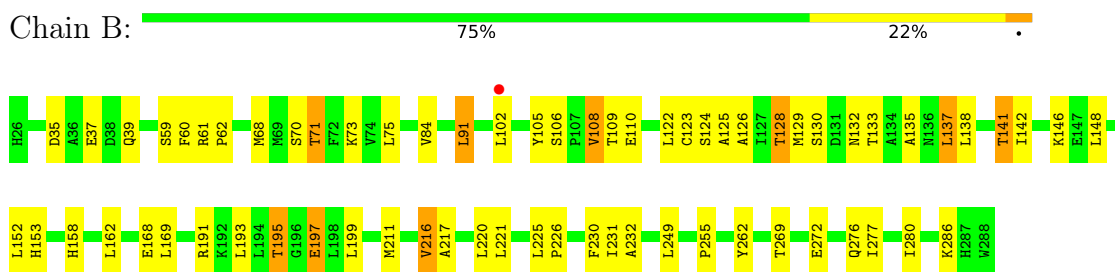
3 Residue-property plots [i](#)

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.

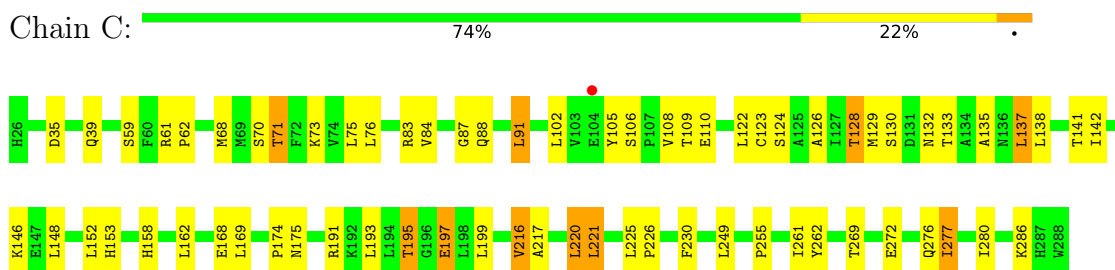
- Molecule 1: Beta-lactamase TEM



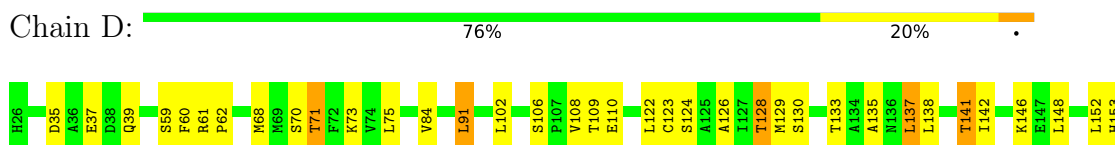
- Molecule 1: Beta-lactamase TEM



- Molecule 1: Beta-lactamase TEM

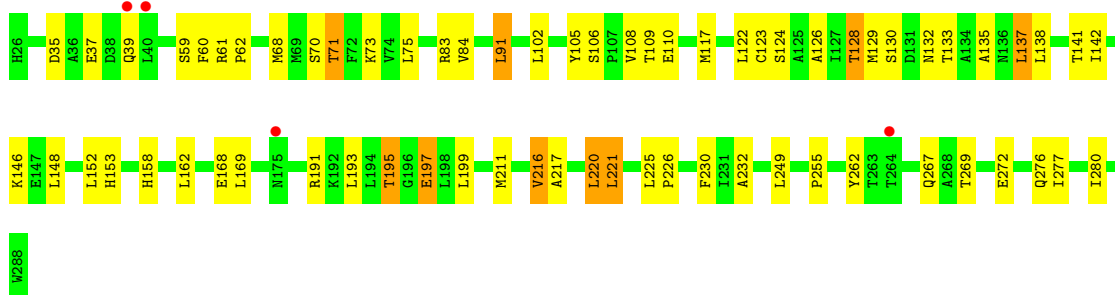
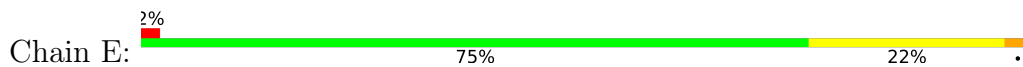


- Molecule 1: Beta-lactamase TEM

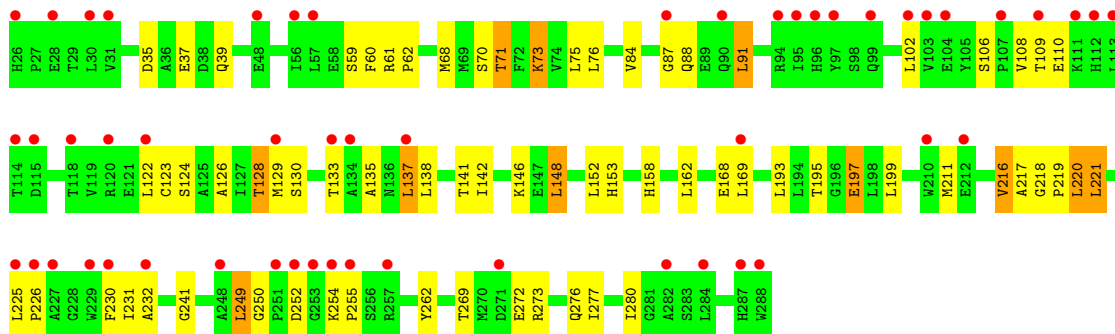
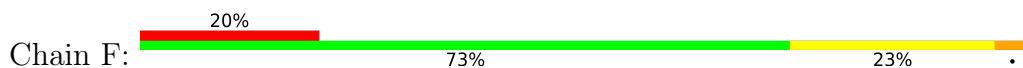




