Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 05:45 PM JST

PDB ID	:	6JL4
Title	:	Crystal structure of aspartate transcarbamoylase from Trypanosoma cruzi in complex with carbamoyl aspartate (CA) and phosphate (Pi)
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	:	2019-03-04
Resolution	:	2.40 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:

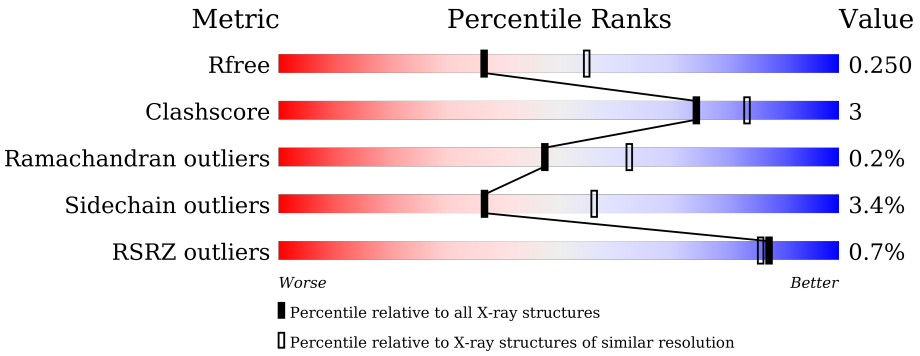
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	327	.% 86% 8% 6%
1	B	327	91% 7% •
1	C	327	86% 12% ••
1	D	327	2% 87% 10% •
1	E	327	.% 83% 12% 5%

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Mol	Chain	Length	Quality of chain
1	F	327	86% 12%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15205 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.

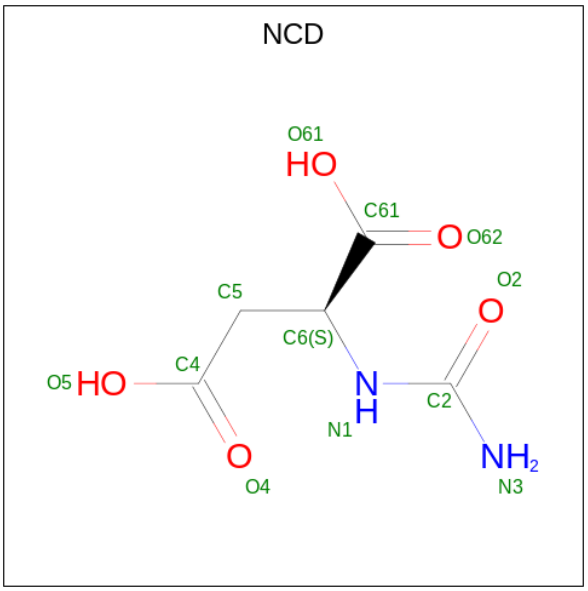
- Molecule 1 is a protein called Aspartate carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	307	2375	1500	417	441	17	0	0	0
1	B	319	2457	1551	431	458	17	0	0	0
1	C	323	2493	1570	438	468	17	0	0	0
1	D	319	2464	1555	434	458	17	0	0	0
1	E	310	2407	1520	423	447	17	0	0	0
1	F	322	2491	1572	437	465	17	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

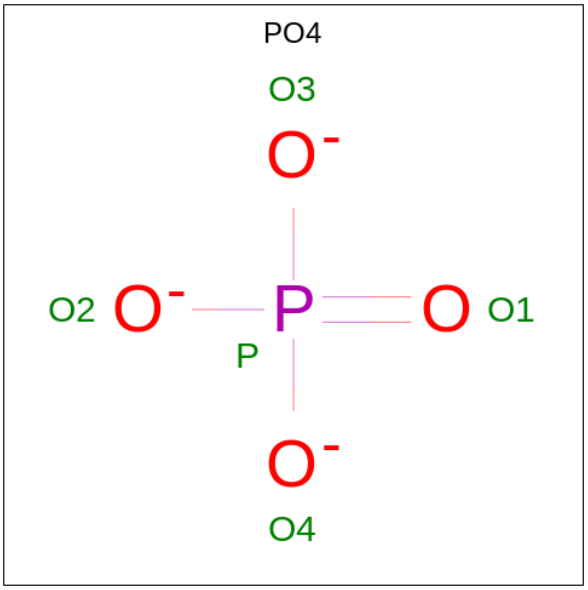
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP O15636
B	0	SER	-	expression tag	UNP O15636
C	0	SER	-	expression tag	UNP O15636
D	0	SER	-	expression tag	UNP O15636
E	0	SER	-	expression tag	UNP O15636
F	0	SER	-	expression tag	UNP O15636

