Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 08:47 AM GMT

PDB ID	:	3FZ8
Title	:	Crystal structure of glutamate decarboxylase beta from Escherichia coli: reduced Schiff base with PLP
Authors	:	Malashkevich, V.N.; De Biase, D.; Bossa, F.
Deposited on	:	2009-01-23
Resolution	:	3.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

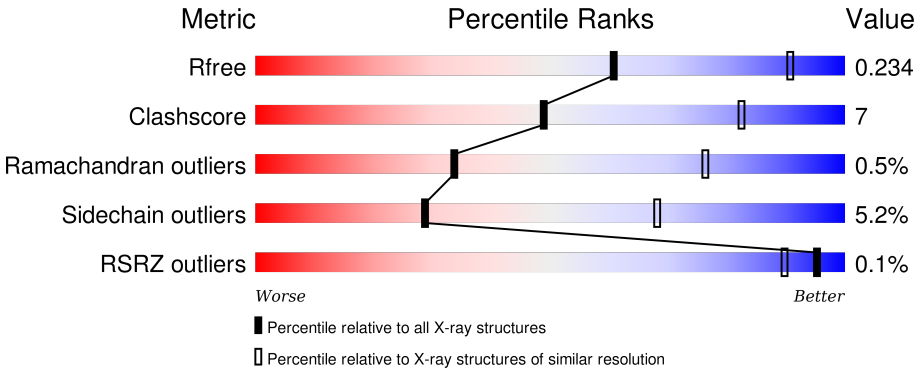
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	84% 13%
1	B	466	76% 23%
1	C	466	79% 17%
1	D	466	77% 19%
1	E	466	78% 20%

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Mol	Chain	Length	Quality of chain
1	F	466	

2 Entry composition

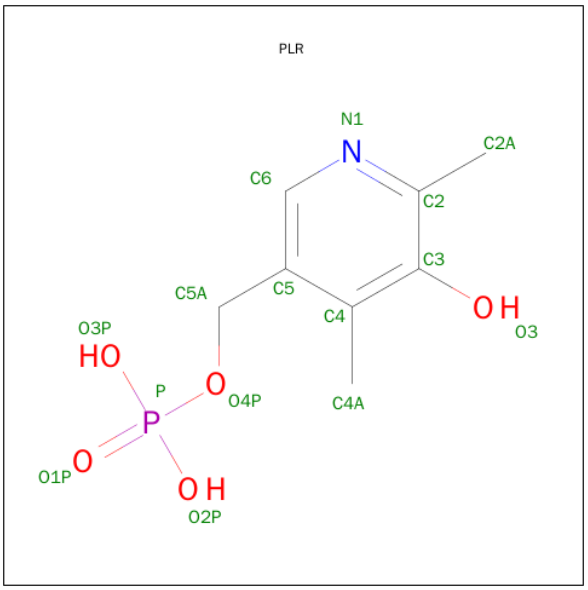
There are 3 unique types of molecules in this entry. The entry contains 21985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	B	463	Total	C	N	O	S	0	0	0
			3681	2347	630	680	24			
1	C	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	D	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			
1	E	464	Total	C	N	O	S	0	0	0
			3690	2353	632	681	24			
1	F	455	Total	C	N	O	S	0	0	0
			3616	2308	617	667	24			

- Molecule 2 is (5-HYDROXY-4,6-DIMETHYLPYRIDIN-3-YL)METHYL DIHYDROGEN PHOSPHATE (three-letter code: PLR) (formula: $C_8H_{12}NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is water.

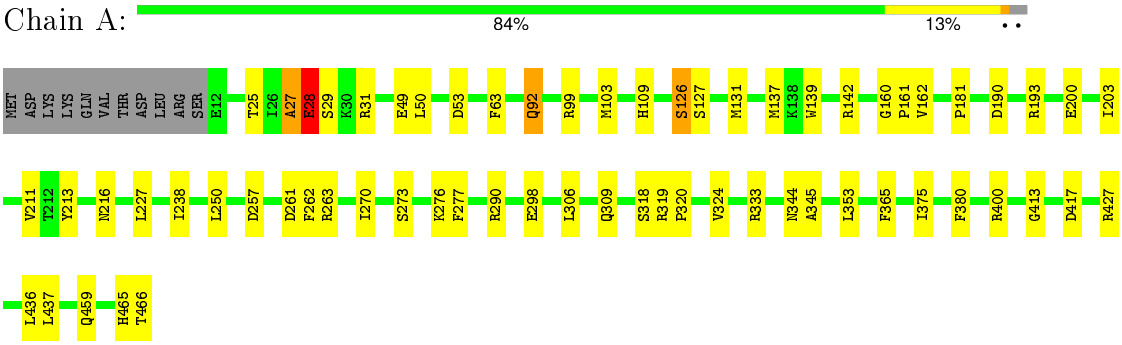
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	60	Total	O	0	0
			60	60		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

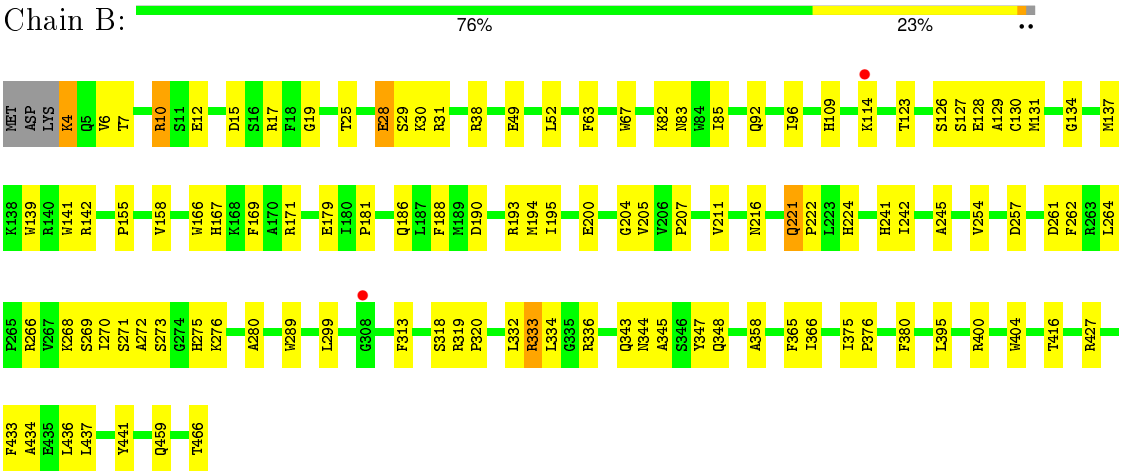
- Molecule 1: Glutamate decarboxylase beta

