Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 04:13 PM JST

PDB ID	:	6JKS
Title	:	Crystal structure of aspartate transcarbamoylase from Trypanosoma cruzi in complex with carbamoyl phosphate (CP) and aspartate (Asp)
Authors	:	Matoba, K.; Shiba, T.; Nara, T.; Aoki, T.; Nagasaki, S.; Hayamizu, R.; Honma, T.; Tanaka, A.; Inoue, M.; Matsuoka, S.; Balogun, E.O.; Inaoka, D.K.; Kita, K.; Harada, S.
Deposited on	:	2019-03-01
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

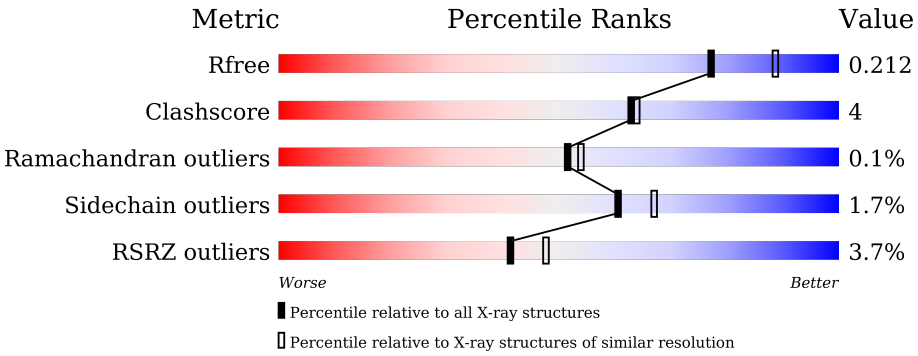
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	328	2% 86% 11% • •
1	B	328	2% 84% 9% • 7%
1	C	328	5% 87% 6% • 7%
1	D	328	6% 92% 8%
1	E	328	3% 81% 10% • 8%

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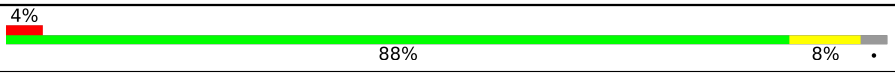
Mol	Chain	Length	Quality of chain
1	F	328	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15321 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.

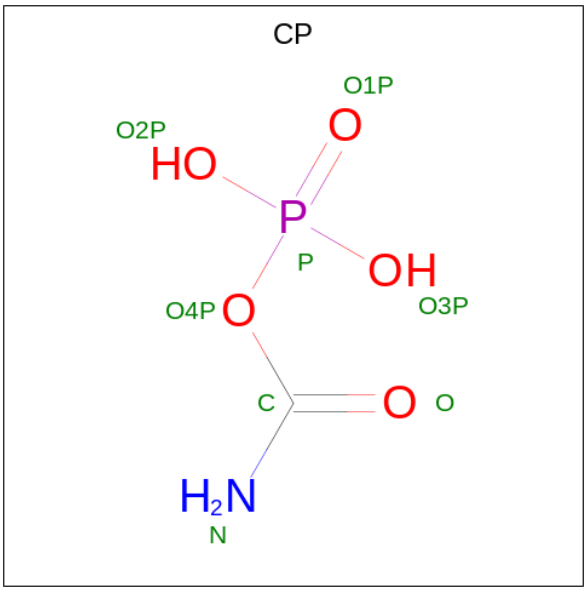
- Molecule 1 is a protein called Aspartate carbamoyltransferase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2482	1565	436	465	16			
1	B	306	Total	C	N	O	S	0	0	0
			2367	1494	415	441	17			
1	C	306	Total	C	N	O	S	0	0	0
			2366	1493	415	441	17			
1	D	328	Total	C	N	O	S	0	0	0
			2527	1592	443	474	18			
1	E	302	Total	C	N	O	S	0	0	0
			2340	1477	411	436	16			
1	F	318	Total	C	N	O	S	0	0	0
			2447	1544	429	457	17			

There are 12 discrepancies between the modelled and reference sequences:

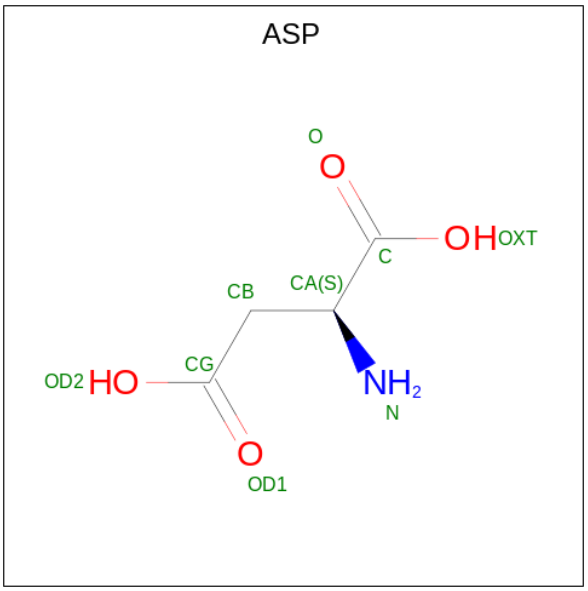
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q4D3W3
A	0	SER	-	expression tag	UNP Q4D3W3
B	-1	GLY	-	expression tag	UNP Q4D3W3
B	0	SER	-	expression tag	UNP Q4D3W3
C	-1	GLY	-	expression tag	UNP Q4D3W3
C	0	SER	-	expression tag	UNP Q4D3W3
D	-1	GLY	-	expression tag	UNP Q4D3W3
D	0	SER	-	expression tag	UNP Q4D3W3
E	-1	GLY	-	expression tag	UNP Q4D3W3
E	0	SER	-	expression tag	UNP Q4D3W3
F	-1	GLY	-	expression tag	UNP Q4D3W3
F	0	SER	-	expression tag	UNP Q4D3W3

- Molecule 2 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula: CH_4NO_5P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			8	1	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			8	1	1	5	1		

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 4 1 4	0	0
3	B	1	Total C N O 9 4 1 4	0	0
3	C	1	Total C N O 9 4 1 4	0	0
3	D	1	Total C N O 9 4 1 4	0	0
3	E	1	Total C N O 9 4 1 4	0	0
3	F	1	Total C N O 9 4 1 4	0	0

- Molecule 4 is water.

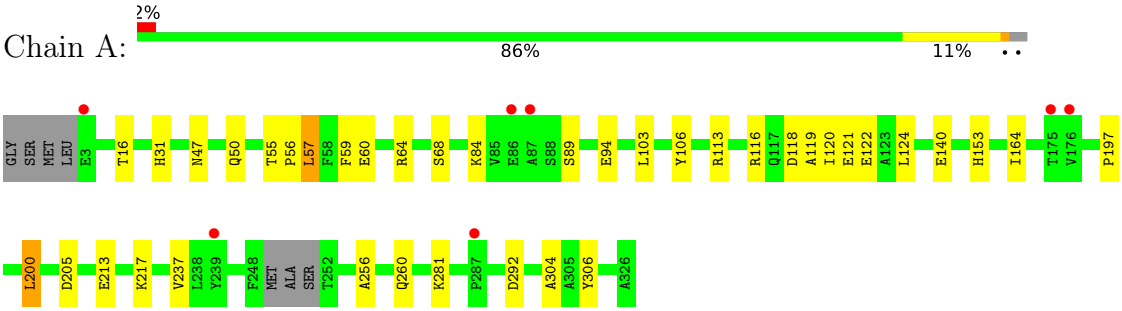
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	130	Total O 130 130	0	0
4	B	133	Total O 133 133	0	0
4	C	88	Total O 88 88	0	0
4	D	111	Total O 111 111	0	0
4	E	101	Total O 101 101	0	0
4	F	127	Total O 127 127	0	0

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.

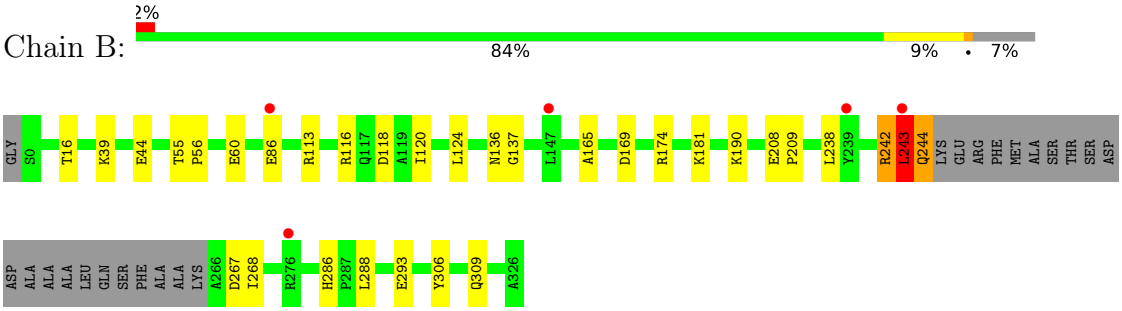
• Molecule 1: Aspartate carbamoyltransferase, putative

Chain A:



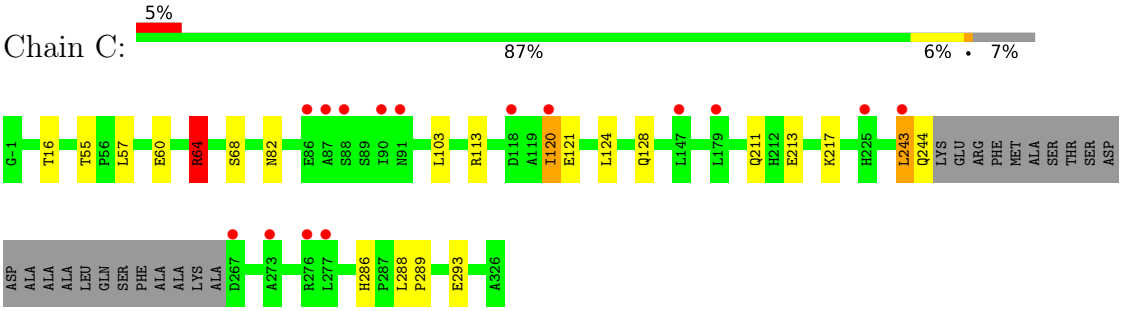
• Molecule 1: Aspartate carbamoyltransferase, putative

Chain B:



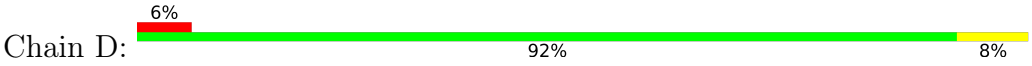
• Molecule 1: Aspartate carbamoyltransferase, putative

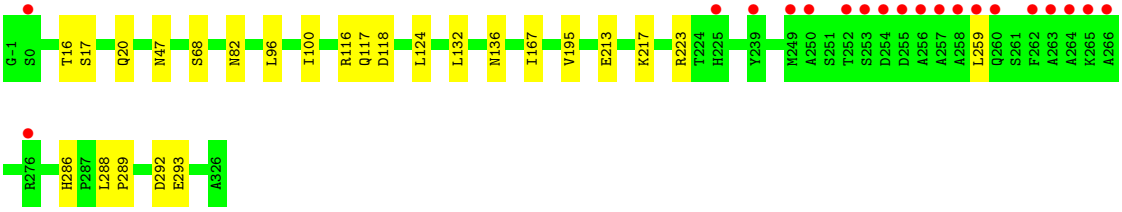
Chain C:



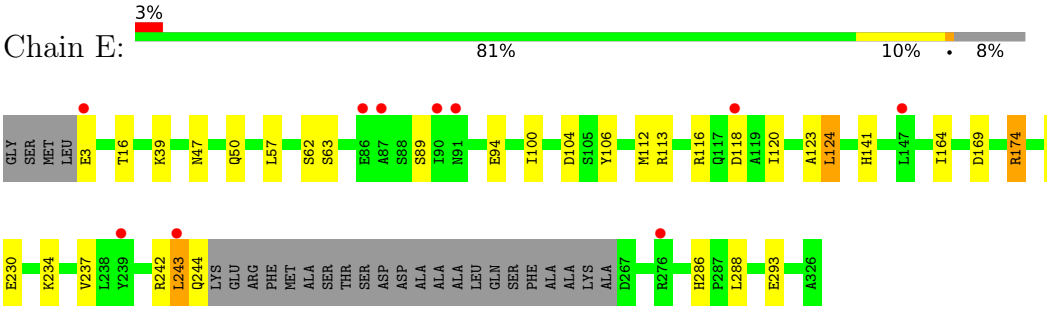
• Molecule 1: Aspartate carbamoyltransferase, putative

Chain D:

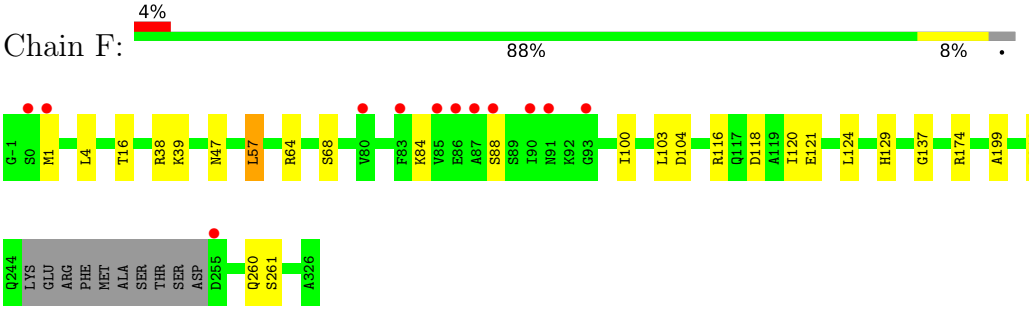




• Molecule 1: Aspartate carbamoyltransferase, putative



• Molecule 1: Aspartate carbamoyltransferase, putative



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.33Å 157.31Å 88.59Å 90.00° 119.73° 90.00°	Depositor
Resolution (Å)	29.44 – 2.10 29.44 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.44-2.10) 99.9 (29.44-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.67 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.166 , 0.212 0.168 , 0.212	Depositor DCC
R_{free} test set	6117 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.007 for -h-l,k,h 0.007 for l,k,-h-l 0.126 for h,-k,-h-l 0.021 for -h-l,-k,l 0.021 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15321	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.76	2/2521 (0.1%)	0.74	1/3407 (0.0%)
1	B	0.73	0/2404	0.72	0/3250
1	C	0.69	0/2403	0.71	1/3248 (0.0%)
1	D	0.71	0/2567	0.71	0/3469
1	E	0.72	0/2377	0.74	2/3214 (0.1%)
1	F	0.74	0/2485	0.76	0/3359
All	All	0.72	2/14757 (0.0%)	0.73	4/19947 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	140	GLU	CD-OE1	-6.15	1.18	1.25
1	A	140	GLU	CD-OE2	-5.74	1.19	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	64	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	E	113	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	E	205	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	205	ASP	CB-CG-OD1	5.06	122.86	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2482	0	2533	25	0
1	B	2367	0	2429	22	0
1	C	2366	0	2427	18	0
1	D	2527	0	2584	16	0
1	E	2340	0	2396	32	0
1	F	2447	0	2507	18	0
2	A	8	0	2	1	0
2	B	8	0	2	0	0
2	C	8	0	2	0	0
2	D	8	0	2	1	0
2	E	8	0	2	1	0
2	F	8	0	2	0	0
3	A	9	0	3	1	0
3	B	9	0	3	0	0
3	C	9	0	3	0	0
3	D	9	0	3	1	0
3	E	9	0	3	3	0
3	F	9	0	3	0	0
4	A	130	0	0	7	0
4	B	133	0	0	3	0
4	C	88	0	0	3	0
4	D	111	0	0	2	0
4	E	101	0	0	4	0
4	F	127	0	0	3	0
All	All	15321	0	14906	127	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 4.