- Molecule 2 is N-CARBAMOYL-L-ASPARTATE (three-letter code: NCD) (formula: $C_5H_8N_2O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	12	5	2	5	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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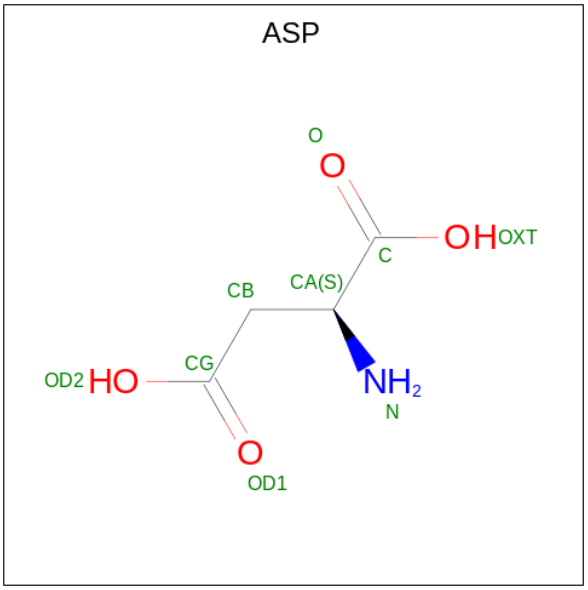
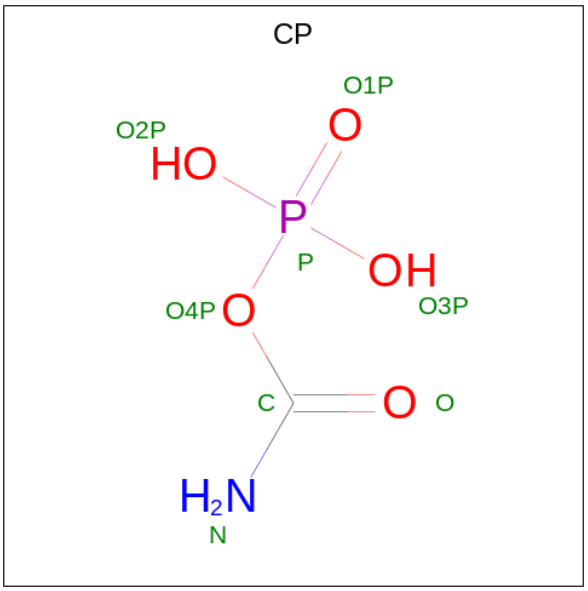
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	P			
3	E	1	5	4	1		0	0
			Total	O	P			
3	F	1	5	4	1		0	0

- Molecule 4 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



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

- Molecule 5 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (three-letter code: CP) (formula: CH_4NO_5P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	8	1	1	5	1	0	0

- Molecule 6 is water.

