Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 05:14 pm BST

PDB ID	:	3FZ7
Title	:	Crystal structure of apo glutamate decarboxylase beta from Escherichia coli
Authors	:	Malashkevich, V.N.; De Biase, D.; Bossa, F.
Deposited on	:	2009-01-23
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

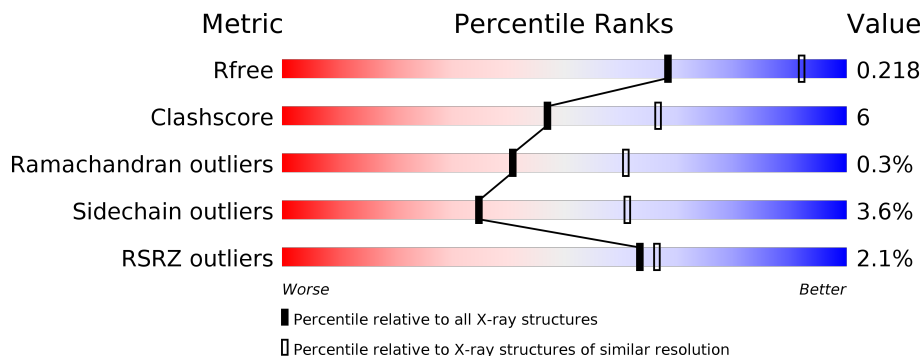|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.50 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	Percentile Ranks	Value
Rfree		0.218
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		3.6%
RSRZ outliers		2.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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.

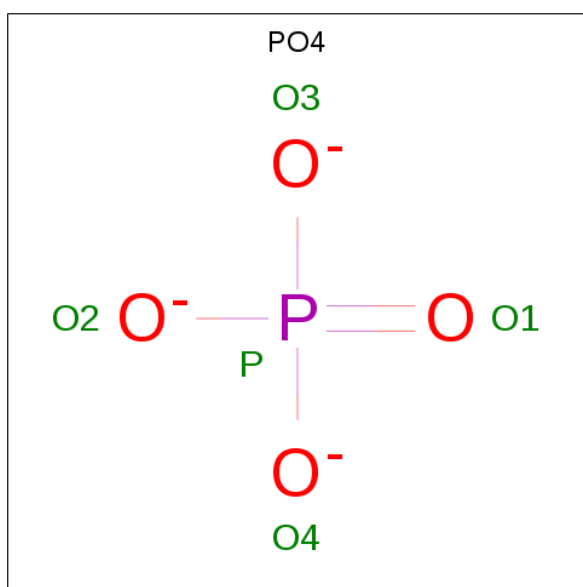| Mol	Chain	Length	Quality of chain
1	A	466	2% / 86% / 10% / · ·
1	B	466	2% / 85% / 11% / · ·
1	C	466	2% / 84% / 14% / · ·
1	D	466	2% / 80% / 15% / · ·
1	E	466	2% / 82% / 14% / · ·
1	F	466	2% / 82% / 14% / · ·

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22845 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 Glutamate decarboxylase beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3607	2303	616	664	24			
1	B	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	C	463	Total	C	N	O	S	0	0	0
			3681	2347	630	680	24			
1	D	454	Total	C	N	O	S	0	0	0
			3607	2303	616	664	24			
1	E	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	F	464	Total	C	N	O	S	0	0	0
			3690	2353	632	681	24			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	998	Total 998	O 998	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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 s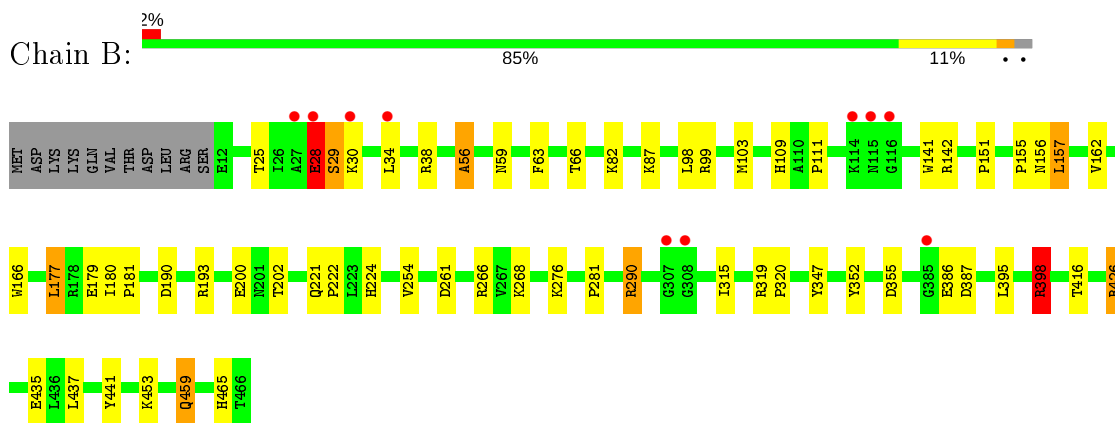hows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit 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.
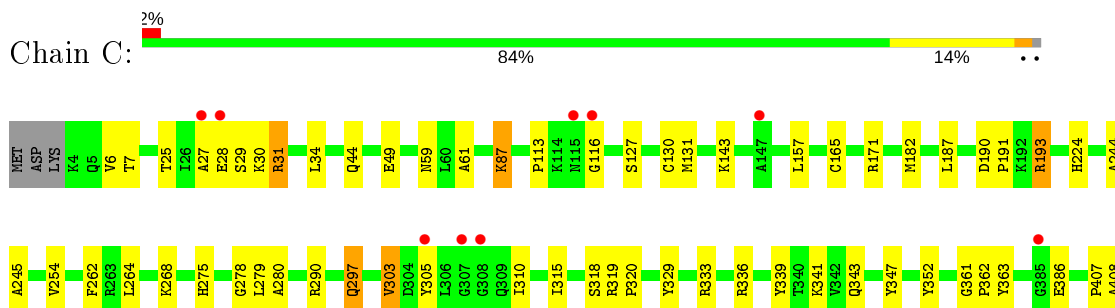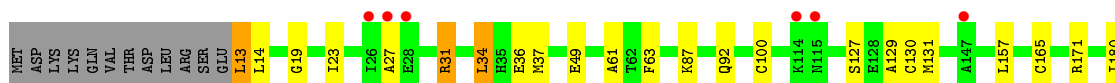
- Molecule 1: Glutamate decarboxylase beta
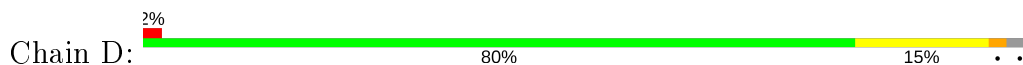