All (127) 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:B:190:LYS:HE2	4:B:620:HOH:O	1.47	1.15
1:E:112:MET:CE	1:E:120:ILE:HD13	1.79	1.11
1:C:243:LEU:O	1:C:244:GLN:HB2	1.44	1.09
1:E:112:MET:HE3	1:E:120:ILE:HD13	1.11	1.06
1:E:47:ASN:HB3	4:E:578:HOH:O	1.59	1.02
1:D:292:ASP:HB3	4:D:598:HOH:O	1.61	0.98
1:B:286:HIS:HD2	1:B:288:LEU:H	1.11	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:MET:HE3	1:E:120:ILE:CD1	1.98	0.93
1:E:286:HIS:HD2	1:E:288:LEU:H	1.17	0.93
1:D:213:GLU:HG3	4:D:607:HOH:O	1.69	0.93
1:D:286:HIS:HD2	1:D:288:LEU:H	1.16	0.92
1:C:243:LEU:O	1:C:244:GLN:CB	2.21	0.89
1:E:112:MET:HE1	1:E:120:ILE:HA	1.59	0.84
1:C:286:HIS:HD2	1:C:288:LEU:H	1.22	0.84
1:A:292:ASP:HB2	4:A:608:HOH:O	1.81	0.80
1:F:199:ALA:H	1:F:260:GLN:HE22	1.32	0.78
1:C:55:THR:HG21	1:C:103:LEU:HD12	1.70	0.73
1:A:116:ARG:NH1	1:A:118:ASP:OD1	2.22	0.72
1:B:286:HIS:CD2	1:B:288:LEU:H	2.02	0.72
1:C:286:HIS:HE1	1:C:293:GLU:OE2	1.71	0.72
1:A:16:THR:HG21	1:A:124:LEU:HD11	1.72	0.71
1:D:16:THR:HG21	1:D:124:LEU:HD11	1.73	0.71
1:E:112:MET:CE	1:E:120:ILE:HA	2.20	0.71
1:B:16:THR:HG21	1:B:124:LEU:HD11	1.72	0.71
1:E:286:HIS:CD2	1:E:288:LEU:H	2.07	0.69
1:B:286:HIS:H	1:B:309:GLN:HE22	1.42	0.68
1:A:57:LEU:HD23	1:A:59:PHE:HE1	1.58	0.68
1:D:286:HIS:CD2	1:D:288:LEU:H	2.04	0.67
1:A:106:TYR:OH	1:C:64:ARG:HB2	1.95	0.66
1:A:197:PRO:HG2	1:A:200:LEU:HB2	1.77	0.65
1:C:286:HIS:CD2	1:C:288:LEU:H	2.11	0.65
1:F:199:ALA:H	1:F:260:GLN:NE2	1.94	0.64
1:E:16:THR:HG21	1:E:124:LEU:HD21	1.79	0.64
1:F:64:ARG:O	1:F:68:SER:HB2	1.98	0.64
1:A:153:HIS:HD2	4:A:507:HOH:O	1.81	0.63
1:A:47:ASN:OD1	1:A:50:GLN:HB2	1.99	0.63
1:F:16:THR:HG21	1:F:124:LEU:HD11	1.81	0.62
1:C:211:GLN:HG3	4:C:552:HOH:O	1.98	0.62
1:B:39:LYS:HE3	1:B:44:GLU:OE1	2.01	0.60
1:C:16:THR:HG21	1:C:124:LEU:HD11	1.84	0.59
1:D:116:ARG:NH1	1:D:118:ASP:OD1	2.35	0.59
1:C:213:GLU:OE1	1:C:217:LYS:HE3	2.02	0.59
1:D:286:HIS:HE1	1:D:293:GLU:OE2	1.86	0.59
1:F:213:GLU:OE1	1:F:217:LYS:HE3	2.02	0.58
1:E:89:SER:HB2	1:E:94:GLU:OE1	2.04	0.56
1:A:164:ILE:HG13	1:A:237:VAL:HG22	1.87	0.56
2:A:401:CP:C	3:A:402:ASP:N	2.70	0.55
1:E:3:GLU:HG3	1:E:39:LYS:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:HIS:HE1	1:B:293:GLU:OE2	1.90	0.54
1:D:223:ARG:HG3	1:D:223:ARG:HH11	1.73	0.54
1:A:120:ILE:HG22	4:A:514:HOH:O	2.07	0.53
1:F:104:ASP:OD1	1:F:129:HIS:HD2	1.92	0.53
1:E:141:HIS:HB2	1:E:174:ARG:HG3	1.90	0.53
1:F:116:ARG:NH1	1:F:118:ASP:OD1	2.42	0.52
1:D:96:LEU:O	1:D:100:ILE:HG12	2.09	0.52
1:C:120:ILE:HG13	4:C:501:HOH:O	2.10	0.52
1:C:55:THR:HG21	1:C:103:LEU:CD1	2.39	0.52
1:A:60:GLU:HG3	1:A:113:ARG:HG2	1.91	0.51
1:A:121:GLU:HG2	4:A:514:HOH:O	2.10	0.51
1:E:164:ILE:HG13	1:E:237:VAL:HG22	1.94	0.50
1:F:57:LEU:HG	1:F:103:LEU:CD1	2.42	0.50
1:D:213:GLU:OE1	1:D:217:LYS:HE3	2.11	0.50
1:B:169:ASP:HB2	1:B:243:LEU:HA	1.93	0.50
1:F:137:GLY:O	1:F:174:ARG:HD3	2.12	0.49
1:B:306:TYR:HA	1:B:309:GLN:HE21	1.77	0.49
1:D:289:PRO:HG3	1:E:89:SER:HB3	1.94	0.49
1:B:267:ASP:HA	4:B:618:HOH:O	2.13	0.48
1:C:286:HIS:CE1	1:C:293:GLU:OE2	2.60	0.48
1:B:268:ILE:C	1:B:268:ILE:HD12	2.34	0.48
1:E:116:ARG:NH1	1:E:118:ASP:OD1	2.46	0.48
1:E:3:GLU:HG3	1:E:39:LYS:CE	2.43	0.48
1:F:100:ILE:O	1:F:104:ASP:HB2	2.14	0.48