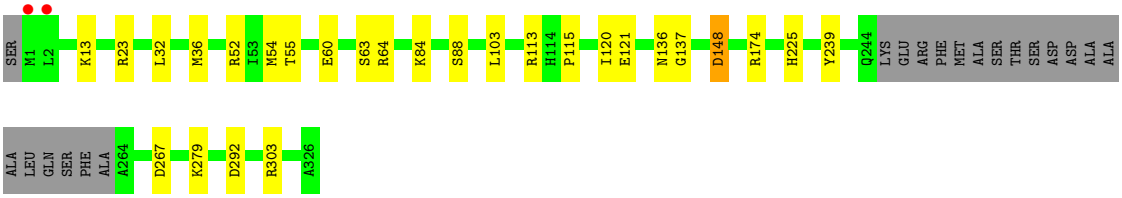
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	65	65	65	0	0
			Total	O		
6	B	71	71	71	0	0
			Total	O		
6	C	73	73	73	0	0
			Total	O		
6	D	73	73	73	0	0
			Total	O		
6	E	72	72	72	0	0
			Total	O		
6	F	74	74	74	0	0

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.

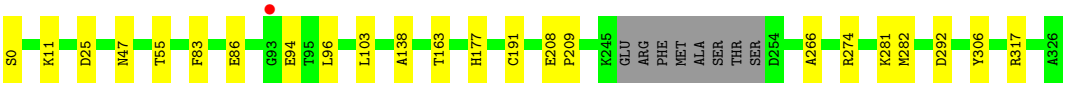
• Molecule 1: Aspartate carbamoyltransferase

Chain A:



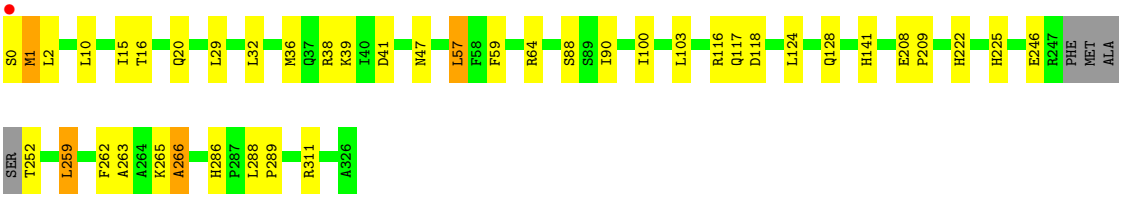
• Molecule 1: Aspartate carbamoyltransferase

Chain B:



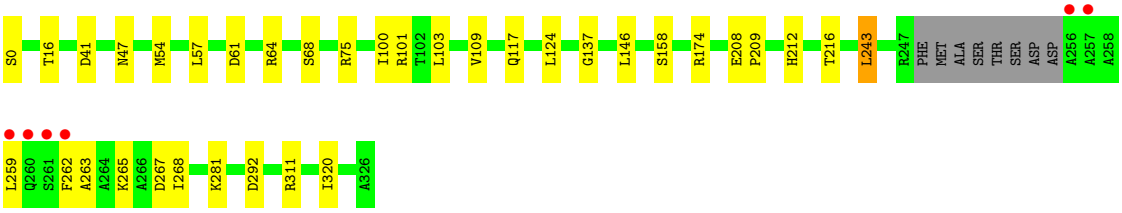
• Molecule 1: Aspartate carbamoyltransferase

Chain C:



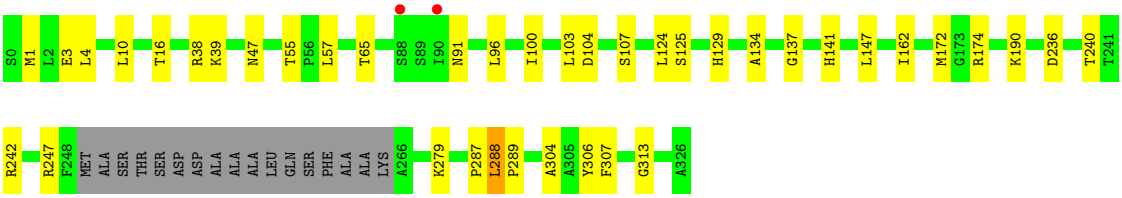
• Molecule 1: Aspartate carbamoyltransferase

Chain D:



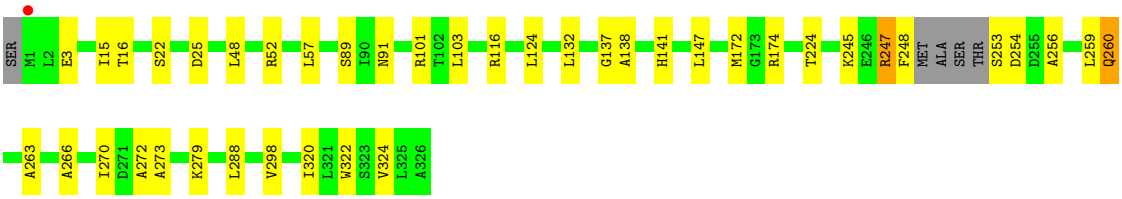
• Molecule 1: Aspartate carbamoyltransferase

Chain E:



• Molecule 1: Aspartate carbamoyltransferase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.99Å 156.98Å 88.30Å 90.00° 119.84° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.34 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.1 (30.00-2.40) 94.9 (29.34-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.176 , 0.250 0.181 , 0.250	Depositor DCC
R_{free} test set	3867 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 18.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.039 for -h-l,k,h 0.039 for l,k,-h-l 0.276 for h,-k,-h-l 0.045 for -h-l,-k,l 0.046 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15205	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CP, NCD

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	0.59	0/2412	0.78	4/3260 (0.1%)
1	B	0.61	0/2495	0.77	2/3372 (0.1%)
1	C	0.60	0/2531	0.81	3/3420 (0.1%)
1	D	0.60	0/2502	0.78	2/3380 (0.1%)
1	E	0.58	0/2445	0.78	0/3303
1	F	0.62	0/2530	0.79	1/3418 (0.0%)
All	All	0.60	0/14915	0.79	12/20153 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	52	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	266	ALA	N-CA-C	6.23	127.82	111.00
1	C	259	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	317	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	148	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	23	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	113	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	75	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	25	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	101	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	52	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	64	ARG	NE-CZ-NH2	-5.06	117.77	120.30