- Molecule 1: Glutamate decarboxylase beta
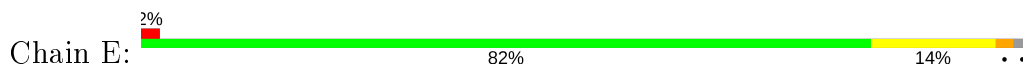

- Molecule 1: Glutamate decarboxylase beta

L411 T416 V420 M421 R422 R426 R427 E435 L436 L437 Q459 T466

● Molecule 1: Glutamate decarboxylase beta

Chain D:

2%
80%　　　15%

MET ASP LYS LYS GLN VAL THR ASP LEU ARG SER GLU L13 L14 G19 I23 I26 A27 E28 R31 L34 H35 E36 M37 E49 A61 T62 F63 K87 Q92 C100 K114 N115 S127 E128 A129 C130 M131 A147 L157 C165 R171 I180

P181 M182 R183 L187 D190 R193 N216 Y217 E218 F219 P220 Q221 P222 L223 H224 A245 V254 A255 P256 D257 F262 R263 I264 P265 R266 V267 K268 S269 A272 W287 V288 W289 R290 D291 N302 V303 D304 Y305 L306 G307 G308 Q309 I310 G311 I315 S318

L332 K341 V342 Q343 N344 Y347 I366 L395 R400 W404 P407 L411 G412 G413 E414 A415 T416 M424 C425 R426 R427 E435 L436 L437 Y441 Q459 Q460 H465 T466

● Molecule 1: Glutamate decarboxylase beta

Chain E:

2%
82%　　　14%

MET ASP LYS LYS GLN VAL THR ASP LEU ARG SER E12 I26 A27 E28 R31 E36 E49 N83 W84 I85 D86 K87 Q92 K114 N115 G116 A136 R142 K143 R144 A147 L157 V162 W166 H167 K168 L177 P181 M182 R183 Q186 L187 F188

M189 D190 R193 E196 N216 P220 H224 A245 D257 W260 L264 P265 R266 H275 A280 P281 L282 R290 E298 F301 N302 V303 D304 Y305 L306 G307 G308 Q309 I310 G311 I315 S318 Q323 E337 G338 Y339 T340 K341 V342 Q343 N344

Q348 G385 Y393 D394 L395 R398 I411 E414 A415 T416 V419 R427 E430 L437 Y441 L454 I457 A458 Q459 Q460 H465 T466

● Molecule 1: Glutamate decarboxylase beta

Chain F:

2%
82%　　　14%

MET ASP K3 K4 Q5 V6 T7 R10 S11 E12 L13 S16 G19 A20 K21 S22 I23 S24 T25 I26 A27 E28 S29 E49 I80 I85 Q92 R99 K114 N115 G116 T123 S127 E128 A129 C130 M131 M137 R142 L157 R171 L177 R178 E179

I180 P181 M182 R183 L187 D190 R193 E200 G204 Q221 P222 L223 H224 A245 V254 F262 R263 L264 K268 S269 I270 S271 A272 C284 V287 I288 W289 R290 V303 D304 Y305 G308 Q309 I310 I315 G322 Q323 Y329 R333 Y339

Q343 Y347 D372 L395 R398 P407 E414 A415 I418 R422 R427 L437 Y441 K446 Q459 T466

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	115.56Å 115.56Å 206.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-2.50) 98.8 (19.92-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.13 (at 2.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.151 , 0.222 0.153 , 0.218	Depositor DCC
R_{free} test set	5253 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	20.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 40.3	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l 0.025 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22845	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PO4

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	0.81	0/3701	0.85	3/5016 (0.1%)
1	B	0.84	0/3710	0.86	5/5028 (0.1%)
1	C	0.82	0/3775	0.86	3/5115 (0.1%)
1	D	0.83	0/3701	0.89	10/5016 (0.2%)
1	E	0.81	0/3710	0.83	4/5028 (0.1%)
1	F	0.85	0/3784	0.86	9/5126 (0.2%)
All	All	0.83	0/22381	0.86	34/30329 (0.1%)