- Molecule 1: Beta-lactamase TEM



- Molecule 1: Beta-lactamase TEM



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	88.10Å 88.10Å 500.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.28 – 2.70 39.40 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.3 (39.28-2.70) 99.8 (39.40-2.70)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.4_95)	Depositor
R, R_{free}	0.230 , 0.260 0.235 , 0.265	Depositor DCC
R_{free} test set	2819 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtrriage
Anisotropy	0.521	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12416	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4991e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 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	0/2056	0.56	0/2784
1	B	0.38	0/2056	0.56	0/2784
1	C	0.39	0/2056	0.56	0/2784
1	D	0.39	0/2056	0.56	0/2784
1	E	0.41	0/2056	0.57	0/2784
1	F	0.49	0/2056	0.56	0/2784
All	All	0.41	0/12336	0.56	0/16704

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	2022	0	2031	38	0
1	B	2022	0	2031	42	0
1	C	2022	0	2031	44	0
1	D	2022	0	2031	39	0
1	E	2022	0	2031	40	0
1	F	2022	0	2031	46	1
2	A	15	0	17	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	15	0	17	0	0
2	C	15	0	17	0	0
2	D	15	0	17	0	0
2	E	15	0	17	0	0
2	F	15	0	17	0	0
3	A	5	0	0	0	0
3	B	5	0	0	1	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
4	A	39	0	0	1	0
4	B	33	0	0	0	0
4	C	47	0	0	2	0
4	D	31	0	0	1	0
4	E	20	0	0	2	0
4	F	4	0	0	0	0
All	All	12416	0	12288	244	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 10.