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	2375	0	2442	12	0
1	B	2457	0	2519	8	0
1	C	2493	0	2552	19	0
1	D	2464	0	2532	15	0
1	E	2407	0	2470	22	0
1	F	2491	0	2549	22	0
2	A	12	0	6	0	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	B	9	0	3	2	0
4	C	9	0	3	0	0
4	D	9	0	3	0	0
4	E	9	0	3	1	0
4	F	9	0	3	1	0
5	B	8	0	2	1	0
6	A	65	0	0	2	0
6	B	71	0	0	0	0
6	C	73	0	0	0	0
6	D	73	0	0	0	0
6	E	72	0	0	0	0
6	F	74	0	0	1	0
All	All	15205	0	15087	96	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 3.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:HA	6:A:535:HOH:O	1.52	1.10
1:A:121:GLU:HG3	6:A:557:HOH:O	1.86	0.74
1:A:55:THR:HG21	1:A:103:LEU:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ALA:O	1:B:274:ARG:NH2	2.27	0.68
1:E:242:ARG:NH2	4:E:401:ASP:OD2	2.24	0.68
1:F:263:ALA:HA	1:F:266:ALA:HB2	1.80	0.64
1:F:288:LEU:O	4:F:401:ASP:HB2	1.98	0.63
1:C:1:MET:SD	1:C:39:LYS:NZ	2.72	0.62
1:A:60:GLU:HG3	1:A:115:PRO:HD3	1.83	0.60
1:E:16:THR:HG21	1:E:124:LEU:HD11	1.84	0.60
1:D:137:GLY:O	1:D:174:ARG:HD3	2.02	0.59
1:F:137:GLY:O	1:F:174:ARG:HD3	2.02	0.59
1:B:163:THR:HG23	1:B:191:CYS:HB3	1.83	0.59
1:E:55:THR:HG21	1:E:103:LEU:HD12	1.85	0.58
1:F:138:ALA:CB	1:F:172:MET:HE3	2.35	0.57
1:F:320:ILE:O	1:F:324:VAL:HG23	2.05	0.56
1:C:263:ALA:HA	1:C:266:ALA:HB2	1.89	0.55
1:F:57:LEU:HD11	1:F:103:LEU:HG	1.89	0.55
1:D:146:LEU:CD1	1:D:320:ILE:HD11	2.37	0.54
1:C:288:LEU:HB3	1:C:289:PRO:HA	1.90	0.53
1:C:32:LEU:O	1:C:36:MET:HG2	2.09	0.53
1:E:104:ASP:OD1	1:E:129:HIS:HD2	1.92	0.53
1:C:41:ASP:OD1	1:C:311:ARG:NH2	2.42	0.52
1:E:137:GLY:O	1:E:174:ARG:HD3	2.10	0.52
1:D:265:LYS:HA	1:D:268:ILE:HG12	1.91	0.51
1:D:243:LEU:HD23	1:D:243:LEU:N	2.25	0.51
1:E:236:ASP:OD1	1:E:279:LYS:NZ	2.44	0.50
4:B:401:ASP:N	5:B:402:CP:O2P	2.45	0.50
1:F:3:GLU:O	1:F:3:GLU:HG2	2.12	0.49
1:D:41:ASP:OD1	1:D:311:ARG:NH2	2.46	0.49
1:D:146:LEU:HD12	1:D:320:ILE:HD11	1.95	0.49
1:C:262:PHE:O	1:C:266:ALA:HB2	2.13	0.48
1:B:83:PHE:CE1	1:B:103:LEU:HD21	2.49	0.48
1:A:279:LYS:O	1:A:303:ARG:NH1	2.43	0.48
1:C:10:LEU:HD22	1:C:29:LEU:HD21	1.95	0.47
1:C:15:ILE:HA	1:C:20:GLN:HE22	1.79	0.47
1:C:15:ILE:HA	1:C:20:GLN:NE2	2.29	0.47
1:C:57:LEU:HD23	1:C:59:PHE:HE1	1.80	0.47
1:C:286:HIS:O	1:C:288:LEU:HG	2.16	0.46
1:C:225:HIS:O	1:C:266:ALA:O	2.34	0.46
1:D:57:LEU:HD21	1:D:103:LEU:HG	1.98	0.46
1:A:137:GLY:O	1:A:174:ARG:HD3	2.16	0.46
1:C:103:LEU:N	1:C:103:LEU:HD22	2.31	0.46
1:E:4:LEU:HD21	1:E:39:LYS:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:138:ALA:HB3	1:F:172:MET:HE3	1.97	0.46
1:F:22:SER:O	1:F:25:ASP:HB2	2.16	0.45