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	F	0	2

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	426	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	D	290	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	D	34	LEU	CB-CG-CD1	-7.85	97.66	111.00
1	C	426	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	B	426	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	D	193	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	290	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	B	157	LEU	CA-CB-CG	6.93	131.25	115.30
1	B	398	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	F	398	ARG	NE-CZ-NH1	6.72	123.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	426	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	E	157	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	290	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	D	332	LEU	CA-CB-CG	6.04	129.18	115.30
1	D	157	LEU	CA-CB-CG	5.94	128.97	115.30
1	F	398	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	178	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	F	372	ASP	CB-CG-OD1	5.74	123.46	118.30
1	D	426	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	F	13	LEU	CA-CB-CG	5.46	127.86	115.30
1	F	193	ARG	NE-CZ-NH2	-5.43	117.59	120.30
1	E	437	LEU	CA-CB-CG	5.40	127.72	115.30
1	F	157	LEU	CA-CB-CG	5.32	127.54	115.30
1	E	427	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	193	ARG	NE-CZ-NH2	-5.23	117.68	120.30
1	C	422	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	D	291	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	237	ASP	CB-CG-OD1	5.19	122.97	118.30
1	E	290	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	290	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	F	177	LEU	CA-CB-CG	5.07	126.95	115.30
1	F	49	GLU	N-CA-CB	5.02	119.64	110.60
1	F	290	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	11	SER	Peptide
1	F	12	GLU	Peptide

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	3607	0	3510	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3616	0	3516	40	0
1	C	3681	0	3586	49	0
1	D	3607	0	3510	59	0
1	E	3616	0	3516	49	0
1	F	3690	0	3599	51	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	D	998	0	0	49	2
All	All	22845	0	21237	266	2

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 6.