Chain A:



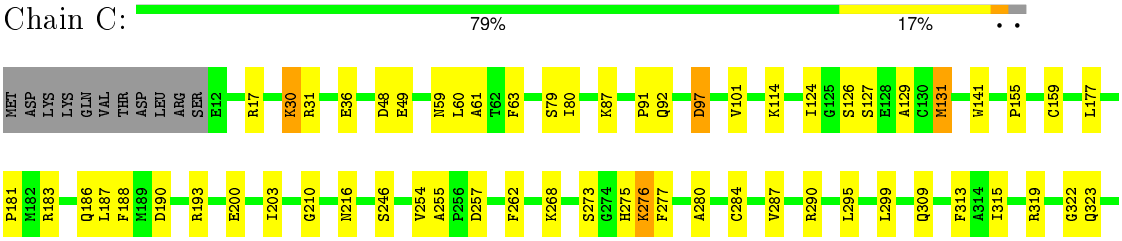
- Molecule 1: Glutamate decarboxylase beta

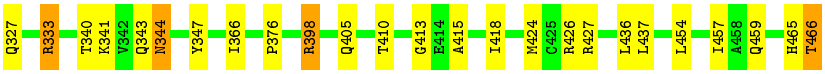
Chain B:



- Molecule 1: Glutamate decarboxylase beta

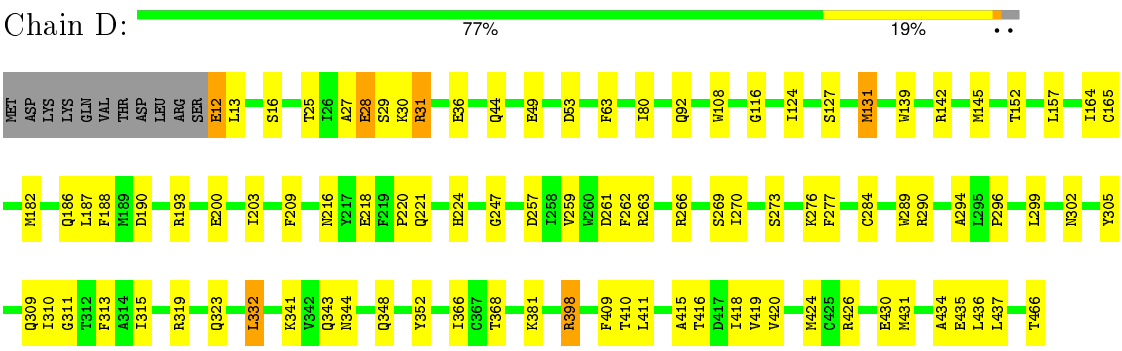
Chain C:





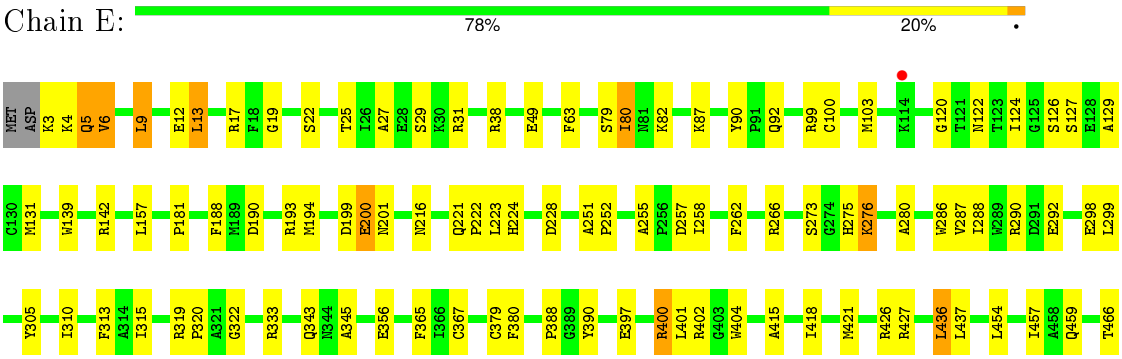
• Molecule 1: Glutamate decarboxylase beta

Chain D:



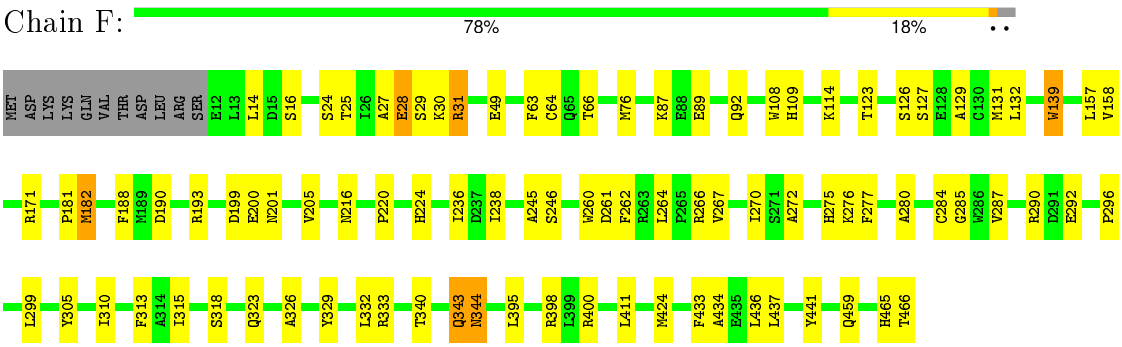
• Molecule 1: Glutamate decarboxylase beta

Chain E:



• Molecule 1: Glutamate decarboxylase beta

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	116.90Å 116.89Å 208.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.88 – 3.00 29.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.4 (19.88-3.00) 95.4 (29.88-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.165 , 0.237 0.166 , 0.234	Depositor DCC
R_{free} test set	3072 reflections (5.33%)	DCC
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 26.6	EDS
Estimated twinning fraction	0.013 for -h,-k,l 0.041 for h,-h-k,-l 0.026 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 60814 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	21985	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PLR