1:B:208:GLU:HB3	1:B:209:PRO:HD3	1.97	0.45
1:E:65:THR:HG21	1:E:134:ALA:HB1	1.99	0.45
1:E:288:LEU:HB3	1:E:289:PRO:HA	1.99	0.45
1:E:172:MET:CE	1:E:247:ARG:HB3	2.47	0.45
1:C:116:ARG:NH2	1:C:118:ASP:OD1	2.44	0.44
1:C:88:SER:OG	1:C:90:ILE:HD12	2.16	0.44
1:F:138:ALA:HB2	1:F:172:MET:CE	2.47	0.44
1:A:148:ASP:OD2	1:A:239:TYR:OH	2.26	0.44
1:D:212:HIS:O	1:D:216:THR:OG1	2.36	0.44
1:C:208:GLU:HB2	1:C:209:PRO:HD3	1.98	0.44
1:E:104:ASP:OD1	1:E:129:HIS:CD2	2.71	0.44
1:E:240:THR:O	1:E:287:PRO:HD2	2.17	0.44
1:F:247:ARG:O	1:F:248:PHE:HB2	2.18	0.44
1:F:247:ARG:O	1:F:248:PHE:CB	2.66	0.44
1:B:55:THR:HG21	1:B:103:LEU:HD12	1.99	0.43
1:C:16:THR:HG21	1:C:124:LEU:HD11	1.98	0.43
1:F:16:THR:HG21	1:F:124:LEU:HD11	2.00	0.43
1:B:138:ALA:O	1:B:177:HIS:CE1	2.71	0.43
1:A:54:MET:HG2	1:A:55:THR:N	2.32	0.43
1:F:270:ILE:HG22	1:F:298:VAL:HG21	1.99	0.43
1:E:55:THR:HG21	1:E:103:LEU:CD1	2.49	0.43
1:E:304:ALA:HB1	1:E:306:TYR:CE2	2.53	0.43
1:F:15:ILE:HD12	1:F:132:LEU:HD22	2.00	0.43
1:B:282:MET:O	1:E:1:MET:HG2	2.18	0.43
1:F:48:LEU:HB3	1:F:322:TRP:CZ3	2.54	0.42
1:D:16:THR:HG21	1:D:124:LEU:HD11	2.01	0.42
1:D:146:LEU:HD13	1:D:320:ILE:HD11	2.00	0.42
1:C:1:MET:HB3	1:C:39:LYS:NZ	2.35	0.42
1:A:120:ILE:HG13	1:A:136:ASN:HB3	2.00	0.42
1:E:103:LEU:HD13	1:E:103:LEU:HA	1.94	0.42
1:A:64:ARG:HH22	1:B:94:GLU:CD	2.23	0.42
1:D:57:LEU:CD1	1:D:100:ILE:HD13	2.50	0.42
1:D:61:ASP:OD2	1:E:91:ASN:ND2	2.48	0.42
1:E:307:PHE:CE1	1:F:101:ARG:HD2	2.54	0.42
1:D:64:ARG:O	1:D:68:SER:CB	2.68	0.42
1:E:96:LEU:O	1:E:100:ILE:HG12	2.19	0.41
1:A:32:LEU:O	1:A:36:MET:HG2	2.20	0.41
1:F:91:ASN:HA	6:F:505:HOH:O	2.19	0.41
1:E:147:LEU:HB2	1:E:313:GLY:HA2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:256:ALA:O	1:F:260:GLN:HB2	2.20	0.41
1:E:172:MET:HE2	1:E:247:ARG:HB3	2.02	0.41
1:D:54:MET:HG2	1:D:109:VAL:HG13	2.01	0.41
1:E:10:LEU:HD12	1:E:10:LEU:N	2.36	0.41
1:F:3:GLU:O	1:F:3:GLU:CG	2.68	0.41
1:F:272:ALA:O	1:F:273:ALA:C	2.59	0.41
1:D:208:GLU:N	1:D:209:PRO:CD	2.84	0.41
1:F:245:LYS:O	1:F:247:ARG:O	2.39	0.40
1:A:84:LYS:O	1:A:88:SER:HB3	2.21	0.40
4:B:401:ASP:N	4:B:401:ASP:OD1	2.52	0.40
1:C:57:LEU:HD22	1:C:100:ILE:CD1	2.52	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	303/327 (93%)	293 (97%)	10 (3%)	0	100	100
1	B	315/327 (96%)	301 (96%)	14 (4%)	0	100	100
1	C	319/327 (98%)	305 (96%)	14 (4%)	0	100	100
1	D	315/327 (96%)	302 (96%)	12 (4%)	1 (0%)	41	55
1	E	306/327 (94%)	290 (95%)	15 (5%)	1 (0%)	41	55
1	F	318/327 (97%)	301 (95%)	15 (5%)	2 (1%)	25	36
All	All	1876/1962 (96%)	1792 (96%)	80 (4%)	4 (0%)	47	62