All (266) 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:E:31:ARG:HG2	1:E:31:ARG:HH21	1.19	1.05
1:F:12:GLU:HB2	1:F:13:LEU:HD13	1.43	1.00
1:B:398:ARG:HD3	3:D:1211:HOH:O	1.70	0.92
1:D:435:GLU:HG2	3:D:1171:HOH:O	1.71	0.91
1:B:28:GLU:O	1:B:30:LYS:N	2.03	0.91
1:F:3:LYS:HE3	1:F:4:LYS:H	1.34	0.88
1:D:310:ILE:HD11	3:D:1291:HOH:O	1.75	0.87
1:B:315:ILE:HG21	1:C:315:ILE:HG21	1.58	0.85
1:E:190:ASP:OD1	1:E:193:ARG:HD3	1.76	0.84
1:A:315:ILE:HG21	1:F:315:ILE:HG21	1.61	0.82
1:C:352:TYR:OH	1:C:435:GLU:OE1	1.96	0.82
1:D:315:ILE:HG21	1:E:315:ILE:HG21	1.61	0.81
1:E:31:ARG:HG2	1:E:31:ARG:NH2	1.92	0.80
1:B:162:VAL:HG22	1:B:166:TRP:CD1	2.17	0.80
1:E:344:ASN:O	1:E:348:GLN:HG3	1.82	0.80
1:A:190:ASP:OD1	1:A:193:ARG:HD3	1.81	0.80
1:F:190:ASP:OD1	1:F:193:ARG:HD3	1.84	0.78
1:B:416:THR:HG23	3:D:855:HOH:O	1.83	0.78
3:D:1308:HOH:O	1:F:398:ARG:HD3	1.82	0.78
1:E:144:ARG:HB3	1:E:144:ARG:HH11	1.47	0.77
3:D:1224:HOH:O	1:E:168:LYS:HE3	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:GLU:HG3	3:D:1434:HOH:O	1.83	0.77
1:F:12:GLU:CB	1:F:13:LEU:HD13	2.14	0.77
1:D:190:ASP:OD1	1:D:193:ARG:HD3	1.85	0.77
1:B:162:VAL:HG22	1:B:166:TRP:HD1	1.51	0.75
1:D:435:GLU:CG	3:D:1171:HOH:O	2.29	0.75
1:B:59:ASN:O	1:B:426:ARG:NH2	2.19	0.75
1:A:424:MET:HG3	3:D:728:HOH:O	1.88	0.74
1:D:305:TYR:HE1	1:D:310:ILE:HG13	1.51	0.74
3:D:596:HOH:O	1:F:427:ARG:HD2	1.89	0.73
1:A:144:ARG:NH1	1:A:237:ASP:O	2.22	0.73
1:B:162:VAL:CG2	1:B:166:TRP:CD1	2.71	0.72
1:B:190:ASP:OD1	1:B:193:ARG:HD3	1.88	0.72
1:C:190:ASP:OD1	1:C:193:ARG:HD3	1.90	0.72
1:A:130:CYS:HG	1:A:165:CYS:HG	1.37	0.71
1:A:200:GLU:HG2	3:D:1221:HOH:O	1.91	0.71
1:C:27:ALA:O	3:D:757:HOH:O	2.08	0.71
1:B:352:TYR:OH	1:B:435:GLU:OE1	2.06	0.70
1:D:305:TYR:CE2	3:D:731:HOH:O	2.42	0.70
1:E:144:ARG:NH1	1:E:144:ARG:HB3	2.05	0.70
1:D:171:ARG:NH2	3:D:498:HOH:O	2.24	0.70
1:E:26:ILE:O	1:E:27:ALA:O	2.08	0.70
1:B:28:GLU:C	1:B:30:LYS:H	1.96	0.68
1:C:59:ASN:O	1:C:426:ARG:NH2	2.16	0.67
1:A:239:ASP:OD2	3:D:1410:HOH:O	2.12	0.67
1:D:305:TYR:HD2	3:D:808:HOH:O	1.76	0.66
1:D:427:ARG:HD2	3:D:1279:HOH:O	1.96	0.66
2:B:467:PO4:O4	1:C:318:SER:HB2	1.95	0.66
1:D:305:TYR:CD2	3:D:808:HOH:O	2.49	0.65
1:A:362:PRO:HB2	1:A:386:GLU:HG2	1.78	0.65
1:B:181:PRO:O	1:B:193:ARG:NH2	2.30	0.65
1:C:341:LYS:HE2	1:D:19:GLY:O	1.95	0.64
3:D:1382:HOH:O	1:E:257:ASP:HB2	1.97	0.64
1:F:181:PRO:O	1:F:193:ARG:NH2	2.26	0.64
1:F:182:MET:HG2	1:F:187:LEU:O	1.99	0.63
1:C:290:ARG:HD3	3:D:693:HOH:O	1.98	0.63
3:D:1440:HOH:O	1:E:303:VAL:HG23	1.99	0.63
1:F:127:SER:O	1:F:131:MET:HG2	1.99	0.63
1:F:221:GLN:HB3	1:F:222:PRO:HD3	1.80	0.62
3:D:531:HOH:O	1:F:446:LYS:HE2	2.00	0.62
1:D:49:GLU:O	1:E:92:GLN:HG2	1.98	0.62
1:A:200:GLU:CG	3:D:1221:HOH:O	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:ARG:HG2	1:D:414:GLU:HB2	1.81	0.61
1:D:254:VAL:HG21	1:D:347:TYR:CE2	2.36	0.61
1:B:398:ARG:HD2	1:B:398:ARG:N	2.14	0.60
1:C:25:THR:O	1:C:29:SER:HB3	2.01	0.60
1:A:23:ILE:HG21	1:A:37:MET:CE	2.32	0.60
1:F:329:TYR:CZ	1:F:333:ARG:HD3	2.37	0.59
1:B:56:ALA:HB1	1:B:66:THR:HG21	1.83	0.59
1:E:183:ARG:HB3	1:E:414:GLU:HB2	1.84	0.59
1:D:305:TYR:HE2	3:D:731:HOH:O	1.82	0.59
1:A:415:ALA:HB1	1:A:418:ILE:HD12	1.85	0.58
1:A:28:GLU:HB3	1:A:31:ARG:HD2	1.84	0.58
1:F:329:TYR:CE2	1:F:333:ARG:HD3	2.39	0.58
1:B:28:GLU:HB3	3:D:1212:HOH:O	2.04	0.58
1:C:427:ARG:HD2	3:D:562:HOH:O	2.04	0.58
1:A:339:TYR:O	1:A:343:GLN:HG2	2.04	0.57
1:C:297:GLN:HA	1:C:297:GLN:NE2	2.18	0.57
1:F:21:LYS:HB3	1:F:21:LYS:NZ	2.20	0.57
1:F:254:VAL:HG21	1:F:347:TYR:CE2	2.39	0.57
1:D:182:MET:HG2	1:D:187:LEU:O	2.05	0.56
1:A:183:ARG:NH2	1:A:186:GLN:OE1	2.33	0.56
1:D:181:PRO:O	1:D:193:ARG:NH2	2.37	0.56
1:A:49:GLU:O	1:F:92:GLN:HG2	2.05	0.56
1:D:23:ILE:HG21	1:D:37:MET:CE	2.36	0.56
1:D:31:ARG:HD3	3:D:838:HOH:O	2.05	0.55
1:B:25:THR:O	1:B:29:SER:HB3	2.05	0.55
1:D:23:ILE:HG21	1:D:37:MET:HE2	1.87	0.55
1:C:329:TYR:CE2	1:C:333:ARG:HD3	2.43	0.54