All (244) 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:D:124:SER:O	1:D:128:THR:HB	1.68	0.93
1:C:124:SER:O	1:C:128:THR:HB	1.68	0.93
1:E:124:SER:O	1:E:128:THR:HB	1.69	0.92
1:F:124:SER:O	1:F:128:THR:HB	1.73	0.89
1:A:124:SER:O	1:A:128:THR:HB	1.74	0.88
1:A:216:VAL:HG12	1:A:217:ALA:H	1.40	0.87
1:B:124:SER:O	1:B:128:THR:HB	1.74	0.86
1:B:216:VAL:HG12	1:B:217:ALA:H	1.41	0.85
1:D:216:VAL:HG12	1:D:217:ALA:H	1.41	0.84
1:F:216:VAL:HG12	1:F:217:ALA:H	1.43	0.83
1:C:216:VAL:HG12	1:C:217:ALA:H	1.42	0.82
1:E:216:VAL:HG12	1:E:217:ALA:H	1.45	0.79
1:D:71:THR:HG21	1:D:262:TYR:OH	1.85	0.77
1:B:71:THR:HG21	1:B:262:TYR:OH	1.84	0.77
1:A:71:THR:HG21	1:A:262:TYR:OH	1.85	0.77
1:F:71:THR:HG21	1:F:262:TYR:OH	1.85	0.77
1:A:68:MET:O	1:A:71:THR:HB	1.87	0.75
1:E:71:THR:HG21	1:E:262:TYR:OH	1.87	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:THR:HG21	1:C:262:TYR:OH	1.88	0.74
1:D:68:MET:O	1:D:71:THR:HB	1.88	0.73
1:C:68:MET:O	1:C:71:THR:HB	1.90	0.72
1:F:128:THR:HG22	1:F:129:MET:HG2	1.72	0.72
1:E:68:MET:O	1:E:71:THR:HB	1.91	0.70
1:F:84:VAL:HG21	1:F:91:LEU:HD13	1.75	0.69
1:A:141:THR:HG22	1:A:142:ILE:HG23	1.74	0.68
1:E:128:THR:HG22	1:E:129:MET:HG2	1.76	0.68
1:D:128:THR:HG22	1:D:129:MET:HG2	1.75	0.68
1:B:68:MET:O	1:B:71:THR:HB	1.94	0.68
1:F:59:SER:HB2	1:F:62:PRO:HG3	1.75	0.68
1:B:128:THR:HG22	1:B:129:MET:HG2	1.76	0.67
1:D:141:THR:HG22	1:D:142:ILE:HG23	1.77	0.67
1:D:84:VAL:HG21	1:D:91:LEU:HD13	1.77	0.66
1:C:128:THR:HG22	1:C:129:MET:HG2	1.77	0.66
1:F:68:MET:O	1:F:71:THR:HB	1.95	0.66
1:D:59:SER:HB2	1:D:62:PRO:HG3	1.78	0.66
1:A:128:THR:HG22	1:A:129:MET:HG2	1.78	0.66
1:B:59:SER:HB2	1:B:62:PRO:HG3	1.78	0.66
1:F:141:THR:HG22	1:F:142:ILE:HG23	1.77	0.66
1:E:59:SER:HB2	1:E:62:PRO:HG3	1.79	0.65
1:E:276:GLN:O	1:E:280:ILE:HG13	1.98	0.63
1:C:84:VAL:HG21	1:C:91:LEU:HD13	1.81	0.63
1:C:59:SER:HB2	1:C:62:PRO:HG3	1.81	0.63
1:E:84:VAL:HG21	1:E:91:LEU:HD13	1.81	0.62
1:C:141:THR:HG22	1:C:142:ILE:HG23	1.82	0.61
1:D:216:VAL:HG12	1:D:217:ALA:N	2.14	0.61
1:B:141:THR:HG22	1:B:142:ILE:HG23	1.83	0.60
1:C:216:VAL:HG12	1:C:217:ALA:N	2.15	0.60
1:E:141:THR:HG22	1:E:142:ILE:HG23	1.83	0.60
1:A:59:SER:HB2	1:A:62:PRO:HG3	1.84	0.60
1:A:84:VAL:HG21	1:A:91:LEU:HD13	1.83	0.60
1:A:276:GLN:O	1:A:280:ILE:HG13	2.01	0.60
1:B:276:GLN:O	1:B:280:ILE:HG13	2.02	0.59
1:E:61:ARG:N	1:E:62:PRO:HD3	2.17	0.59
1:B:231:ILE:HG22	3:B:2:PO4:O1	2.03	0.59
1:E:197:GLU:OE1	1:E:197:GLU:HA	2.03	0.59
1:B:84:VAL:HG21	1:B:91:LEU:HD13	1.85	0.59
1:D:61:ARG:N	1:D:62:PRO:HD3	2.18	0.59
1:B:216:VAL:HG12	1:B:217:ALA:N	2.14	0.59
1:D:126:ALA:O	1:D:130:SER:HA	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:THR:O	4:D:304:HOH:O	2.17	0.58
1:E:126:ALA:O	1:E:130:SER:HA	2.03	0.58
1:E:216:VAL:HG12	1:E:217:ALA:N	2.17	0.58
1:E:162:LEU:HD11	1:E:169:LEU:HD22	1.84	0.58
1:F:276:GLN:O	1:F:280:ILE:HG13	2.03	0.58
1:B:197:GLU:OE1	1:B:197:GLU:HA	2.04	0.58
1:C:138:LEU:O	1:C:141:THR:HB	2.04	0.57
1:D:197:GLU:OE1	1:D:197:GLU:HA	2.02	0.57
1:F:68:MET:HE3	1:F:75:LEU:HD22	1.86	0.57
1:B:61:ARG:N	1:B:62:PRO:HD3	2.18	0.57
1:A:216:VAL:HG12	1:A:217:ALA:N	2.15	0.57
1:F:138:LEU:O	1:F:141:THR:HB	2.05	0.57
1:A:197:GLU:HA	1:A:197:GLU:OE1	2.04	0.56
1:A:106:SER:HB3	1:A:109:THR:OG1	2.05	0.56
1:B:73:LYS:HD3	1:B:135:ALA:HB2	1.88	0.56
1:C:68:MET:HE3	1:C:75:LEU:HD22	1.87	0.56
1:C:276:GLN:O	1:C:280:ILE:HG13	2.06	0.56
1:F:197:GLU:HA	1:F:197:GLU:OE1	2.05	0.56
1:C:197:GLU:HA	1:C:197:GLU:OE1	2.06	0.56
1:E:68:MET:HE3	1:E:75:LEU:HD22	1.88	0.56
1:F:133:THR:HG22	1:F:137:LEU:HD22	1.87	0.56
1:A:133:THR:HG22	1:A:137:LEU:HD22	1.88	0.55