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	0.61	0/3710	0.72	0/5028
1	B	0.63	0/3775	0.74	0/5115
1	C	0.64	1/3710 (0.0%)	0.76	1/5028 (0.0%)
1	D	0.62	0/3710	0.73	0/5028
1	E	0.66	2/3784 (0.1%)	0.76	2/5126 (0.0%)
1	F	0.63	0/3710	0.72	1/5028 (0.0%)
All	All	0.63	3/22399 (0.0%)	0.74	4/30353 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	276	LYS	CE-NZ	-7.00	1.31	1.49
1	E	367	CYS	CB-SG	-6.29	1.71	1.82
1	E	100	CYS	CB-SG	-5.21	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	276	LYS	CD-CE-NZ	8.67	131.63	111.70
1	E	157	LEU	CA-CB-CG	8.24	134.25	115.30
1	E	436	LEU	CA-CB-CG	6.66	130.62	115.30
1	F	157	LEU	CA-CB-CG	5.43	127.78	115.30

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	3616	0	3514	42	0
1	B	3681	0	3584	69	0
1	C	3616	0	3513	56	0
1	D	3616	0	3514	59	0
1	E	3690	0	3597	64	0
1	F	3616	0	3514	57	0
2	A	15	0	9	2	0
2	B	15	0	9	0	0
2	C	15	0	9	0	0
2	D	15	0	9	0	0
2	E	15	0	9	0	0
2	F	15	0	8	1	0
3	E	60	0	0	2	0
All	All	21985	0	21289	309	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 7.