1:A:168:LYS:HE2	3:D:782:HOH:O	2.07	0.54
1:F:22:SER:OG	1:F:23:ILE:N	2.40	0.54
1:D:13:LEU:HD23	1:D:14:LEU:HG	1.89	0.54
1:F:305:TYR:CE1	1:F:310:ILE:HG13	2.43	0.54
1:D:305:TYR:CE1	1:D:310:ILE:HG13	2.37	0.54
1:D:262:PHE:O	1:D:290:ARG:NH2	2.39	0.54
1:E:188:PHE:HZ	1:E:216:ASN:HD22	1.54	0.54
1:E:282:LEU:O	1:E:323:GLN:HG2	2.08	0.54
1:D:303:VAL:HG12	1:E:465:HIS:CD2	2.43	0.53
1:C:319:ARG:HB2	1:C:320:PRO:HD2	1.89	0.53
1:D:183:ARG:NE	1:D:414:GLU:OE1	2.38	0.53
1:B:465:HIS:NE2	1:C:303:VAL:HG12	2.24	0.53
1:C:275:HIS:HA	1:C:280:ALA:O	2.09	0.53
1:D:218:GLU:O	1:D:220:PRO:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLU:HB3	1:C:31:ARG:HD2	1.91	0.53
3:D:982:HOH:O	1:E:427:ARG:HD2	2.09	0.52
1:A:398:ARG:N	1:A:398:ARG:HD2	2.23	0.52
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.45	0.52
1:A:92:GLN:HG2	1:F:49:GLU:O	2.10	0.52
1:A:23:ILE:HG21	1:A:37:MET:HE1	1.92	0.52
1:C:30:LYS:HB2	3:D:1399:HOH:O	2.09	0.52
1:F:177:LEU:HD13	1:F:179:GLU:HB2	1.91	0.52
1:C:31:ARG:HH21	1:C:34:LEU:HD11	1.75	0.52
1:D:127:SER:O	1:D:131:MET:HG2	2.10	0.52
1:D:310:ILE:HG22	1:D:311:GLY:H	1.74	0.52
1:C:262:PHE:O	1:C:290:ARG:NH2	2.43	0.51
1:A:181:PRO:O	1:A:193:ARG:NH2	2.41	0.51
1:D:435:GLU:HG3	3:D:1171:HOH:O	2.06	0.51
3:D:950:HOH:O	1:F:322:GLY:HA3	2.09	0.51
1:A:129:ALA:HB1	1:A:287:VAL:HB	1.93	0.51
1:F:5:GLN:HG3	1:F:10:ARG:HD2	1.91	0.51
1:B:99:ARG:O	1:B:103:MET:HG3	2.11	0.51
1:F:398:ARG:N	1:F:398:ARG:HD2	2.25	0.51
3:D:1380:HOH:O	1:E:167:HIS:HE1	1.94	0.51
1:B:416:THR:CG2	3:D:855:HOH:O	2.50	0.50
1:A:362:PRO:CB	1:A:386:GLU:HG2	2.41	0.50
1:D:460:GLN:HG2	1:E:306:LEU:O	2.12	0.50
1:C:6:VAL:HA	1:D:257:ASP:HB2	1.94	0.50
1:E:341:LYS:HE2	1:F:19:GLY:O	2.11	0.50
1:E:395:LEU:HD21	1:E:441:TYR:CZ	2.47	0.50
1:C:87:LYS:HD3	1:C:87:LYS:H	1.76	0.50
3:D:1308:HOH:O	1:F:398:ARG:CD	2.51	0.50
1:E:430:GLU:OE2	1:F:16:SER:OG	2.29	0.49
3:D:1093:HOH:O	1:F:11:SER:HB2	2.12	0.49
1:B:111:PRO:HD2	1:B:290:ARG:O	2.12	0.49
1:D:435:GLU:HA	1:D:435:GLU:OE1	2.11	0.49
1:D:465:HIS:O	1:D:466:THR:HB	2.13	0.49
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.48	0.49
1:D:221:GLN:HB3	1:D:222:PRO:HD3	1.95	0.48
1:E:143:LYS:HE2	1:E:298:GLU:OE1	2.12	0.48
1:F:3:LYS:HE3	1:F:4:LYS:N	2.16	0.48
1:C:61:ALA:HA	3:D:736:HOH:O	2.12	0.48
1:E:275:HIS:HA	1:E:280:ALA:O	2.13	0.48
1:B:156:ASN:OD1	1:B:202:THR:HA	2.13	0.48
1:D:92:GLN:HG2	1:E:49:GLU:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:224:HIS:CD2	1:E:266:ARG:HB2	2.49	0.48
1:A:28:GLU:C	1:A:30:LYS:H	2.16	0.48
1:B:109:HIS:HD2	1:B:261:ASP:OD2	1.97	0.48
1:B:98:LEU:HD23	3:D:1124:HOH:O	2.12	0.48
1:C:305:TYR:CE1	1:C:310:ILE:HG13	2.48	0.48
1:D:269:SER:HB3	1:D:289:TRP:CD1	2.49	0.48
1:A:23:ILE:HG21	1:A:37:MET:HE2	1.95	0.48
1:F:137:MET:SD	1:F:204:GLY:HA3	2.54	0.48
1:A:63:PHE:CZ	1:A:212:THR:HG23	2.48	0.48
1:B:281:PRO:HD3	3:D:668:HOH:O	2.13	0.48
1:E:186:GLN:HB3	1:E:186:GLN:HE21	1.48	0.48
1:E:305:TYR:HE1	1:E:310:ILE:HG13	1.79	0.47
1:B:254:VAL:HG21	1:B:347:TYR:CE2	2.49	0.47
1:C:127:SER:O	1:C:131:MET:HG2	2.15	0.47
1:C:278:GLY:O	1:C:279:LEU:HB2	2.14	0.47
1:A:141:TRP:CD2	1:A:203:ILE:HG22	2.48	0.47
1:F:183:ARG:HB3	1:F:414:GLU:HB2	1.97	0.47
1:C:339:TYR:O	1:C:343:GLN:HG2	2.15	0.47
1:B:224:HIS:NE2	1:B:266:ARG:HG3	2.30	0.47
1:C:459:GLN:HE21	1:C:459:GLN:HB3	1.43	0.47
1:E:183:ARG:HE	1:E:186:GLN:HB2	1.80	0.47
1:C:130:CYS:SG	1:C:165:CYS:SG	3.10	0.47
1:F:284:CYS:HB2	1:F:323:GLN:HB3	1.97	0.47
1:B:151:PRO:HA	3:D:803:HOH:O	2.14	0.46
1:A:63:PHE:HB2	1:A:276:LYS:HG2	1.98	0.46
1:B:395:LEU:HD21	1:B:441:TYR:CZ	2.51	0.46
1:A:29:SER:HB2	1:F:99:ARG:HG2	1.96	0.46
1:E:224:HIS:CD2	1:E:264:LEU:HB3	2.50	0.46
1:E:87:LYS:HG2	1:E:310:ILE:HD12	1.96	0.46
1:F:262:PHE:CE2	1:F:270:ILE:HD12	2.51	0.46
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.98	0.46
1:E:301:PHE:O	1:E:311:GLY:HA2	2.15	0.46
1:A:337:GLU:HB2	3:D:683:HOH:O	2.16	0.46
1:C:411:LEU:HA	1:C:411:LEU:HD23	1.77	0.46
1:D:130:CYS:HG	1:D:165:CYS:HG	1.59	0.46