1:C:61:ARG:N	1:C:62:PRO:HD3	2.21	0.55
1:F:126:ALA:O	1:F:130:SER:HA	2.06	0.55
1:A:73:LYS:HD3	1:A:135:ALA:HB2	1.88	0.55
1:C:133:THR:HG22	1:C:137:LEU:HD22	1.88	0.55
1:E:267:GLN:NE2	4:E:293:HOH:O	2.27	0.55
1:F:61:ARG:N	1:F:62:PRO:HD3	2.22	0.55
1:D:106:SER:HB3	1:D:109:THR:OG1	2.07	0.54
1:E:133:THR:HG22	1:E:137:LEU:HD22	1.87	0.54
1:D:133:THR:HG22	1:D:137:LEU:HD22	1.89	0.54
1:D:138:LEU:O	1:D:141:THR:HB	2.07	0.54
1:F:73:LYS:HD3	1:F:135:ALA:HB2	1.90	0.54
1:A:138:LEU:O	1:A:141:THR:HB	2.08	0.54
1:A:162:LEU:HD11	1:A:169:LEU:HD22	1.90	0.54
1:E:138:LEU:O	1:E:141:THR:HB	2.08	0.54
1:F:106:SER:HB3	1:F:109:THR:OG1	2.06	0.54
1:B:133:THR:HG22	1:B:137:LEU:HD22	1.90	0.54
1:D:153:HIS:CD2	1:D:158:HIS:HD2	2.25	0.54
1:F:153:HIS:CD2	1:F:158:HIS:HD2	2.25	0.54
1:A:35:ASP:O	1:A:39:GLN:HG2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:ALA:O	1:B:130:SER:HA	2.08	0.54
1:D:73:LYS:HD3	1:D:135:ALA:HB2	1.89	0.54
1:E:35:ASP:O	1:E:39:GLN:HG2	2.07	0.54
1:E:106:SER:HB3	1:E:109:THR:OG1	2.08	0.54
1:A:216:VAL:HG11	2:A:3380:EPE:H61	1.90	0.53
1:B:153:HIS:CD2	1:B:158:HIS:HD2	2.26	0.53
1:B:106:SER:O	1:B:110:GLU:HG3	2.08	0.53
1:B:162:LEU:HD11	1:B:169:LEU:HD22	1.91	0.53
1:C:162:LEU:HD11	1:C:169:LEU:HD22	1.90	0.53
1:E:70:SER:O	1:E:73:LYS:HG3	2.09	0.53
1:B:226:PRO:HG3	1:F:88:GLN:HB3	1.88	0.53
1:F:153:HIS:NE2	1:F:158:HIS:HD2	2.07	0.53
1:C:70:SER:O	1:C:73:LYS:HG3	2.09	0.53
1:E:83:ARG:NH2	4:E:300:HOH:O	2.40	0.53
1:A:126:ALA:O	1:A:130:SER:HA	2.08	0.53
1:A:106:SER:O	1:A:110:GLU:HG3	2.09	0.53
1:B:106:SER:HB3	1:B:109:THR:OG1	2.08	0.53
1:C:106:SER:HB3	1:C:109:THR:OG1	2.08	0.53
1:F:216:VAL:HG12	1:F:217:ALA:N	2.18	0.52
1:B:153:HIS:NE2	1:B:158:HIS:HD2	2.07	0.52
1:B:138:LEU:O	1:B:141:THR:HB	2.09	0.52
1:C:153:HIS:CD2	1:C:158:HIS:HD2	2.27	0.52
1:E:73:LYS:HD3	1:E:135:ALA:HB2	1.91	0.52
1:F:153:HIS:CE1	1:F:158:HIS:CD2	2.98	0.52
1:A:68:MET:HE3	1:A:75:LEU:HD22	1.92	0.52
1:A:153:HIS:CE1	1:A:158:HIS:CD2	2.98	0.51
1:E:106:SER:O	1:E:110:GLU:HG3	2.10	0.51
1:F:230:PHE:CD2	1:F:255:PRO:HB3	2.45	0.51
1:A:153:HIS:CD2	1:A:158:HIS:HD2	2.28	0.51
1:C:126:ALA:O	1:C:130:SER:HA	2.11	0.51
1:C:269:THR:HB	1:C:272:GLU:HG3	1.93	0.51
1:A:153:HIS:NE2	1:A:158:HIS:HD2	2.09	0.51
1:B:153:HIS:CE1	1:B:158:HIS:CD2	2.98	0.51
1:F:70:SER:O	1:F:73:LYS:HG3	2.11	0.50
1:A:153:HIS:CE1	1:A:158:HIS:HD2	2.29	0.50
1:C:106:SER:O	1:C:110:GLU:HG3	2.12	0.50
1:A:269:THR:HB	1:A:272:GLU:HG3	1.93	0.50
1:C:35:ASP:O	1:C:39:GLN:HG2	2.11	0.50
1:A:61:ARG:N	1:A:62:PRO:HD3	2.26	0.50
1:D:153:HIS:NE2	1:D:158:HIS:HD2	2.09	0.50
1:D:269:THR:HB	1:D:272:GLU:HG3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:LEU:HD11	1:D:169:LEU:HD22	1.93	0.49
1:B:35:ASP:O	1:B:39:GLN:HG2	2.12	0.49
1:D:276:GLN:O	1:D:280:ILE:HG13	2.11	0.49
1:E:153:HIS:CD2	1:E:158:HIS:HD2	2.29	0.49
1:C:153:HIS:NE2	1:C:158:HIS:HD2	2.10	0.49
1:B:71:THR:HG21	1:B:262:TYR:HH	1.76	0.49
1:B:286:LYS:HA	1:F:87:GLY:O	2.13	0.49
1:D:35:ASP:O	1:D:39:GLN:HG2	2.11	0.49
1:F:153:HIS:CE1	1:F:158:HIS:HD2	2.30	0.49
1:B:269:THR:HB	1:B:272:GLU:HG3	1.95	0.49
1:C:153:HIS:CE1	1:C:158:HIS:CD2	3.01	0.49
1:B:153:HIS:CE1	1:B:158:HIS:HD2	2.31	0.48
1:F:35:ASP:O	1:F:39:GLN:HG2	2.13	0.48
1:F:37:GLU:OE2	1:F:60:PHE:HE2	1.96	0.48
1:C:68:MET:CE	1:C:75:LEU:HD22	2.44	0.48
1:F:162:LEU:HD11	1:F:169:LEU:HD22	1.96	0.48
1:F:70:SER:CB	1:F:73:LYS:HE2	2.44	0.48
1:B:68:MET:HE3	1:B:75:LEU:HD22	1.96	0.48
1:D:153:HIS:CE1	1:D:158:HIS:CD2	3.02	0.47
1:E:269:THR:HB	1:E:272:GLU:HG3	1.96	0.47
1:E:153:HIS:CE1	1:E:158:HIS:CD2	3.03	0.47
1:D:68:MET:HE3	1:D:75:LEU:HD22	1.96	0.47