All (309) 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:188:PHE:HZ	1:D:216:ASN:HD22	1.02	0.99
1:E:305:TYR:HE1	1:E:310:ILE:HG13	1.35	0.90
1:F:188:PHE:HZ	1:F:216:ASN:HD22	1.20	0.86
1:E:188:PHE:HZ	1:E:216:ASN:ND2	1.74	0.85
1:E:188:PHE:HZ	1:E:216:ASN:HD22	1.20	0.85
1:F:28:GLU:OE2	1:F:28:GLU:HA	1.77	0.84
1:D:190:ASP:OD1	1:D:193:ARG:HD3	1.78	0.83
1:C:183:ARG:HG3	1:C:186:GLN:HB3	1.59	0.82
1:E:5:GLN:HG3	1:E:5:GLN:O	1.77	0.82
1:E:305:TYR:CE1	1:E:310:ILE:HG13	2.16	0.81
1:B:221:GLN:HB3	1:B:222:PRO:HD3	1.63	0.81
1:B:273:SER:HB2	1:B:276:LYS:HG3	1.63	0.80
1:E:228:ASP:HA	1:E:266:ARG:HH21	1.46	0.79
1:E:92:GLN:HG2	1:F:49:GLU:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:LEU:HB3	1:E:313:PHE:CE1	2.18	0.78
1:E:25:THR:O	1:E:29:SER:HB3	1.84	0.77
1:C:49:GLU:O	1:D:92:GLN:HG2	1.85	0.77
1:A:27:ALA:O	1:A:29:SER:N	2.18	0.77
1:D:188:PHE:HZ	1:D:216:ASN:ND2	1.81	0.76
1:D:31:ARG:HD3	3:E:502:HOH:O	1.84	0.76
1:F:190:ASP:OD1	1:F:193:ARG:HD3	1.86	0.75
1:C:183:ARG:CG	1:C:186:GLN:HB3	2.17	0.75
1:A:127:SER:O	1:A:131:MET:HG2	1.87	0.73
1:E:127:SER:O	1:E:131:MET:HG3	1.89	0.73
1:B:343:GLN:OE1	1:B:343:GLN:HA	1.87	0.73
1:B:190:ASP:OD1	1:B:193:ARG:HD3	1.89	0.72
1:E:188:PHE:CZ	1:E:216:ASN:ND2	2.54	0.72
1:B:109:HIS:HD2	1:B:261:ASP:OD2	1.71	0.72
1:D:273:SER:HB2	1:D:276:LYS:HG3	1.69	0.72
1:B:188:PHE:HZ	1:B:216:ASN:HD22	1.36	0.71
1:E:190:ASP:OD1	1:E:193:ARG:HD3	1.91	0.71
1:A:190:ASP:OD1	1:A:193:ARG:HD3	1.90	0.70
1:E:343:GLN:OE1	1:E:343:GLN:HA	1.92	0.69
1:A:63:PHE:HB3	1:A:276:LYS:HG2	1.73	0.69
1:B:10:ARG:HH11	1:B:10:ARG:HB2	1.58	0.69
1:E:13:LEU:O	1:E:22:SER:HB2	1.93	0.68
1:B:273:SER:CB	1:B:276:LYS:HG3	2.24	0.68
1:E:224:HIS:CD2	1:E:266:ARG:HB2	2.30	0.67
1:F:114:LYS:HE2	1:F:292:GLU:HG3	1.75	0.67
1:D:124:ILE:HD11	1:D:319:ARG:HD2	1.77	0.65
1:F:188:PHE:HZ	1:F:216:ASN:ND2	1.95	0.65
1:E:13:LEU:O	1:E:22:SER:N	2.27	0.65
1:B:19:GLY:O	1:C:341:LYS:HE2	1.97	0.65
1:F:190:ASP:OD1	1:F:193:ARG:CD	2.46	0.64
1:C:465:HIS:O	1:C:466:THR:HB	1.97	0.64
1:C:181:PRO:O	1:C:193:ARG:NH2	2.29	0.64
1:A:99:ARG:O	1:A:103:MET:HG3	1.98	0.64
1:B:25:THR:O	1:B:29:SER:HB3	1.99	0.62
1:C:188:PHE:HZ	1:C:216:ASN:ND2	1.96	0.62
1:D:431:MET:O	1:D:434:ALA:HB3	1.99	0.62
1:A:92:GLN:HG2	1:B:49:GLU:O	1.99	0.62
1:E:63:PHE:HB3	1:E:276:LYS:HG2	1.81	0.61
1:E:49:GLU:O	1:F:92:GLN:HG2	1.99	0.61
1:D:218:GLU:O	1:D:220:PRO:HD3	2.00	0.61
1:D:188:PHE:CZ	1:D:216:ASN:ND2	2.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:PHE:CZ	1:C:216:ASN:ND2	2.69	0.60
1:E:13:LEU:H	1:E:22:SER:HB3	1.66	0.60
1:F:343:GLN:HA	1:F:343:GLN:OE1	2.02	0.60
1:E:13:LEU:O	1:E:22:SER:CB	2.49	0.60
1:C:190:ASP:OD1	1:C:193:ARG:HD3	2.01	0.60
1:D:299:LEU:HB3	1:D:313:PHE:CE1	2.37	0.59
1:B:211:VAL:HG23	1:B:216:ASN:O	2.02	0.59
1:A:181:PRO:O	1:A:193:ARG:NH2	2.36	0.59
1:F:182:MET:HE2	1:F:411:LEU:HD13	1.85	0.59
1:C:63:PHE:HB3	1:C:276:LYS:HG2	1.84	0.58
1:B:92:GLN:O	1:B:96:ILE:HG13	2.02	0.58
1:A:92:GLN:CG	1:B:49:GLU:O	2.51	0.58
1:C:415:ALA:HB1	1:C:418:ILE:HD12	1.84	0.58
1:D:27:ALA:O	1:D:29:SER:N	2.36	0.58
1:F:64:CYS:O	1:F:66:THR:HG23	2.04	0.57
1:E:194:MET:SD	1:E:223:LEU:HD22	2.44	0.57
1:D:145:MET:HB3	1:D:152:THR:HG22	1.85	0.57
1:F:398:ARG:N	1:F:398:ARG:HD2	2.19	0.57
1:F:126:SER:HB2	2:F:500:PLR:O4P	2.04	0.57
1:F:129:ALA:HB1	1:F:287:VAL:HB	1.87	0.57
1:E:181:PRO:O	1:E:193:ARG:NH2	2.36	0.57
1:C:188:PHE:HZ	1:C:216:ASN:HD22	1.51	0.57
1:C:299:LEU:HD13	1:C:313:PHE:CZ	2.40	0.56
1:E:99:ARG:O	1:E:103:MET:HG3	2.04	0.56
1:B:365:PHE:CD2	1:B:380:PHE:HB3	2.40	0.56
1:F:284:CYS:HB2	1:F:323:GLN:HB3	1.88	0.56
1:A:298:GLU:O	1:B:171:ARG:NH1	2.39	0.56
1:B:137:MET:CE	1:B:241:HIS:HB3	2.36	0.56
1:F:109:HIS:HD2	1:F:261:ASP:OD2	1.89	0.56
1:B:137:MET:HE1	1:B:241:HIS:HB3	1.87	0.55
1:D:352:TYR:OH	1:D:435:GLU:OE1	2.14	0.55
1:E:251:ALA:HB3	1:E:252:PRO:HD3	1.88	0.55
1:A:262:PHE:CE2	1:A:270:ILE:HD12	2.41	0.55
1:D:269:SER:HB3	1:D:289:TRP:CD1	2.42	0.55
1:B:4:LYS:HD3	1:B:4:LYS:C	2.27	0.55
1:D:430:GLU:HG3	1:E:17:ARG:NH2	2.22	0.54
1:E:221:GLN:HB3	1:E:222:PRO:HD3	1.90	0.54
1:F:236:ILE:HG22	1:F:238:ILE:HG13	1.89	0.54
1:E:388:PRO:HB2	1:E:390:TYR:CE2	2.43	0.54
1:C:254:VAL:HG21	1:C:347:TYR:CE2	2.42	0.54
1:F:127:SER:O	1:F:131:MET:HG2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:VAL:HG11	1:F:270:ILE:HD11	1.88	0.54
1:D:224:HIS:CD2	1:D:266:ARG:HB2	2.43	0.54
1:A:250:LEU:HD21	1:A:277:PHE:CD1	2.42	0.54
1:B:299:LEU:HB3	1:B:313:PHE:CE1	2.43	0.54
1:C:216:ASN:HD21	1:C:366:ILE:HG22	1.73	0.53
1:C:59:ASN:OD1	1:C:61:ALA:N	2.41	0.53
1:A:25:THR:O	1:A:29:SER:HB2	2.09	0.53
1:D:25:THR:O	1:D:29:SER:HB3	2.08	0.53
1:B:207:PRO:HG2	1:B:242:ILE:HD13	1.91	0.53