1:C:143:LYS:NZ	3:D:957:HOH:O	2.47	0.46
1:C:87:LYS:N	1:C:87:LYS:HD3	2.30	0.45
1:C:244:ALA:O	1:C:245:ALA:C	2.54	0.45
1:D:216:ASN:HD21	1:D:366:ILE:HG22	1.81	0.45
3:D:516:HOH:O	1:E:136:ALA:HB3	2.15	0.45
1:B:398:ARG:CD	3:D:1211:HOH:O	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:454:LEU:O	1:E:457:ILE:HG13	2.16	0.45
1:F:339:TYR:O	1:F:343:GLN:HG2	2.17	0.45
1:B:319:ARG:HB2	1:B:320:PRO:HD2	1.98	0.45
1:C:305:TYR:HE1	1:C:310:ILE:HG13	1.81	0.45
1:F:10:ARG:O	1:F:12:GLU:HG3	2.17	0.45
1:A:269:SER:HB3	1:A:289:TRP:CD1	2.52	0.45
1:C:182:MET:HG2	1:C:187:LEU:O	2.16	0.45
1:D:411:LEU:O	1:D:416:THR:HA	2.16	0.45
1:D:63:PHE:HA	1:D:424:MET:HE2	1.98	0.44
1:C:7:THR:HA	1:D:255:ALA:HA	2.00	0.44
1:D:36:GLU:HG3	1:E:337:GLU:HG2	1.99	0.44
1:E:162:VAL:HG21	1:E:166:TRP:HB2	1.99	0.44
1:F:303:VAL:O	1:F:309:GLN:HB2	2.17	0.44
1:F:129:ALA:HB1	1:F:287:VAL:HB	2.00	0.44
1:C:44:GLN:HG2	3:D:630:HOH:O	2.18	0.44
1:D:224:HIS:NE2	1:D:266:ARG:HB2	2.33	0.44
1:E:393:TYR:HE2	1:E:419:VAL:HG21	1.82	0.43
1:C:61:ALA:HB2	1:C:407:PRO:HD3	2.00	0.43
1:A:25:THR:O	1:A:29:SER:HB3	2.19	0.43
1:C:362:PRO:CB	1:C:386:GLU:HG2	2.49	0.43
1:F:25:THR:O	1:F:29:SER:HB3	2.19	0.43
1:A:17:ARG:NH1	1:A:48:ASP:OD2	2.44	0.43
1:D:224:HIS:CD2	1:D:264:LEU:HB3	2.54	0.43
1:B:177:LEU:HD13	1:B:179:GLU:HB2	2.01	0.43
1:B:453:LYS:HE2	1:B:453:LYS:HB3	1.73	0.43
1:D:61:ALA:HB2	1:D:407:PRO:HD3	2.01	0.43
1:E:411:LEU:HB2	1:E:415:ALA:O	2.19	0.43
1:C:28:GLU:HG2	1:C:31:ARG:HH11	1.83	0.43
1:E:83:ASN:OD1	1:E:85:ILE:HG22	2.18	0.43
1:C:361:GLY:HA3	1:C:363:TYR:CZ	2.54	0.43
2:D:467:PO4:O1	1:E:318:SER:HB2	2.19	0.43
1:F:3:LYS:HE3	1:F:3:LYS:HB2	1.61	0.42
1:F:407:PRO:HD2	1:F:422:ARG:O	2.18	0.42
1:C:28:GLU:HG2	1:C:31:ARG:NH1	2.35	0.42
1:D:224:HIS:CD2	1:D:266:ARG:HB2	2.54	0.42
1:D:411:LEU:HA	1:D:411:LEU:HD23	1.81	0.42
1:D:343:GLN:OE1	1:D:343:GLN:HA	2.19	0.42
1:F:269:SER:HB3	1:F:289:TRP:CD1	2.53	0.42
1:C:113:PRO:HB2	1:C:116:GLY:H	1.85	0.42
1:D:180:ILE:N	1:D:180:ILE:HD12	2.34	0.42
1:D:318:SER:OG	1:E:466:THR:HG21	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:LYS:NZ	1:E:36:GLU:OE2	2.40	0.42
1:A:63:PHE:HA	1:A:424:MET:HE2	2.02	0.42
1:F:123:THR:HB	1:F:128:GLU:HB3	2.02	0.42
1:C:254:VAL:HG21	1:C:347:TYR:CE2	2.54	0.42
1:D:100:CYS:HB3	1:D:286:TRP:CH2	2.54	0.42
1:F:85:ILE:HA	1:F:85:ILE:HD12	1.93	0.42
1:B:82:LYS:O	1:B:320:PRO:HA	2.20	0.42
1:D:129:ALA:HB1	1:D:287:VAL:HB	2.01	0.42
1:E:344:ASN:HA	1:E:344:ASN:HD22	1.70	0.42
1:F:23:ILE:HA	1:F:23:ILE:HD13	1.59	0.42
1:E:220:PRO:HG2	1:E:260:TRP:HB2	2.02	0.42
1:E:393:TYR:CE2	1:E:419:VAL:HG21	2.54	0.41
1:B:38:ARG:HB3	1:B:38:ARG:HE	1.54	0.41
1:E:181:PRO:O	1:E:193:ARG:NH2	2.48	0.41
1:E:183:ARG:NE	1:E:186:GLN:HB2	2.35	0.41
1:D:305:TYR:CZ	3:D:731:HOH:O	2.63	0.41
1:F:245:ALA:HA	1:F:272:ALA:HA	2.02	0.41
1:C:191:PRO:HD2	3:D:497:HOH:O	2.19	0.41
1:B:63:PHE:HB3	1:B:276:LYS:HG2	2.02	0.41
1:C:224:HIS:CD2	1:C:264:LEU:HB3	2.56	0.41
1:F:80:ILE:HG21	1:F:80:ILE:HD13	1.76	0.41
1:D:395:LEU:HD21	1:D:441:TYR:CZ	2.55	0.41
1:A:343:GLN:HA	1:A:343:GLN:OE1	2.21	0.41
1:E:280:ALA:HB1	1:E:281:PRO:HD2	2.03	0.41
1:F:200:GLU:HG3	1:F:200:GLU:H	1.58	0.41
1:F:224:HIS:CD2	1:F:264:LEU:HB3	2.56	0.41
1:B:459:GLN:HB3	1:B:459:GLN:HE21	1.71	0.41
1:C:361:GLY:HA3	1:C:363:TYR:CE2	2.56	0.40
1:D:400:ARG:HA	1:D:404:TRP:O	2.20	0.40
1:E:339:TYR:O	1:E:343:GLN:HG2	2.21	0.40
1:F:415:ALA:HB1	1:F:418:ILE:HD12	2.02	0.40
1:B:34:LEU:HD23	1:C:336:ARG:HD2	2.04	0.40
1:D:220:PRO:O	1:D:224:HIS:N	2.50	0.40
1:A:112:ALA:HA	1:A:113:PRO:HD3	1.86	0.40
1:A:200:GLU:HG3	3:D:1221:HOH:O	2.19	0.40
1:C:408:ALA:HA	1:C:420:VAL:O	2.21	0.40
1:A:459:GLN:HB3	3:D:922:HOH:O	2.20	0.40
1:D:245:ALA:HA	1:D:272:ALA:HA	2.03	0.40
1:A:410:THR:HA	1:A:418:ILE:O	2.22	0.40
1:C:31:ARG:NH2	1:C:34:LEU:HD11	2.35	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:649:HOH:O	3:D:803:HOH:O[1_455]	1.88	0.32
3:D:810:HOH:O	3:D:869:HOH:O[3_555]	2.10	0.10