1:A:57:LEU:CD2	1:A:59:PHE:HE1	2.26	0.47
1:F:199:ALA:N	1:F:260:GLN:HE22	2.07	0.46
1:C:121:GLU:HG2	4:C:501:HOH:O	2.14	0.46
1:E:47:ASN:CB	4:E:578:HOH:O	2.36	0.46
1:A:64:ARG:O	1:A:68:SER:HB2	2.15	0.46
1:B:116:ARG:NH1	1:B:118:ASP:OD1	2.49	0.45
1:B:208:GLU:HB3	1:B:209:PRO:HD3	1.98	0.45
1:A:106:TYR:CZ	1:C:68:SER:HB3	2.52	0.45
1:D:17:SER:O	1:D:20:GLN:HG2	2.16	0.45
1:C:60:GLU:HG3	1:C:113:ARG:HD3	1.99	0.45
1:B:60:GLU:HG3	1:B:113:ARG:HG2	1.99	0.45
1:E:112:MET:HE1	1:E:123:ALA:HB3	1.99	0.45
1:A:304:ALA:HB1	1:A:306:TYR:CE1	2.52	0.44
1:E:174:ARG:CD	3:E:402:ASP:OXT	2.65	0.44
1:C:288:LEU:HB3	1:C:289:PRO:HA	1.98	0.44
1:E:169:ASP:OD2	1:E:244:GLN:HB2	2.17	0.44
1:F:243:LEU:HD23	1:F:261:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:LYS:O	1:F:88:SER:HB3	2.18	0.44
1:B:242:ARG:O	1:B:244:GLN:N	2.49	0.44
1:E:141:HIS:HB2	1:E:174:ARG:CG	2.48	0.43
1:E:112:MET:HE2	1:E:120:ILE:HD13	1.89	0.43
1:A:89:SER:HB2	1:A:94:GLU:OE1	2.18	0.43
1:A:119:ALA:HB3	4:A:516:HOH:O	2.19	0.43
1:A:256:ALA:O	1:A:260:GLN:HG2	2.18	0.43
1:B:286:HIS:HD2	1:B:288:LEU:N	1.94	0.43
1:E:63:SER:OG	1:F:88:SER:HB2	2.19	0.43
1:B:55:THR:HA	1:B:56:PRO:HD3	1.91	0.42
1:E:243:LEU:N	4:E:506:HOH:O	2.51	0.42
1:F:120:ILE:CG2	4:F:531:HOH:O	2.66	0.42
2:E:401:CP:O3P	3:E:402:ASP:N	2.52	0.42
1:F:120:ILE:HG23	4:F:531:HOH:O	2.18	0.42
1:B:243:LEU:N	1:B:243:LEU:CD2	2.83	0.42
1:E:230:GLU:HG3	1:E:234:LYS:HE2	2.02	0.42
1:A:89:SER:HB3	1:C:289:PRO:HG3	2.01	0.42
1:E:286:HIS:HE1	1:E:293:GLU:OE2	2.03	0.42
1:F:121:GLU:HG2	4:F:531:HOH:O	2.19	0.42
1:A:31:HIS:HD2	4:A:620:HOH:O	2.02	0.41
1:D:47:ASN:HD21	1:E:50:GLN:HE22	1.68	0.41
1:B:120:ILE:HG13	1:B:136:ASN:HB3	2.02	0.41
1:B:165:ALA:HB3	1:B:238:LEU:HD23	2.03	0.41
1:D:68:SER:HB3	1:E:106:TYR:CZ	2.56	0.41
1:F:4:LEU:HD11	1:F:39:LYS:HD2	2.02	0.41
1:E:286:HIS:HD2	1:E:288:LEU:N	2.00	0.41
1:A:55:THR:HA	1:A:56:PRO:HD3	1.94	0.40
1:A:213:GLU:OE2	1:A:217:LYS:HE3	2.21	0.40
1:D:117:GLN:HG2	1:D:136:ASN:O	2.21	0.40
1:B:181:LYS:HE2	4:B:544:HOH:O	2.21	0.40
1:E:190:LYS:HE3	4:E:600:HOH:O	2.22	0.40
1:E:242:ARG:HH21	3:E:402:ASP:CG	2.25	0.40
1:A:122:GLU:HB3	4:A:593:HOH:O	2.21	0.40
1:B:137:GLY:O	1:B:174:ARG:HD3	2.20	0.40
2:D:401:CP:O1P	3:D:402:ASP:N	2.54	0.40
1:E:100:ILE:O	1:E:104:ASP:HB2	2.21	0.40
1:A:55:THR:HG21	1:A:103:LEU:HD12	2.04	0.40
1:D:167:ILE:HA	1:D:195:VAL:O	2.20	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	317/328 (97%)	307 (97%)	10 (3%)	0	100	100
1	B	302/328 (92%)	294 (97%)	7 (2%)	1 (0%)	41	41
1	C	302/328 (92%)	293 (97%)	9 (3%)	0	100	100
1	D	326/328 (99%)	318 (98%)	8 (2%)	0	100	100
1	E	298/328 (91%)	290 (97%)	8 (3%)	0	100	100
1	F	314/328 (96%)	306 (98%)	8 (2%)	0	100	100
All	All	1859/1968 (94%)	1808 (97%)	50 (3%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	243	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	270/275 (98%)	266 (98%)	4 (2%)	65	71
1	B	260/275 (94%)	256 (98%)	4 (2%)	65	71
1	C	260/275 (94%)	254 (98%)	6 (2%)	50	55
1	D	275/275 (100%)	272 (99%)	3 (1%)	73	79
1	E	257/275 (94%)	252 (98%)	5 (2%)	57	63
1	F	266/275 (97%)	262 (98%)	4 (2%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1588/1650 (96%)	1562 (98%)	26 (2%)	60 69