1:A:92:GLN:HG2	1:B:52:LEU:HB2	1.91	0.53
1:D:415:ALA:HB1	1:D:418:ILE:HD12	1.90	0.53
1:B:15:ASP:OD1	1:B:17:ARG:HB2	2.09	0.53
1:E:466:THR:HG21	1:F:318:SER:OG	2.09	0.53
1:A:227:LEU:HD22	1:A:238:ILE:HB	1.90	0.53
1:C:79:SER:CB	1:C:322:GLY:HA2	2.39	0.53
1:B:262:PHE:CE2	1:B:270:ILE:HD12	2.45	0.52
1:A:319:ARG:HB2	1:A:320:PRO:HD2	1.91	0.52
1:D:63:PHE:HB3	1:D:276:LYS:HD3	1.92	0.52
1:A:49:GLU:O	1:B:92:GLN:HG2	2.09	0.52
1:D:27:ALA:O	1:D:28:GLU:C	2.48	0.52
1:F:275:HIS:HA	1:F:280:ALA:O	2.09	0.51
1:B:181:PRO:O	1:B:193:ARG:NH2	2.43	0.51
1:E:79:SER:CB	1:E:322:GLY:HA2	2.40	0.51
1:F:24:SER:HB3	1:F:27:ALA:HB3	1.92	0.51
1:E:400:ARG:HA	1:E:404:TRP:O	2.11	0.51
1:C:127:SER:O	1:C:131:MET:HG2	2.11	0.51
1:D:348:GLN:OE1	1:E:13:LEU:HD12	2.10	0.51
1:B:83:ASN:OD1	1:B:85:ILE:HG22	2.10	0.51
1:C:124:ILE:HD11	1:C:319:ARG:HD2	1.93	0.51
1:C:30:LYS:HE2	1:D:116:GLY:O	2.11	0.51
1:C:276:LYS:NZ	1:C:466:THR:OG1	2.44	0.50
1:E:80:ILE:HD11	1:F:76:MET:HG3	1.92	0.50
1:E:87:LYS:HG2	1:E:310:ILE:HD12	1.93	0.50
1:A:273:SER:CB	1:A:276:LYS:HD2	2.41	0.50
1:C:131:MET:CE	1:D:315:ILE:HG23	2.42	0.50
1:D:411:LEU:O	1:D:416:THR:HA	2.12	0.50
1:F:245:ALA:HA	1:F:272:ALA:HA	1.94	0.50
1:C:159:CYS:SG	1:C:177:LEU:HD11	2.51	0.50
1:C:60:LEU:O	1:C:424:MET:HB2	2.12	0.50
1:E:415:ALA:HB1	1:E:418:ILE:HD12	1.93	0.49
1:F:224:HIS:NE2	1:F:266:ARG:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:PHE:HB3	1:B:276:LYS:HD3	1.94	0.49
1:C:340:THR:O	1:C:344:ASN:HB2	2.12	0.49
1:B:245:ALA:HA	1:B:272:ALA:HA	1.94	0.49
1:B:129:ALA:HB1	1:B:271:SER:HB2	1.94	0.49
1:D:262:PHE:O	1:D:290:ARG:NH2	2.45	0.49
1:F:139:TRP:HB3	1:F:296:PRO:HG2	1.94	0.49
1:C:275:HIS:HA	1:C:280:ALA:O	2.12	0.49
1:F:262:PHE:O	1:F:290:ARG:NH2	2.46	0.49
1:D:216:ASN:HD21	1:D:366:ILE:HG22	1.77	0.49
1:C:366:ILE:HG22	1:C:366:ILE:O	2.13	0.49
1:F:224:HIS:CD2	1:F:266:ARG:HB2	2.47	0.49
1:F:28:GLU:CD	1:F:31:ARG:HD2	2.33	0.49
1:D:294:ALA:O	1:D:296:PRO:HD3	2.13	0.49
1:A:109:HIS:HD2	1:A:261:ASP:OD2	1.94	0.49
1:E:299:LEU:HD13	1:E:313:PHE:CZ	2.48	0.48
1:D:344:ASN:O	1:D:348:GLN:HG3	2.13	0.48
1:B:400:ARG:HA	1:B:404:TRP:O	2.13	0.48
1:E:319:ARG:HB2	1:E:320:PRO:HD2	1.95	0.48
1:A:276:LYS:HE2	1:A:466:THR:OG1	2.13	0.48
1:C:131:MET:HE2	1:D:315:ILE:HG23	1.95	0.48
1:C:36:GLU:OE2	1:D:341:LYS:NZ	2.25	0.48
1:C:126:SER:O	1:C:127:SER:C	2.52	0.48
1:C:59:ASN:OD1	1:C:59:ASN:C	2.52	0.48
1:C:92:GLN:HG2	1:D:49:GLU:O	2.14	0.48
1:F:277:PHE:O	1:F:343:GLN:NE2	2.46	0.47
1:B:319:ARG:HB2	1:B:320:PRO:HD2	1.96	0.47
1:A:25:THR:O	1:A:29:SER:CB	2.63	0.47
1:C:284:CYS:HB2	1:C:323:GLN:HB3	1.96	0.47
1:B:224:HIS:CD2	1:B:266:ARG:HB2	2.49	0.47
1:B:216:ASN:HD21	1:B:366:ILE:HG22	1.80	0.47
1:D:262:PHE:CE2	1:D:270:ILE:HD12	2.49	0.47
1:B:333:ARG:HG2	1:B:334:LEU:N	2.28	0.47
1:A:466:THR:HB	2:A:500:PLR:H4A3	1.95	0.47
1:D:305:TYR:HE1	1:D:310:ILE:HG13	1.80	0.47
1:E:315:ILE:HG21	1:F:315:ILE:HG21	1.96	0.47
1:D:284:CYS:HB2	1:D:323:GLN:HB3	1.96	0.47
1:F:220:PRO:HG2	1:F:260:TRP:HB2	1.96	0.47
1:A:126:SER:HB2	2:A:500:PLR:O4P	2.15	0.47
1:D:164:ILE:HG23	1:D:165:CYS:N	2.30	0.46
1:D:108:TRP:O	1:D:261:ASP:HB2	2.15	0.46
1:B:343:GLN:OE1	1:B:343:GLN:CA	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:PHE:HB3	1:F:276:LYS:HG2	1.96	0.46
1:C:141:TRP:CD2	1:C:203:ILE:HG22	2.51	0.46
1:E:333:ARG:NH2	1:E:427:ARG:HH12	2.14	0.46
1:A:137:MET:HB3	1:A:203:ILE:HD12	1.98	0.46
1:F:158:VAL:O	1:F:205:VAL:HA	2.15	0.46
1:D:63:PHE:CD1	1:D:466:THR:HA	2.51	0.46
1:E:379:CYS:HA	1:E:421:MET:O	2.16	0.46
1:C:315:ILE:HG23	1:D:131:MET:CE	2.45	0.46
1:E:5:GLN:CG	1:E:5:GLN:O	2.56	0.45
1:F:132:LEU:HB3	1:F:313:PHE:CE2	2.52	0.45
1:F:25:THR:O	1:F:29:SER:HB3	2.16	0.45
1:F:199:ASP:O	1:F:201:ASN:N	2.50	0.45
1:D:12:GLU:HB2	1:D:13:LEU:H	1.62	0.45
1:E:3:LYS:C	1:E:5:GLN:H	2.20	0.45
1:C:273:SER:HB2	1:C:276:LYS:HB2	1.98	0.45
1:C:17:ARG:HD3	1:C:48:ASP:OD2	2.16	0.45
1:E:273:SER:HB2	1:E:276:LYS:HD2	1.99	0.45
1:C:454:LEU:HA	1:C:457:ILE:HD12	1.98	0.45
1:B:275:HIS:HA	1:B:280:ALA:O	2.17	0.45
1:E:262:PHE:O	1:E:290:ARG:NH2	2.50	0.45
1:B:141:TRP:CZ3	1:B:155:PRO:HB3	2.51	0.45
1:C:97:ASP:O	1:C:101:VAL:HG23	2.17	0.45
1:A:28:GLU:HG3	3:E:488:HOH:O	2.16	0.45
1:F:108:TRP:CZ3	1:F:270:ILE:HG22	2.52	0.44
1:B:345:ALA:O	1:B:348:GLN:HB2	2.17	0.44
1:B:254:VAL:HG21	1:B:347:TYR:CE2	2.53	0.44
1:E:365:PHE:CD2	1:E:380:PHE:HB3	2.52	0.44
1:B:269:SER:HB3	1:B:289:TRP:CD1	2.52	0.44
1:B:333:ARG:NH2	1:B:427:ARG:HH12	2.16	0.44
1:B:7:THR:HA	1:C:255:ALA:HA	1.98	0.44
1:F:181:PRO:O	1:F:193:ARG:NH2	2.50	0.44
1:F:465:HIS:O	1:F:466:THR:HB	2.16	0.44
1:B:333:ARG:NH2	1:B:427:ARG:NH1	2.65	0.44
1:E:9:LEU:HA	1:E:9:LEU:HD12	1.72	0.44