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	452/466 (97%)	436 (96%)	16 (4%)	0	100	100
1	B	453/466 (97%)	431 (95%)	17 (4%)	5 (1%)	14	26
1	C	461/466 (99%)	437 (95%)	24 (5%)	0	100	100
1	D	452/466 (97%)	435 (96%)	16 (4%)	1 (0%)	47	68
1	E	453/466 (97%)	433 (96%)	18 (4%)	2 (0%)	34	54
1	F	462/466 (99%)	441 (96%)	21 (4%)	0	100	100
All	All	2733/2796 (98%)	2613 (96%)	112 (4%)	8 (0%)	41	61

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	29	SER
1	D	27	ALA
1	E	27	ALA
1	B	386	GLU
1	B	56	ALA
1	B	28	GLU
1	B	387	ASP
1	E	245	ALA

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	378/390 (97%)	366 (97%)	12 (3%)	39	65
1	B	379/390 (97%)	367 (97%)	12 (3%)	39	65
1	C	387/390 (99%)	376 (97%)	11 (3%)	43	70
1	D	378/390 (97%)	365 (97%)	13 (3%)	37	63
1	E	379/390 (97%)	364 (96%)	15 (4%)	31	56
1	F	388/390 (100%)	369 (95%)	19 (5%)	25	47
All	All	2289/2340 (98%)	2207 (96%)	82 (4%)	35	61

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	28	GLU
1	A	31	ARG
1	A	164	ILE
1	A	171	ARG
1	A	180	ILE
1	A	183	ARG
1	A	200	GLU
1	A	355	ASP
1	A	398	ARG
1	A	437	LEU
1	A	459	GLN
1	B	28	GLU
1	B	87	LYS
1	B	142	ARG
1	B	157	LEU
1	B	177	LEU
1	B	180	ILE
1	B	200	GLU
1	B	268	LYS
1	B	355	ASP
1	B	398	ARG

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Mol	Chain	Res	Type
1	B	437	LEU
1	B	459	GLN
1	C	31	ARG
1	C	49	GLU
1	C	87	LYS
1	C	157	LEU
1	C	171	ARG
1	C	268	LYS
1	C	297	GLN
1	C	303	VAL
1	C	416	THR
1	C	437	LEU
1	C	459	GLN
1	D	13	LEU
1	D	31	ARG
1	D	34	LEU
1	D	87	LYS
1	D	268	LYS
1	D	303	VAL
1	D	304	ASP
1	D	310	ILE
1	D	344	ASN
1	D	416	THR
1	D	435	GLU
1	D	437	LEU
1	D	459	GLN
1	E	28	GLU
1	E	31	ARG
1	E	87	LYS
1	E	142	ARG
1	E	157	LEU
1	E	177	LEU
1	E	183	ARG
1	E	186	GLN
1	E	196	GLU
1	E	303	VAL
1	E	398	ARG
1	E	416	THR
1	E	437	LEU
1	E	459	GLN
1	E	466	THR
1	F	3	LYS