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	84	LYS
1	A	200	LEU
1	A	281	LYS
1	B	86	GLU
1	B	242	ARG
1	B	243	LEU
1	B	244	GLN
1	C	57	LEU
1	C	64	ARG
1	C	82	ASN
1	C	120	ILE
1	C	128	GLN
1	C	243	LEU
1	D	82	ASN
1	D	132	LEU
1	D	259	LEU
1	E	57	LEU
1	E	62	SER
1	E	124	LEU
1	E	174	ARG
1	E	243	LEU
1	F	1	MET
1	F	38	ARG
1	F	47	ASN
1	F	57	LEU

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

Mol	Chain	Res	Type
1	A	153	HIS
1	B	129	HIS
1	B	225	HIS
1	B	286	HIS
1	B	309	GLN
1	C	50	GLN

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Mol	Chain	Res	Type
1	C	128	GLN
1	C	129	HIS
1	C	211	GLN
1	C	286	HIS
1	D	31	HIS
1	D	91	ASN
1	D	129	HIS
1	D	212	HIS
1	D	286	HIS
1	E	50	GLN
1	E	82	ASN
1	E	129	HIS
1	E	212	HIS
1	E	286	HIS
1	E	291	ASN
1	F	31	HIS
1	F	82	ASN
1	F	129	HIS
1	F	260	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

12 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	$\#\|Z\| > 2$
2	CP	F	401	-	6,7,7	0.96	0	7,10,10	1.43	1 (14%)
3	ASP	F	402	-	6,8,8	1.28	1 (16%)	8,10,10	1.85	2 (25%)
3	ASP	E	402	-	6,8,8	1.38	1 (16%)	8,10,10	1.85	2 (25%)
2	CP	B	401	-	6,7,7	1.40	1 (16%)	7,10,10	1.28	1 (14%)
2	CP	E	401	-	6,7,7	1.62	1 (16%)	7,10,10	1.41	1 (14%)
2	CP	D	401	-	6,7,7	2.08	3 (50%)	7,10,10	2.51	3 (42%)
3	ASP	A	402	-	6,8,8	1.34	1 (16%)	8,10,10	1.76	2 (25%)
3	ASP	B	402	-	6,8,8	1.32	1 (16%)	8,10,10	1.70	2 (25%)
3	ASP	D	402	-	6,8,8	1.29	1 (16%)	8,10,10	1.99	2 (25%)
3	ASP	C	402	-	6,8,8	1.13	0	8,10,10	1.36	1 (12%)
2	CP	C	401	-	6,7,7	1.31	1 (16%)	7,10,10	1.36	1 (14%)
2	CP	A	401	-	6,7,7	1.06	0	7,10,10	0.98	0

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	CP	F	401	-	-	0/3/5/5	-
3	ASP	F	402	-	-	3/8/8/8	-
3	ASP	E	402	-	-	2/8/8/8	-
2	CP	B	401	-	-	0/3/5/5	-
2	CP	E	401	-	-	0/3/5/5	-
2	CP	D	401	-	-	0/3/5/5	-
3	ASP	A	402	-	-	0/8/8/8	-
3	ASP	B	402	-	-	2/8/8/8	-
3	ASP	D	402	-	-	2/8/8/8	-
3	ASP	C	402	-	-	3/8/8/8	-
2	CP	C	401	-	-	0/3/5/5	-
2	CP	A	401	-	-	0/3/5/5	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	CP	P-O4P	3.26	1.64	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	CP	P-O3P	-3.12	1.42	1.54
2	D	401	CP	P-O2P	-2.79	1.44	1.54
2	C	401	CP	P-O4P	2.69	1.63	1.59
3	E	402	ASP	OXT-C	-2.55	1.22	1.30
2	B	401	CP	O-C	2.42	1.25	1.21
3	F	402	ASP	OXT-C	-2.23	1.23	1.30
2	D	401	CP	P-O1P	-2.21	1.43	1.50
3	A	402	ASP	OXT-C	-2.20	1.23	1.30
3	D	402	ASP	OXT-C	-2.14	1.23	1.30
3	B	402	ASP	OXT-C	-2.01	1.24	1.30

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	CP	O-C-N	-5.61	116.25	125.51
3	D	402	ASP	OXT-C-O	-4.54	113.78	124.09
3	E	402	ASP	OXT-C-O	-3.55	116.03	124.09
3	F	402	ASP	OXT-C-O	-3.48	116.19	124.09
3	F	402	ASP	OXT-C-CA	3.35	124.79	113.38
3	E	402	ASP	OXT-C-CA	3.24	124.42	113.38
3	A	402	ASP	OXT-C-CA	3.14	124.09	113.38
3	B	402	ASP	OXT-C-CA	3.13	124.06	113.38
3	A	402	ASP	OXT-C-O	-2.98	117.32	124.09
2	F	401	CP	O4P-P-O1P	-2.77	99.47	109.32
3	D	402	ASP	OXT-C-CA	2.75	122.76	113.38
3	C	402	ASP	OXT-C-O	-2.70	117.96	124.09
2	B	401	CP	O4P-P-O1P	-2.55	100.25	109.32
3	B	402	ASP	OXT-C-O	-2.54	118.32	124.09
2	C	401	CP	O3P-P-O2P	2.53	117.30	107.64
2	E	401	CP	O-C-N	-2.51	121.37	125.51
2	D	401	CP	O3P-P-O2P	2.20	116.06	107.64
2	D	401	CP	O3P-P-O4P	-2.18	98.60	105.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	ASP	N-CA-CB-CG
3	F	402	ASP	N-CA-CB-CG
3	C	402	ASP	C-CA-CB-CG
3	D	402	ASP	O-C-CA-CB
3	F	402	ASP	CA-CB-CG-OD1