1:A:262:PHE:O	1:A:290:ARG:NH2	2.51	0.44
1:D:398:ARG:HH22	1:E:397:GLU:CD	2.21	0.44
1:A:465:HIS:O	1:A:466:THR:HB	2.18	0.43
1:F:262:PHE:CZ	1:F:270:ILE:HD12	2.53	0.43
1:D:157:LEU:HD23	1:D:203:ILE:HD11	2.00	0.43
1:E:343:GLN:OE1	1:E:343:GLN:CA	2.64	0.43
1:F:89:GLU:HG3	1:F:89:GLU:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LEU:HA	1:B:334:LEU:HD23	1.80	0.43
1:A:160:GLY:O	1:A:162:VAL:N	2.51	0.43
1:E:27:ALA:C	1:E:29:SER:N	2.72	0.43
1:A:276:LYS:CE	1:A:466:THR:OG1	2.67	0.43
1:C:343:GLN:HA	1:C:343:GLN:OE1	2.18	0.43
1:E:129:ALA:HB1	1:E:287:VAL:HB	1.99	0.43
1:B:433:PHE:O	1:B:434:ALA:C	2.56	0.43
1:A:365:PHE:CD2	1:A:380:PHE:HB3	2.53	0.43
1:A:50:LEU:O	1:A:53:ASP:HB2	2.18	0.43
1:F:424:MET:HE2	1:F:424:MET:HB3	1.87	0.43
1:A:353:LEU:HA	1:A:353:LEU:HD23	1.64	0.43
1:D:309:GLN:O	1:D:309:GLN:HG3	2.19	0.43
1:D:273:SER:CB	1:D:276:LYS:HG3	2.43	0.43
1:A:273:SER:HB2	1:A:276:LYS:HD2	2.01	0.43
1:D:410:THR:HA	1:D:418:ILE:O	2.18	0.43
1:A:306:LEU:HD11	1:B:400:ARG:NH1	2.34	0.43
1:B:224:HIS:CD2	1:B:264:LEU:HB3	2.53	0.43
1:B:123:THR:HB	1:B:128:GLU:HB3	2.01	0.43
1:F:326:ALA:O	1:F:329:TYR:HB3	2.19	0.43
1:B:158:VAL:O	1:B:205:VAL:HA	2.19	0.42
1:B:67:TRP:CE2	1:C:17:ARG:HG2	2.53	0.42
1:B:375:ILE:HB	1:B:376:PRO:CD	2.49	0.42
1:C:333:ARG:NH2	1:C:427:ARG:HH12	2.17	0.42
1:B:395:LEU:HD21	1:B:441:TYR:CZ	2.53	0.42
1:A:427:ARG:HD2	1:F:16:SER:O	2.19	0.42
1:E:275:HIS:HA	1:E:280:ALA:O	2.20	0.42
1:F:305:TYR:CE1	1:F:310:ILE:HG13	2.54	0.42
1:D:343:GLN:HA	1:D:343:GLN:OE1	2.20	0.42
1:F:433:PHE:O	1:F:434:ALA:C	2.58	0.42
1:E:120:GLY:HA3	1:E:288:ILE:HD13	2.00	0.42
1:B:318:SER:O	1:B:319:ARG:HB3	2.20	0.42
1:D:409:PHE:O	1:D:419:VAL:HA	2.20	0.42
1:E:122:ASN:HB2	1:E:286:TRP:CZ3	2.54	0.42
1:C:262:PHE:O	1:C:290:ARG:NH2	2.52	0.42
1:B:38:ARG:HB3	1:B:38:ARG:HE	1.43	0.42
1:F:395:LEU:HD21	1:F:441:TYR:CZ	2.54	0.42
1:B:358:ALA:HB2	1:B:365:PHE:CE1	2.55	0.42
1:B:194:MET:O	1:B:195:ILE:C	2.57	0.42
1:A:99:ARG:HG2	1:B:29:SER:HB2	2.02	0.42
1:C:59:ASN:HA	1:C:405:GLN:HB3	2.02	0.42
1:A:250:LEU:CD1	1:A:375:ILE:HG22	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:199:ASP:O	1:E:201:ASN:N	2.53	0.41
1:E:5:GLN:O	1:E:6:VAL:C	2.59	0.41
1:A:92:GLN:HG3	1:B:49:GLU:O	2.20	0.41
1:E:103:MET:CE	1:F:29:SER:HA	2.50	0.41
1:B:167:HIS:HE1	1:B:179:GLU:OE1	2.03	0.41
1:C:277:PHE:CZ	1:C:376:PRO:HD2	2.56	0.41
1:B:224:HIS:NE2	1:B:266:ARG:HB2	2.36	0.41
1:B:6:VAL:O	1:C:255:ALA:HA	2.21	0.41
1:B:130:CYS:HB3	1:B:166:TRP:CZ2	2.55	0.41
1:D:302:ASN:HA	1:D:311:GLY:HA2	2.01	0.41
1:D:289:TRP:HB3	1:D:294:ALA:HB3	2.02	0.41
1:B:134:GLY:HA3	1:B:169:PHE:CE1	2.56	0.41
1:C:63:PHE:HB3	1:C:276:LYS:CG	2.51	0.41
1:F:299:LEU:HB3	1:F:313:PHE:CE1	2.55	0.41
1:C:187:LEU:HA	1:C:187:LEU:HD23	1.75	0.41
1:D:16:SER:HB3	1:E:345:ALA:HB3	2.02	0.41
1:E:402:ARG:HG2	1:E:402:ARG:HH11	1.86	0.41
1:D:332:LEU:HA	1:D:332:LEU:HD23	1.86	0.41
1:A:211:VAL:HG12	1:A:213:TYR:H	1.86	0.41
1:C:410:THR:HA	1:C:418:ILE:O	2.21	0.41
1:E:99:ARG:HG2	1:F:29:SER:HB2	2.03	0.41
1:B:137:MET:SD	1:B:204:GLY:HA3	2.61	0.41
1:A:50:LEU:HD22	1:B:82:LYS:HE3	2.02	0.41
1:F:340:THR:O	1:F:344:ASN:HB2	2.21	0.41
1:D:209:PHE:CD2	1:D:247:GLY:HA3	2.56	0.41
1:E:82:LYS:HA	1:E:90:TYR:CE1	2.56	0.41
1:F:123:THR:O	1:F:285:GLY:N	2.47	0.41
1:D:277:PHE:CE2	1:D:424:MET:HE1	2.55	0.41
1:C:398:ARG:HD2	1:C:398:ARG:N	2.36	0.41
1:E:454:LEU:HA	1:E:457:ILE:HD12	2.03	0.41
1:F:224:HIS:CD2	1:F:264:LEU:HB3	2.56	0.41
1:C:129:ALA:HB1	1:C:287:VAL:HB	2.03	0.41
1:A:109:HIS:CD2	1:A:263:ARG:HE	2.39	0.40
1:C:315:ILE:HG23	1:D:131:MET:HE3	2.04	0.40
1:D:381:LYS:HB3	1:D:420:VAL:HG12	2.03	0.40
1:C:91:PRO:HD2	1:D:53:ASP:HA	2.02	0.40
1:B:358:ALA:HB2	1:B:365:PHE:HE1	1.87	0.40
1:E:298:GLU:O	1:F:171:ARG:NH1	2.55	0.40
1:B:221:GLN:HB3	1:B:222:PRO:CD	2.43	0.40
1:C:295:LEU:HD11	1:C:313:PHE:CD2	2.56	0.40
1:D:341:LYS:HE3	1:E:19:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:356:GLU:HA	1:E:356:GLU:OE2	2.21	0.40
1:E:255:ALA:HB1	1:E:258:ILE:HG13	2.04	0.40
1:A:318:SER:OG	1:B:466:THR:HG21	2.22	0.40
1:F:114:LYS:HB2	1:F:114:LYS:HE3	1.82	0.40
1:C:141:TRP:CZ3	1:C:155:PRO:HB3	2.56	0.40
1:D:182:MET:HG2	1:D:187:LEU:O	2.21	0.40
1:D:259:VAL:HG22	1:D:263:ARG:NH1	2.35	0.40
1:A:345:ALA:HB2	1:F:14:LEU:HB2	2.03	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	453/466 (97%)	422 (93%)	27 (6%)	4 (1%)	21	64
1	B	461/466 (99%)	431 (94%)	28 (6%)	2 (0%)	39	80
1	C	453/466 (97%)	424 (94%)	27 (6%)	2 (0%)	39	80
1	D	453/466 (97%)	425 (94%)	27 (6%)	1 (0%)	52	88
1	E	462/466 (99%)	429 (93%)	28 (6%)	5 (1%)	17	58
1	F	453/466 (97%)	424 (94%)	29 (6%)	0	100	100
All	All	2735/2796 (98%)	2555 (93%)	166 (6%)	14 (0%)	34	76