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	263	ALA

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Mol	Chain	Res	Type
1	F	89	SER
1	F	279	LYS
1	E	288	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	260/275 (94%)	256 (98%)	4 (2%)	65	80
1	B	267/275 (97%)	259 (97%)	8 (3%)	41	61
1	C	272/275 (99%)	258 (95%)	14 (5%)	24	39
1	D	268/275 (98%)	258 (96%)	10 (4%)	34	53
1	E	264/275 (96%)	255 (97%)	9 (3%)	37	56
1	F	271/275 (98%)	262 (97%)	9 (3%)	38	57
All	All	1602/1650 (97%)	1548 (97%)	54 (3%)	37	56

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	63	SER
1	A	225	HIS
1	A	292	ASP
1	B	0	SER
1	B	11	LYS
1	B	47	ASN
1	B	86	GLU
1	B	96	LEU
1	B	281	LYS
1	B	292	ASP
1	B	306	TYR
1	C	0	SER
1	C	1	MET
1	C	2	LEU

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Mol	Chain	Res	Type
1	C	38	ARG
1	C	47	ASN
1	C	57	LEU
1	C	117	GLN
1	C	128	GLN
1	C	141	HIS
1	C	222	HIS
1	C	246	GLU
1	C	252	THR
1	C	259	LEU
1	C	265	LYS
1	D	0	SER
1	D	47	ASN
1	D	117	GLN
1	D	158	SER
1	D	243	LEU
1	D	259	LEU
1	D	262	PHE
1	D	267	ASP
1	D	281	LYS
1	D	292	ASP
1	E	3	GLU
1	E	38	ARG
1	E	47	ASN
1	E	57	LEU
1	E	107	SER
1	E	125	SER
1	E	141	HIS
1	E	162	ILE
1	E	190	LYS
1	F	116	ARG
1	F	141	HIS
1	F	147	LEU
1	F	224	THR
1	F	247	ARG
1	F	253	SER
1	F	254	ASP
1	F	259	LEU
1	F	260	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	ASN
1	B	129	HIS
1	B	186	ASN
1	B	225	HIS
1	C	37	GLN
1	C	50	GLN
1	C	129	HIS
1	C	186	ASN
1	C	291	ASN
1	D	50	GLN
1	D	129	HIS
1	E	37	GLN
1	E	50	GLN
1	E	82	ASN
1	E	129	HIS
1	E	186	ASN
1	E	212	HIS
1	F	129	HIS

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)

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	$\#\|Z\| > 2$
4	ASP	D	401	-	6,8,8	1.20	0	8,10,10	1.54	3 (37%)
4	ASP	E	401	-	6,8,8	1.40	1 (16%)	8,10,10	1.14	0
3	PO4	E	402	-	4,4,4	0.91	0	6,6,6	0.62	0
3	PO4	F	402	-	4,4,4	0.95	0	6,6,6	0.50	0
3	PO4	A	402	-	4,4,4	0.83	0	6,6,6	0.52	0
2	NCD	A	401	-	11,11,11	0.91	0	13,14,14	1.87	2 (15%)
4	ASP	F	401	-	6,8,8	1.54	1 (16%)	8,10,10	1.43	2 (25%)
4	ASP	B	401	-	6,8,8	1.17	1 (16%)	8,10,10	1.10	0
3	PO4	C	402	-	4,4,4	0.84	0	6,6,6	1.01	0
3	PO4	D	402	-	4,4,4	1.10	0	6,6,6	0.62	0
4	ASP	C	401	-	6,8,8	1.17	0	8,10,10	1.35	2 (25%)
5	CP	B	402	-	6,7,7	0.83	0	7,10,10	1.63	1 (14%)