1:E:153:HIS:NE2	1:E:158:HIS:HD2	2.12	0.47
1:B:230:PHE:CD2	1:B:255:PRO:HB3	2.50	0.47
1:F:106:SER:O	1:F:110:GLU:HG3	2.15	0.47
1:C:220:LEU:HB3	1:C:221:LEU:H	1.53	0.47
1:F:269:THR:HB	1:F:272:GLU:HG3	1.97	0.46
1:E:191:ARG:O	1:E:195:THR:HB	2.15	0.46
1:A:70:SER:O	1:A:73:LYS:HG3	2.16	0.46
1:F:220:LEU:HB3	1:F:221:LEU:H	1.49	0.46
1:E:153:HIS:CE1	1:E:158:HIS:HD2	2.34	0.46
1:E:68:MET:CE	1:E:75:LEU:HD22	2.45	0.46
1:F:68:MET:CE	1:F:75:LEU:HD22	2.46	0.46
1:C:73:LYS:HD3	1:C:135:ALA:HB2	1.98	0.45
1:C:191:ARG:O	1:C:195:THR:HB	2.16	0.45
1:B:226:PRO:CG	1:F:88:GLN:HB3	2.45	0.45
1:C:153:HIS:CE1	1:C:158:HIS:HD2	2.34	0.45
1:B:70:SER:O	1:B:73:LYS:HG3	2.17	0.45
1:F:70:SER:HB3	1:F:73:LYS:HE2	1.98	0.45
1:F:153:HIS:NE2	1:F:158:HIS:CD2	2.84	0.45
1:B:153:HIS:NE2	1:B:158:HIS:CD2	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:LEU:HA	1:D:226:PRO:HD3	1.83	0.45
1:A:230:PHE:CD2	1:A:255:PRO:HB3	2.52	0.45
1:D:153:HIS:CE1	1:D:158:HIS:HD2	2.35	0.45
1:A:286:LYS:HA	1:C:87:GLY:O	2.16	0.45
1:F:241:GLY:HA2	1:F:273:ARG:NH1	2.32	0.44
1:F:225:LEU:HA	1:F:226:PRO:HD3	1.85	0.44
1:A:68:MET:CE	1:A:75:LEU:HD22	2.48	0.44
1:C:76:LEU:HD21	1:C:138:LEU:HB2	1.99	0.44
1:D:106:SER:O	1:D:110:GLU:HG3	2.17	0.44
1:E:230:PHE:CD2	1:E:255:PRO:HB3	2.52	0.44
1:C:261:ILE:HG21	1:C:277:ILE:HD11	2.00	0.44
1:E:117:MET:HB3	1:E:117:MET:HE2	1.88	0.44
1:F:211:MET:HB2	1:F:232:ALA:HB1	2.00	0.44
1:D:230:PHE:CD2	1:D:255:PRO:HB3	2.52	0.44
1:E:105:TYR:HB3	1:E:132:ASN:ND2	2.33	0.44
1:D:70:SER:O	1:D:73:LYS:HG3	2.18	0.44
1:D:70:SER:CB	1:D:73:LYS:HE2	2.48	0.44
1:F:76:LEU:HD21	1:F:138:LEU:HB2	2.00	0.44
1:A:216:VAL:CG1	2:A:3380:EPE:H61	2.48	0.43
1:D:220:LEU:HB3	1:D:221:LEU:H	1.52	0.43
1:A:191:ARG:O	1:A:195:THR:HB	2.18	0.43
1:C:174:PRO:O	1:C:175:ASN:HB2	2.19	0.43
1:C:230:PHE:CD2	1:C:255:PRO:HB3	2.53	0.43
1:C:225:LEU:HA	1:C:226:PRO:HD3	1.83	0.43
1:A:153:HIS:NE2	1:A:158:HIS:CD2	2.87	0.43
1:B:108:VAL:CG1	1:B:125:ALA:HB1	2.49	0.43
1:D:216:VAL:CG1	1:D:217:ALA:H	2.18	0.43
1:B:211:MET:HB2	1:B:232:ALA:HB1	2.01	0.43
1:E:61:ARG:N	1:E:62:PRO:CD	2.82	0.43
1:C:105:TYR:HB3	1:C:132:ASN:ND2	2.34	0.42
1:C:105:TYR:HB3	1:C:132:ASN:HD22	1.84	0.42
1:F:250:GLY:HA3	1:F:254:LYS:O	2.20	0.42
1:A:105:TYR:HA	4:A:7:HOH:O	2.19	0.42
1:D:191:ARG:O	1:D:195:THR:HB	2.19	0.42
1:F:218:GLY:N	1:F:219:PRO:CD	2.82	0.42
1:E:225:LEU:HA	1:E:226:PRO:HD3	1.84	0.42
1:B:225:LEU:HA	1:B:226:PRO:HD3	1.82	0.42
1:D:68:MET:HE3	1:D:186:MET:CE	2.50	0.42
1:F:231:ILE:O	1:F:231:ILE:HG23	2.20	0.42
1:A:225:LEU:HA	1:A:226:PRO:HD3	1.82	0.42
1:C:153:HIS:NE2	1:C:158:HIS:CD2	2.87	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:HIS:NE2	1:D:158:HIS:CD2	2.87	0.42
1:E:37:GLU:OE2	1:E:60:PHE:HE2	2.02	0.42
1:F:230:PHE:O	1:F:249:LEU:HA	2.20	0.42
1:B:37:GLU:OE2	1:B:60:PHE:HE2	2.03	0.41
1:C:83:ARG:NE	4:C:289:HOH:O	2.43	0.41
1:E:211:MET:HB2	1:E:232:ALA:HB1	2.01	0.41
1:C:216:VAL:CG1	1:C:217:ALA:H	2.19	0.41
1:C:286:LYS:NZ	4:C:318:HOH:O	2.52	0.41
1:B:68:MET:CE	1:B:75:LEU:HD22	2.51	0.41
1:B:70:SER:CB	1:B:73:LYS:HE2	2.51	0.41
1:B:191:ARG:O	1:B:195:THR:HB	2.21	0.41
1:C:70:SER:CB	1:C:73:LYS:HE2	2.51	0.41
1:D:68:MET:CE	1:D:75:LEU:HD22	2.51	0.41
1:A:226:PRO:HG3	1:C:88:GLN:HB3	2.01	0.41
1:D:37:GLU:OE2	1:D:60:PHE:HE2	2.04	0.41
1:E:220:LEU:HB3	1:E:221:LEU:H	1.50	0.40
1:D:174:PRO:O	1:D:175:ASN:HB2	2.22	0.40
1:A:141:THR:HG22	1:A:142:ILE:CG2	2.46	0.40
1:B:105:TYR:HB3	1:B:132:ASN:ND2	2.36	0.40
1:E:105:TYR:HB3	1:E:132:ASN:HD22	1.85	0.40
1:F:148:LEU:HD23	1:F:148:LEU:HA	1.90	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:252:ASP:OD1	1:F:252:ASP:OD1[8_555]	2.11	0.09