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	D	28	GLU
1	A	27	ALA
1	B	186	GLN

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Mol	Chain	Res	Type
1	C	413	GLY
1	E	4	LYS
1	E	6	VAL
1	B	28	GLU
1	E	459	GLN
1	E	200	GLU
1	E	292	GLU
1	A	161	PRO
1	A	413	GLY
1	C	210	GLY

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	379/390 (97%)	361 (95%)	18 (5%)	32	72
1	B	387/390 (99%)	363 (94%)	24 (6%)	23	60
1	C	379/390 (97%)	358 (94%)	21 (6%)	27	65
1	D	379/390 (97%)	359 (95%)	20 (5%)	28	67
1	E	388/390 (100%)	369 (95%)	19 (5%)	31	71
1	F	379/390 (97%)	363 (96%)	16 (4%)	36	76
All	All	2291/2340 (98%)	2173 (95%)	118 (5%)	29	68

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLU
1	A	31	ARG
1	A	92	GLN
1	A	126	SER
1	A	139	TRP
1	A	142	ARG
1	A	200	GLU
1	A	216	ASN

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Mol	Chain	Res	Type
1	A	257	ASP
1	A	309	GLN
1	A	324	VAL
1	A	333	ARG
1	A	344	ASN
1	A	400	ARG
1	A	417	ASP
1	A	436	LEU
1	A	437	LEU
1	A	459	GLN
1	B	4	LYS
1	B	10	ARG
1	B	12	GLU
1	B	28	GLU
1	B	30	LYS
1	B	31	ARG
1	B	114	LYS
1	B	126	SER
1	B	127	SER
1	B	131	MET
1	B	139	TRP
1	B	142	ARG
1	B	200	GLU
1	B	221	GLN
1	B	257	ASP
1	B	268	LYS
1	B	332	LEU
1	B	333	ARG
1	B	336	ARG
1	B	344	ASN
1	B	416	THR
1	B	436	LEU
1	B	437	LEU
1	B	459	GLN
1	C	30	LYS
1	C	31	ARG
1	C	80	ILE
1	C	87	LYS
1	C	97	ASP
1	C	114	LYS
1	C	131	MET
1	C	200	GLU

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Mol	Chain	Res	Type
1	C	246	SER
1	C	257	ASP
1	C	268	LYS
1	C	309	GLN
1	C	327	GLN
1	C	333	ARG
1	C	344	ASN
1	C	398	ARG
1	C	426	ARG
1	C	436	LEU
1	C	437	LEU
1	C	459	GLN
1	C	466	THR
1	D	12	GLU
1	D	30	LYS
1	D	31	ARG
1	D	36	GLU
1	D	44	GLN
1	D	80	ILE
1	D	127	SER
1	D	131	MET
1	D	139	TRP
1	D	142	ARG
1	D	186	GLN
1	D	200	GLU
1	D	221	GLN
1	D	257	ASP
1	D	332	LEU
1	D	368	THR
1	D	398	ARG
1	D	426	ARG
1	D	436	LEU
1	D	437	LEU
1	E	5	GLN
1	E	9	LEU
1	E	12	GLU
1	E	13	LEU
1	E	31	ARG
1	E	38	ARG
1	E	80	ILE
1	E	124	ILE
1	E	126	SER