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	NCD	A	401	-	-	5/12/12/12	-
4	ASP	F	401	-	-	7/8/8/8	-
4	ASP	B	401	-	-	1/8/8/8	-
4	ASP	D	401	-	-	0/8/8/8	-
4	ASP	E	401	-	-	4/8/8/8	-
4	ASP	C	401	-	-	0/8/8/8	-
5	CP	B	402	-	-	0/3/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	ASP	OD2-CG	-2.87	1.21	1.30
4	E	401	ASP	OD2-CG	-2.18	1.23	1.30
4	B	401	ASP	OD2-CG	-2.06	1.23	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	NCD	O2-C2-N3	-4.83	114.93	123.22
5	B	402	CP	O-C-N	-3.17	120.28	125.51
4	D	401	ASP	OXT-C-O	-2.38	118.69	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	ASP	OXT-C-CA	2.34	121.35	113.38
4	C	401	ASP	OXT-C-O	-2.29	118.90	124.09
2	A	401	NCD	O4-C4-C5	-2.18	115.81	122.80
4	F	401	ASP	OD2-CG-CB	2.15	120.95	114.07
4	C	401	ASP	OXT-C-CA	2.14	120.67	113.38
4	F	401	ASP	O-C-CA	-2.08	114.81	122.14
4	D	401	ASP	OD2-CG-CB	2.04	120.61	114.07

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NCD	O2-C2-N1-C6
2	A	401	NCD	N3-C2-N1-C6
4	E	401	ASP	O-C-CA-N
4	F	401	ASP	OXT-C-CA-N
4	E	401	ASP	OXT-C-CA-N
4	E	401	ASP	C-CA-CB-CG
4	F	401	ASP	O-C-CA-N
4	F	401	ASP	C-CA-CB-CG
4	E	401	ASP	N-CA-CB-CG
4	F	401	ASP	OXT-C-CA-CB
4	F	401	ASP	CA-CB-CG-OD2
4	B	401	ASP	N-CA-CB-CG
4	F	401	ASP	CA-CB-CG-OD1
4	F	401	ASP	O-C-CA-CB
2	A	401	NCD	C5-C6-C61-O62
2	A	401	NCD	C5-C6-C61-O61
2	A	401	NCD	C5-C6-N1-C2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	401	ASP	1	0
4	F	401	ASP	1	0
4	B	401	ASP	2	0
5	B	402	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 (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	307/327 (93%)	-0.67	2 (0%)	87	86	25, 34, 58, 104	0
1	B	319/327 (97%)	-0.68	1 (0%)	94	93	24, 34, 61, 90	0
1	C	323/327 (98%)	-0.72	1 (0%)	94	93	25, 36, 56, 70	0
1	D	319/327 (97%)	-0.57	6 (1%)	66	64	22, 32, 60, 146	0
1	E	310/327 (94%)	-0.69	2 (0%)	89	88	23, 36, 57, 81	0
1	F	322/327 (98%)	-0.70	1 (0%)	94	93	23, 33, 54, 97	0
All	All	1900/1962 (96%)	-0.67	13 (0%)	87	86	22, 34, 57, 146	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	ALA	11.6
1	D	260	GLN	10.5
1	D	259	LEU	8.3
1	D	257	ALA	7.4
1	D	261	SER	5.9
1	D	262	PHE	4.5
1	B	93	GLY	3.4
1	A	2	LEU	3.2
1	E	88	SER	2.8
1	F	1	MET	2.6
1	C	0	SER	2.1
1	E	90	ILE	2.1
1	A	1	MET	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(Å^2)	Q<0.9
4	ASP	B	401	9/9	0.84	0.22	49,59,64,67	0
4	ASP	E	401	9/9	0.91	0.12	36,37,40,40	0
2	NCD	A	401	12/12	0.92	0.15	44,53,64,67	0
3	PO4	A	402	5/5	0.92	0.16	59,64,66,70	0
4	ASP	F	401	9/9	0.94	0.12	34,35,42,47	0
3	PO4	C	402	5/5	0.96	0.13	44,49,53,61	0
4	ASP	D	401	9/9	0.96	0.12	32,33,37,38	0
4	ASP	C	401	9/9	0.97	0.13	30,32,33,34	0
3	PO4	E	402	5/5	0.97	0.09	58,61,64,64	0
3	PO4	D	402	5/5	0.98	0.10	42,43,47,49	0
5	CP	B	402	8/8	0.98	0.12	46,53,60,62	0
3	PO4	F	402	5/5	0.99	0.08	44,48,50,56	0

6.5 Other polymers (i)

There are no such residues in this entry.