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	261/263 (99%)	249 (95%)	11 (4%)	1 (0%)	34	60
1	B	261/263 (99%)	249 (95%)	11 (4%)	1 (0%)	34	60
1	C	261/263 (99%)	248 (95%)	12 (5%)	1 (0%)	34	60
1	D	261/263 (99%)	247 (95%)	13 (5%)	1 (0%)	34	60
1	E	261/263 (99%)	248 (95%)	12 (5%)	1 (0%)	34	60
1	F	261/263 (99%)	249 (95%)	11 (4%)	1 (0%)	34	60
All	All	1566/1578 (99%)	1490 (95%)	70 (4%)	6 (0%)	34	60

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	VAL
1	B	216	VAL
1	C	216	VAL
1	D	216	VAL
1	E	216	VAL
1	F	216	VAL

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	216/216 (100%)	195 (90%)	21 (10%)	8	19
1	B	216/216 (100%)	195 (90%)	21 (10%)	8	19
1	C	216/216 (100%)	196 (91%)	20 (9%)	9	21
1	D	216/216 (100%)	195 (90%)	21 (10%)	8	19
1	E	216/216 (100%)	196 (91%)	20 (9%)	9	21
1	F	216/216 (100%)	195 (90%)	21 (10%)	8	19
All	All	1296/1296 (100%)	1172 (90%)	124 (10%)	8	19

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	91	LEU
1	A	102	LEU
1	A	108	VAL
1	A	122	LEU
1	A	123	CYS
1	A	128	THR
1	A	137	LEU
1	A	141	THR
1	A	146	LYS
1	A	148	LEU
1	A	152	LEU
1	A	168	GLU
1	A	193	LEU
1	A	195	THR
1	A	197	GLU
1	A	199	LEU
1	A	220	LEU
1	A	221	LEU
1	A	249	LEU
1	A	277	ILE
1	B	71	THR
1	B	91	LEU
1	B	102	LEU
1	B	108	VAL
1	B	122	LEU
1	B	123	CYS
1	B	128	THR
1	B	137	LEU
1	B	141	THR
1	B	146	LYS
1	B	148	LEU
1	B	152	LEU
1	B	168	GLU
1	B	193	LEU
1	B	195	THR
1	B	197	GLU
1	B	199	LEU
1	B	220	LEU
1	B	221	LEU
1	B	249	LEU
1	B	277	ILE
1	C	71	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	91	LEU
1	C	102	LEU
1	C	108	VAL
1	C	122	LEU
1	C	123	CYS
1	C	128	THR
1	C	137	LEU
1	C	146	LYS
1	C	148	LEU
1	C	152	LEU
1	C	168	GLU
1	C	193	LEU
1	C	195	THR
1	C	197	GLU
1	C	199	LEU
1	C	220	LEU
1	C	221	LEU
1	C	249	LEU
1	C	277	ILE
1	D	71	THR
1	D	91	LEU
1	D	102	LEU
1	D	108	VAL
1	D	122	LEU
1	D	123	CYS
1	D	128	THR
1	D	137	LEU
1	D	141	THR
1	D	146	LYS
1	D	148	LEU
1	D	152	LEU
1	D	168	GLU
1	D	193	LEU
1	D	195	THR
1	D	197	GLU
1	D	199	LEU
1	D	220	LEU
1	D	221	LEU
1	D	249	LEU
1	D	277	ILE
1	E	71	THR
1	E	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	102	LEU
1	E	108	VAL
1	E	122	LEU
1	E	123	CYS
1	E	128	THR
1	E	137	LEU
1	E	146	LYS
1	E	148	LEU
1	E	152	LEU
1	E	168	GLU
1	E	193	LEU
1	E	195	THR
1	E	197	GLU
1	E	199	LEU
1	E	220	LEU
1	E	221	LEU
1	E	249	LEU
1	E	277	ILE
1	F	71	THR
1	F	73	LYS
1	F	91	LEU
1	F	102	LEU
1	F	108	VAL
1	F	122	LEU
1	F	123	CYS
1	F	128	THR
1	F	137	LEU
1	F	146	LYS
1	F	148	LEU
1	F	152	LEU
1	F	168	GLU
1	F	193	LEU
1	F	195	THR
1	F	197	GLU
1	F	199	LEU
1	F	220	LEU
1	F	221	LEU
1	F	249	LEU
1	F	277	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	HIS
1	A	158	HIS
1	A	205	GLN
1	A	267	GLN
1	B	112	HIS
1	B	158	HIS
1	B	205	GLN
1	B	267	GLN
1	C	112	HIS
1	C	158	HIS
1	C	205	GLN
1	C	267	GLN
1	D	112	HIS
1	D	158	HIS
1	D	205	GLN
1	D	267	GLN
1	E	112	HIS
1	E	158	HIS
1	E	205	GLN
1	E	267	GLN
1	F	112	HIS
1	F	158	HIS
1	F	205	GLN
1	F	267	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