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Mol	Chain	Res	Type
1	F	7	THR
1	F	10	ARG
1	F	13	LEU
1	F	21	LYS
1	F	23	ILE
1	F	24	SER
1	F	49	GLU
1	F	142	ARG
1	F	171	ARG
1	F	177	LEU
1	F	183	ARG
1	F	200	GLU
1	F	221	GLN
1	F	268	LYS
1	F	303	VAL
1	F	398	ARG
1	F	437	LEU
1	F	459	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	221	GLN
1	A	344	ASN
1	A	459	GLN
1	B	71	ASN
1	B	92	GLN
1	B	109	HIS
1	B	309	GLN
1	B	344	ASN
1	B	459	GLN
1	C	5	GLN
1	C	109	HIS
1	C	186	GLN
1	C	297	GLN
1	C	309	GLN
1	C	459	GLN
1	D	109	HIS
1	D	216	ASN
1	D	221	GLN
1	D	309	GLN

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Mol	Chain	Res	Type
1	D	459	GLN
1	E	167	HIS
1	E	186	GLN
1	E	309	GLN
1	E	344	ASN
1	E	459	GLN
1	F	5	GLN
1	F	109	HIS
1	F	309	GLN
1	F	344	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	PO4	D	467	-	4,4,4	1.62	1 (25%)	6,6,6	1.18	0
2	PO4	B	467	-	4,4,4	1.24	0	6,6,6	1.09	0
2	PO4	C	467	-	4,4,4	1.19	0	6,6,6	0.54	0
2	PO4	E	467	-	4,4,4	1.00	0	6,6,6	0.66	0

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Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PO4	A	467	-	4,4,4	1.11	0	6,6,6	1.17	1 (16%)
2	PO4	F	467	-	4,4,4	1.25	0	6,6,6	0.80	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	467	PO4	P-O4	-2.22	1.47	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	467	PO4	O3-P-O2	2.52	116.05	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	467	PO4	1	0
2	B	467	PO4	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(Å²)	Q<0.9
1	A	454/466 (97%)	-0.66	9 (1%)	65	68	3, 12, 35, 58	0
1	B	455/466 (97%)	-0.61	10 (2%)	62	65	4, 13, 36, 58	0
1	C	463/466 (99%)	-0.54	10 (2%)	62	65	3, 13, 36, 55	0
1	D	454/466 (97%)	-0.66	11 (2%)	59	62	3, 11, 37, 60	0
1	E	455/466 (97%)	-0.55	8 (1%)	68	71	4, 14, 38, 60	0
1	F	464/466 (99%)	-0.60	11 (2%)	59	62	3, 11, 38, 60	0
All	All	2745/2796 (98%)	-0.60	59 (2%)	63	66	3, 12, 37, 60	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	114	LYS	5.3
1	F	115	ASN	4.7
1	D	115	ASN	4.6
1	D	308	GLY	4.1
1	E	116	GLY	4.0
1	C	115	ASN	4.0
1	E	385	GLY	3.9
1	A	115	ASN	3.9
1	B	115	ASN	3.8
1	D	114	LYS	3.8
1	E	115	ASN	3.6
1	E	147	ALA	3.6
1	B	114	LYS	3.4
1	A	385	GLY	3.4
1	C	308	GLY	3.4
1	C	147	ALA	3.3
1	C	416	THR	3.2
1	D	28	GLU	3.1
1	D	147	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	114	LYS	3.1
1	C	307	GLY	3.1
1	F	12	GLU	3.1
1	C	27	ALA	3.0
1	B	27	ALA	3.0
1	B	308	GLY	2.9
1	E	308	GLY	2.8
1	F	23	ILE	2.8
1	B	116	GLY	2.8
1	B	307	GLY	2.7
1	B	385	GLY	2.7
1	C	28	GLU	2.7
1	A	417	ASP	2.7
1	F	308	GLY	2.7
1	A	148	ALA	2.7
1	F	310	ILE	2.6
1	D	307	GLY	2.6
1	D	413	GLY	2.6
1	A	114	LYS	2.5
1	A	116	GLY	2.5
1	D	302	ASN	2.5
1	B	30	LYS	2.4
1	A	147	ALA	2.4
1	F	27	ALA	2.4
1	A	28	GLU	2.4
1	E	459	GLN	2.3
1	F	19	GLY	2.3
1	C	305	TYR	2.3
1	C	116	GLY	2.3
1	D	27	ALA	2.2
1	E	460	GLN	2.2
1	F	309	GLN	2.2
1	F	116	GLY	2.2
1	D	305	TYR	2.1
1	B	34	LEU	2.1
1	A	27	ALA	2.1
1	F	305	TYR	2.1
1	D	26	ILE	2.1
1	C	385	GLY	2.1
1	B	28	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates 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	PO4	D	467	5/5	0.99	0.12	13,29,31,33	0
2	PO4	B	467	5/5	0.99	0.09	11,19,23,26	0
2	PO4	C	467	5/5	0.99	0.09	11,20,22,28	0
2	PO4	E	467	5/5	0.99	0.10	13,28,33,37	0
2	PO4	A	467	5/5	0.99	0.08	11,13,19,20	0
2	PO4	F	467	5/5	1.00	0.07	6,11,17,22	0

6.5 Other polymers (i)

There are no such residues in this entry.