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Mol	Chain	Res	Type	Atoms
3	D	402	ASP	OXT-C-CA-CB
3	B	402	ASP	N-CA-CB-CG
3	E	402	ASP	N-CA-CB-CG
3	F	402	ASP	CA-CB-CG-OD2
3	C	402	ASP	O-C-CA-N
3	B	402	ASP	C-CA-CB-CG
3	E	402	ASP	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	402	ASP	3	0
2	E	401	CP	1	0
2	D	401	CP	1	0
3	A	402	ASP	1	0
3	D	402	ASP	1	0
2	A	401	CP	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

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, 95^{th} 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	321/328 (97%)	-0.04	7 (2%)	62	66	16, 24, 38, 52	0
1	B	306/328 (93%)	-0.15	5 (1%)	72	75	16, 23, 36, 49	0
1	C	306/328 (93%)	0.14	15 (4%)	29	35	16, 28, 45, 63	0
1	D	328/328 (100%)	0.06	20 (6%)	21	26	18, 27, 51, 65	0
1	E	302/328 (92%)	0.06	10 (3%)	46	53	18, 26, 42, 60	0
1	F	318/328 (96%)	-0.03	12 (3%)	40	46	16, 25, 45, 61	0
All	All	1881/1968 (95%)	0.01	69 (3%)	41	48	16, 25, 43, 65	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	ILE	6.3
1	D	259	LEU	6.3
1	C	86	GLU	4.9
1	D	249	MET	4.7
1	D	253	SER	4.6
1	F	93	GLY	4.3
1	F	91	ASN	4.2
1	C	91	ASN	4.2
1	F	87	ALA	4.1
1	D	250	ALA	3.9
1	E	86	GLU	3.8
1	D	266	ALA	3.6
1	D	257	ALA	3.5
1	A	3	GLU	3.5
1	D	255	ASP	3.4
1	D	252	THR	3.4
1	E	90	ILE	3.3
1	F	90	ILE	3.3
1	C	243	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	258	ALA	3.2
1	F	86	GLU	3.2
1	D	264	ALA	3.1
1	D	262	PHE	3.1
1	E	243	LEU	3.1
1	F	255	ASP	3.1
1	A	87	ALA	3.0
1	C	87	ALA	3.0
1	C	88	SER	3.0
1	D	254	ASP	3.0
1	D	265	LYS	3.0
1	E	3	GLU	3.0
1	F	0	SER	2.9
1	F	83	PHE	2.8
1	E	91	ASN	2.8
1	D	260	GLN	2.8
1	A	287	PRO	2.7
1	D	263	ALA	2.6
1	A	175	THR	2.6
1	D	276	ARG	2.6
1	A	86	GLU	2.6
1	B	243	LEU	2.6
1	E	87	ALA	2.5
1	D	256	ALA	2.5
1	A	239	TYR	2.5
1	C	120	ILE	2.4
1	C	273	ALA	2.4
1	F	85	VAL	2.4
1	E	239	TYR	2.4
1	D	225	HIS	2.4
1	E	276	ARG	2.4
1	E	147	LEU	2.4
1	E	118	ASP	2.4
1	C	147	LEU	2.3
1	D	0	SER	2.3
1	F	88	SER	2.3
1	F	1	MET	2.2
1	C	276	ARG	2.2
1	B	276	ARG	2.2
1	D	239	TYR	2.2
1	B	147	LEU	2.2
1	C	179	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	239	TYR	2.1
1	B	86	GLU	2.1
1	A	176	VAL	2.1
1	C	118	ASP	2.0
1	C	225	HIS	2.0
1	C	267	ASP	2.0
1	F	80	VAL	2.0
1	C	277	LEU	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, 95^{th} 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
3	ASP	F	402	9/9	0.78	0.23	46,47,52,55	0
3	ASP	E	402	9/9	0.83	0.18	38,39,44,46	0
3	ASP	C	402	9/9	0.85	0.17	35,38,43,44	0
3	ASP	B	402	9/9	0.91	0.12	35,37,43,48	0
2	CP	E	401	8/8	0.91	0.14	46,47,49,49	0
2	CP	B	401	8/8	0.96	0.08	29,30,33,34	0
3	ASP	D	402	9/9	0.96	0.12	28,29,34,39	0
3	ASP	A	402	9/9	0.97	0.11	24,26,28,29	0
2	CP	D	401	8/8	0.97	0.09	31,34,35,35	0
2	CP	C	401	8/8	0.97	0.10	33,35,36,36	0
2	CP	A	401	8/8	0.98	0.10	25,27,28,29	0
2	CP	F	401	8/8	0.99	0.09	23,24,25,26	0

6.5 Other polymers (i)

There are no such residues in this entry.