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	PO4	A	1	-	4,4,4	0.70	0	6,6,6	1.29	1 (16%)
3	PO4	B	2	-	4,4,4	0.65	0	6,6,6	0.88	0
3	PO4	E	3	-	4,4,4	0.65	0	6,6,6	0.99	0
2	EPE	F	3380	-	15,15,15	0.81	1 (6%)	18,20,20	2.02	6 (33%)
2	EPE	E	3380	-	15,15,15	0.53	0	18,20,20	2.08	5 (27%)
2	EPE	C	3380	-	15,15,15	0.95	1 (6%)	18,20,20	1.85	5 (27%)
2	EPE	A	3380	-	15,15,15	0.81	1 (6%)	18,20,20	1.97	6 (33%)
2	EPE	B	3380	-	15,15,15	0.85	1 (6%)	18,20,20	1.83	5 (27%)
3	PO4	C	4	-	4,4,4	0.68	0	6,6,6	0.71	0
2	EPE	D	3380	-	15,15,15	0.91	1 (6%)	18,20,20	1.86	6 (33%)

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
2	EPE	F	3380	-	-	3/9/19/19	0/1/1/1
2	EPE	E	3380	-	-	4/9/19/19	0/1/1/1
2	EPE	C	3380	-	-	3/9/19/19	0/1/1/1
2	EPE	A	3380	-	-	7/9/19/19	0/1/1/1
2	EPE	B	3380	-	-	4/9/19/19	0/1/1/1
2	EPE	D	3380	-	-	5/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3380	EPE	C10-S	3.26	1.82	1.77
2	D	3380	EPE	C10-S	2.99	1.81	1.77
2	B	3380	EPE	C10-S	2.83	1.81	1.77
2	F	3380	EPE	C10-S	2.62	1.81	1.77
2	A	3380	EPE	C10-S	2.58	1.81	1.77

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3380	EPE	C5-N4-C3	4.46	118.87	108.83
2	E	3380	EPE	O3S-S-C10	4.41	112.89	105.77
2	E	3380	EPE	C5-N4-C3	4.21	118.30	108.83
2	A	3380	EPE	C5-N4-C3	3.91	117.63	108.83
2	F	3380	EPE	O1S-S-C10	3.82	111.52	106.92
2	A	3380	EPE	C6-N1-C2	3.75	117.26	108.83
2	C	3380	EPE	O3S-S-C10	3.64	111.65	105.77
2	E	3380	EPE	C7-N4-C3	3.60	120.45	111.23
2	B	3380	EPE	O3S-S-C10	3.56	111.53	105.77
2	B	3380	EPE	C5-N4-C3	3.52	116.75	108.83
2	A	3380	EPE	C7-N4-C3	3.48	120.13	111.23
2	D	3380	EPE	C5-N4-C3	3.36	116.40	108.83
2	C	3380	EPE	C5-N4-C3	3.34	116.34	108.83
2	D	3380	EPE	O2S-S-C10	3.33	110.92	106.92
2	A	3380	EPE	O3S-S-C10	3.24	111.01	105.77
2	F	3380	EPE	C7-N4-C3	3.22	119.47	111.23
2	F	3380	EPE	C7-N4-C5	3.17	119.34	111.23
2	E	3380	EPE	C7-N4-C5	3.17	119.33	111.23
2	F	3380	EPE	O2S-S-C10	3.12	110.67	106.92
2	B	3380	EPE	C7-N4-C3	3.11	119.20	111.23
2	C	3380	EPE	O2S-S-C10	3.09	110.64	106.92
2	D	3380	EPE	C7-N4-C5	3.08	119.10	111.23
2	D	3380	EPE	C7-N4-C3	3.00	118.90	111.23
2	E	3380	EPE	O1S-S-C10	2.92	110.44	106.92
2	B	3380	EPE	O2S-S-C10	2.88	110.39	106.92
2	D	3380	EPE	O3S-S-C10	2.86	110.40	105.77
2	C	3380	EPE	C7-N4-C5	2.72	118.20	111.23
2	D	3380	EPE	C6-N1-C2	2.65	114.80	108.83
3	A	1	PO4	O3-P-O2	2.61	116.35	107.97
2	B	3380	EPE	C7-N4-C5	2.58	117.84	111.23
2	C	3380	EPE	C7-N4-C3	2.45	117.51	111.23
2	A	3380	EPE	C7-N4-C5	2.41	117.39	111.23
2	A	3380	EPE	C2-C3-N4	2.19	115.13	110.64
2	F	3380	EPE	O2S-S-O1S	-2.05	106.85	113.95