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Mol	Chain	Res	Type
1	E	139	TRP
1	E	142	ARG
1	E	200	GLU
1	E	257	ASP
1	E	276	LYS
1	E	400	ARG
1	E	401	LEU
1	E	426	ARG
1	E	436	LEU
1	E	437	LEU
1	F	28	GLU
1	F	30	LYS
1	F	31	ARG
1	F	87	LYS
1	F	139	TRP
1	F	182	MET
1	F	200	GLU
1	F	246	SER
1	F	332	LEU
1	F	333	ARG
1	F	343	GLN
1	F	344	ASN
1	F	400	ARG
1	F	436	LEU
1	F	437	LEU
1	F	459	GLN

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

Mol	Chain	Res	Type
1	A	109	HIS
1	A	167	HIS
1	A	216	ASN
1	A	309	GLN
1	A	459	GLN
1	B	5	GLN
1	B	109	HIS
1	B	167	HIS
1	B	216	ASN
1	B	309	GLN
1	B	459	GLN
1	C	216	ASN

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Mol	Chain	Res	Type
1	C	309	GLN
1	C	459	GLN
1	D	109	HIS
1	D	216	ASN
1	D	309	GLN
1	D	459	GLN
1	E	109	HIS
1	E	167	HIS
1	E	216	ASN
1	E	459	GLN
1	F	109	HIS
1	F	309	GLN
1	F	459	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 carbohydrates in this entry.

5.6 Ligand geometry

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	PLR	A	500	1	15,15,15	0.91	0	21,22,22	1.43	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PLR	B	500	1	15,15,15	0.85	1 (6%)	21,22,22	1.26	3 (14%)
2	PLR	C	500	1	15,15,15	0.99	1 (6%)	21,22,22	1.38	3 (14%)
2	PLR	D	500	1	15,15,15	1.21	1 (6%)	21,22,22	1.15	2 (9%)
2	PLR	E	500	1	15,15,15	0.81	1 (6%)	21,22,22	1.33	2 (9%)
2	PLR	F	500	1	15,15,15	1.17	2 (13%)	21,22,22	1.69	5 (23%)

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	PLR	A	500	1	-	0/6/6/6	0/1/1/1
2	PLR	B	500	1	-	0/6/6/6	0/1/1/1
2	PLR	C	500	1	-	0/6/6/6	0/1/1/1
2	PLR	D	500	1	-	0/6/6/6	0/1/1/1
2	PLR	E	500	1	-	0/6/6/6	0/1/1/1
2	PLR	F	500	1	-	0/6/6/6	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PLR	C3-C2	-3.47	1.38	1.40
2	C	500	PLR	C3-C2	-2.88	1.38	1.40
2	B	500	PLR	C3-C2	-2.55	1.39	1.40
2	F	500	PLR	C4A-C4	-2.45	1.46	1.51
2	F	500	PLR	C3-C2	-2.31	1.39	1.40
2	E	500	PLR	C5-C4	-2.20	1.38	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	500	PLR	C4A-C4-C5	-4.35	116.35	120.88
2	E	500	PLR	O4P-P-O1P	-3.74	97.63	107.14
2	C	500	PLR	O4P-P-O1P	-3.19	99.02	107.14
2	A	500	PLR	C4A-C4-C5	-2.86	117.90	120.88
2	F	500	PLR	C2A-C2-C3	-2.71	117.77	121.04
2	D	500	PLR	C4A-C4-C5	-2.64	118.13	120.88
2	F	500	PLR	O3P-P-O4P	-2.48	99.43	106.56
2	B	500	PLR	C4A-C4-C5	-2.29	118.50	120.88
2	B	500	PLR	C5-C6-N1	-2.25	119.95	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	500	PLR	C3-C4-C5	2.06	121.02	118.78
2	F	500	PLR	C2A-C2-N1	2.25	122.93	117.95
2	E	500	PLR	O3P-P-O2P	2.31	116.16	107.38
2	A	500	PLR	O4P-C5A-C5	2.44	113.03	108.99
2	A	500	PLR	C3-C4-C5	2.51	121.52	118.78
2	D	500	PLR	O3P-P-O2P	2.53	117.00	107.38
2	F	500	PLR	O3P-P-O2P	2.53	117.03	107.38
2	C	500	PLR	O3P-P-O2P	2.59	117.24	107.38
2	B	500	PLR	O3P-P-O2P	2.67	117.56	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	PLR	2	0
2	F	500	PLR	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	455/466 (97%)	-0.85	0 100 100	2, 10, 35, 53	0
1	B	463/466 (99%)	-0.84	2 (0%) 93 80	2, 9, 34, 53	0
1	C	455/466 (97%)	-0.91	0 100 100	2, 9, 34, 52	0
1	D	455/466 (97%)	-0.88	0 100 100	2, 10, 36, 52	0
1	E	464/466 (99%)	-0.90	1 (0%) 95 87	2, 8, 33, 51	0
1	F	455/466 (97%)	-0.92	0 100 100	2, 9, 34, 51	0
All	All	2747/2796 (98%)	-0.88	3 (0%) 95 90	2, 9, 35, 53	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	LYS	2.8
1	E	114	LYS	2.7
1	B	308	GLY	2.3

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

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	LLDF	B-factors(Å^2)	Q<0.9
2	PLR	D	500	15/15	0.97	0.14	0.84	3,10,14,15	0
2	PLR	E	500	15/15	0.99	0.13	-0.20	2,4,11,13	0
2	PLR	F	500	15/15	0.98	0.11	-0.27	2,5,13,14	0
2	PLR	A	500	15/15	0.99	0.13	-0.48	11,14,15,15	0
2	PLR	B	500	15/15	0.98	0.11	-0.67	3,11,13,13	0
2	PLR	C	500	15/15	0.99	0.10	-1.03	2,5,13,14	0

6.5 Other polymers (i)

There are no such residues in this entry.