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3380	EPE	C10-C9-N1-C2
2	A	3380	EPE	C10-C9-N1-C6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	3380	EPE	C9-C10-S-O2S
2	A	3380	EPE	C9-C10-S-O3S
2	B	3380	EPE	N4-C7-C8-O8
2	B	3380	EPE	C9-C10-S-O2S
2	C	3380	EPE	C9-C10-S-O1S
2	C	3380	EPE	C9-C10-S-O3S
2	D	3380	EPE	C9-C10-S-O1S
2	D	3380	EPE	C9-C10-S-O2S
2	E	3380	EPE	C8-C7-N4-C5
2	E	3380	EPE	C9-C10-S-O1S
2	E	3380	EPE	C9-C10-S-O2S
2	F	3380	EPE	C8-C7-N4-C3
2	F	3380	EPE	N4-C7-C8-O8
2	D	3380	EPE	C9-C10-S-O3S
2	A	3380	EPE	N4-C7-C8-O8
2	F	3380	EPE	C8-C7-N4-C5
2	E	3380	EPE	C9-C10-S-O3S
2	D	3380	EPE	C10-C9-N1-C2
2	D	3380	EPE	C10-C9-N1-C6
2	A	3380	EPE	C9-C10-S-O1S
2	B	3380	EPE	C9-C10-S-O1S
2	C	3380	EPE	C9-C10-S-O2S
2	A	3380	EPE	C8-C7-N4-C5
2	B	3380	EPE	C9-C10-S-O3S

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	PO4	1	0
2	A	3380	EPE	2	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	263/263 (100%)	-0.13	0 100 100	38, 50, 69, 86	11 (4%)
1	B	263/263 (100%)	-0.09	1 (0%) 92 93	39, 53, 72, 88	11 (4%)
1	C	263/263 (100%)	-0.07	1 (0%) 92 93	37, 50, 70, 87	11 (4%)
1	D	263/263 (100%)	-0.09	0 100 100	38, 51, 70, 87	11 (4%)
1	E	263/263 (100%)	-0.02	4 (1%) 73 76	40, 53, 72, 88	11 (4%)
1	F	263/263 (100%)	0.88	52 (19%) 1 0	45, 57, 76, 93	11 (4%)
All	All	1578/1578 (100%)	0.08	58 (3%) 41 41	37, 53, 72, 93	66 (4%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	102	LEU	5.4
1	F	227	ALA	5.4
1	F	114	THR	4.6
1	F	97	TYR	4.3
1	F	99	GLN	3.9
1	F	229	TRP	3.7
1	F	122	LEU	3.6
1	F	103	VAL	3.5
1	F	26	HIS	3.5
1	F	253	GLY	3.5
1	F	113	LEU	3.5
1	F	57	LEU	3.4
1	F	112	HIS	3.3
1	F	48	GLU	3.2
1	F	226	PRO	3.2
1	E	175	ASN	3.0
1	F	230	PHE	3.0
1	F	254	LYS	3.0
1	E	40	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	248	ALA	2.9
1	F	96	HIS	2.8
1	F	137	LEU	2.8
1	F	288	TRP	2.7
1	F	252	ASP	2.7
1	F	134	ALA	2.7
1	F	95	ILE	2.6
1	F	94	ARG	2.6
1	F	87	GLY	2.6
1	F	284	LEU	2.5
1	F	133	THR	2.5
1	F	115	ASP	2.5
1	E	39	GLN	2.4
1	F	118	THR	2.4
1	F	287	HIS	2.4
1	F	282	ALA	2.4
1	F	271	ASP	2.4
1	F	225	LEU	2.3
1	F	111	LYS	2.3
1	F	232	ALA	2.3
1	F	210	TRP	2.3
1	F	107	PRO	2.3
1	F	109	THR	2.3
1	F	28	GLU	2.3
1	F	257	ARG	2.3
1	F	251	PRO	2.2
1	F	129	MET	2.2
1	F	31	VAL	2.2
1	F	120	ARG	2.2
1	F	30	LEU	2.2
1	B	102	LEU	2.2
1	F	90	GLN	2.1
1	C	104	GLU	2.1
1	F	169	LEU	2.1
1	F	104	GLU	2.1
1	F	212	GLU	2.1
1	F	56	ILE	2.0
1	E	264	THR	2.0
1	F	255	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
3	PO4	C	4	5/5	0.82	0.25	71,85,89,121	0
3	PO4	A	1	5/5	0.91	0.35	65,67,76,106	0
2	EPE	F	3380	15/15	0.94	0.15	78,87,100,103	11
2	EPE	A	3380	15/15	0.94	0.22	51,73,97,100	0
3	PO4	B	2	5/5	0.94	0.32	53,79,86,87	0
2	EPE	E	3380	15/15	0.94	0.17	46,58,61,66	10
3	PO4	E	3	5/5	0.94	0.23	62,72,86,102	0
2	EPE	D	3380	15/15	0.96	0.14	44,61,65,67	9
2	EPE	C	3380	15/15	0.97	0.15	40,61,74,76	9
2	EPE	B	3380	15/15	0.97	0.21	46,66,78,80	10

6.5 Other polymers [i](#)

There are no such residues in this entry.