Full wwPDB X-ray Structure Validation Report (i)

Dec 2, 2023 – 07:04 pm GMT

PDB ID	:	2BQ1
Title	:	Ribonucleotide reductase class 1b holocomplex R1E,R2F from Salmonella typhimurium
Authors	:	Uppsten, M.; Farnegardh, M.; Domkin, V.; Uhlin, U.
Deposited on	:	2005-04-26
Resolution	:	3.99 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:

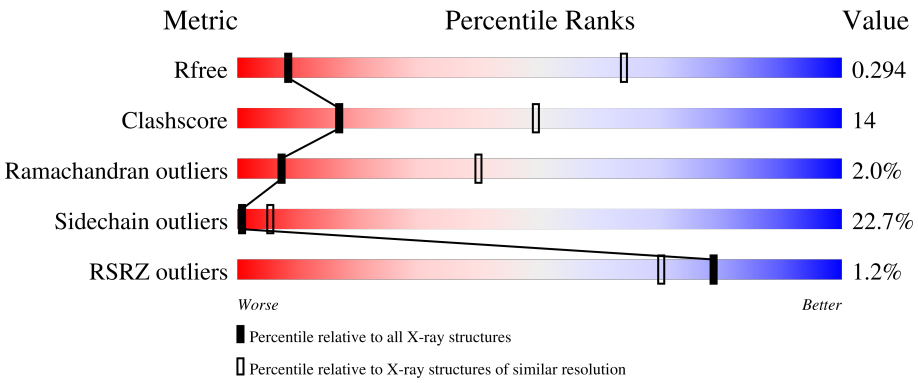
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 3.99 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	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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	E	714	.% 52% 36% 7% 5%
1	F	714	.% 52% 36% 7% .
2	I	319	48% 35% 8% 8%
2	J	319	3% 40% 40% 8% 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15520 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.

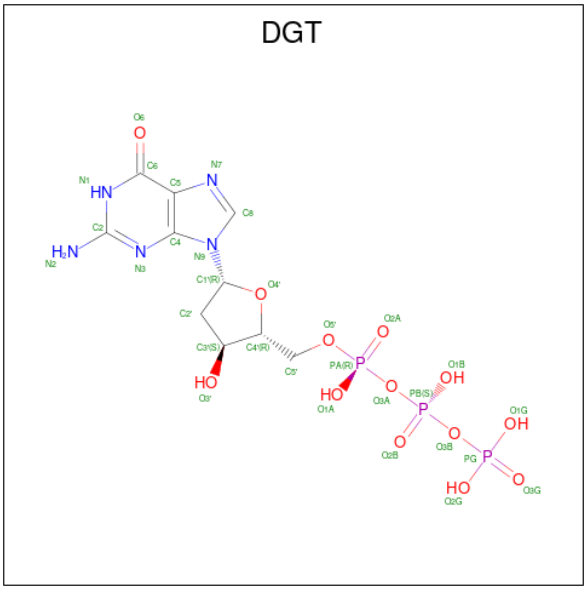
- Molecule 1 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	676	5389	3420	949	998	22	0	0	1
1	F	685	5465	3464	964	1015	22	0	0	1

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	294	2343	1522	376	437	8	0	0	0
2	J	281	2255	1463	362	422	8	0	0	0

- Molecule 3 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	E	1	31	10	5	13	3	0	0
3	F	1	31	10	5	13	3	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	E	1	1	1	0	0
4	F	1	1	1	0	0

- Molecule 5 is FE (III) ION (three-letter code: FE) (formula: Fe).

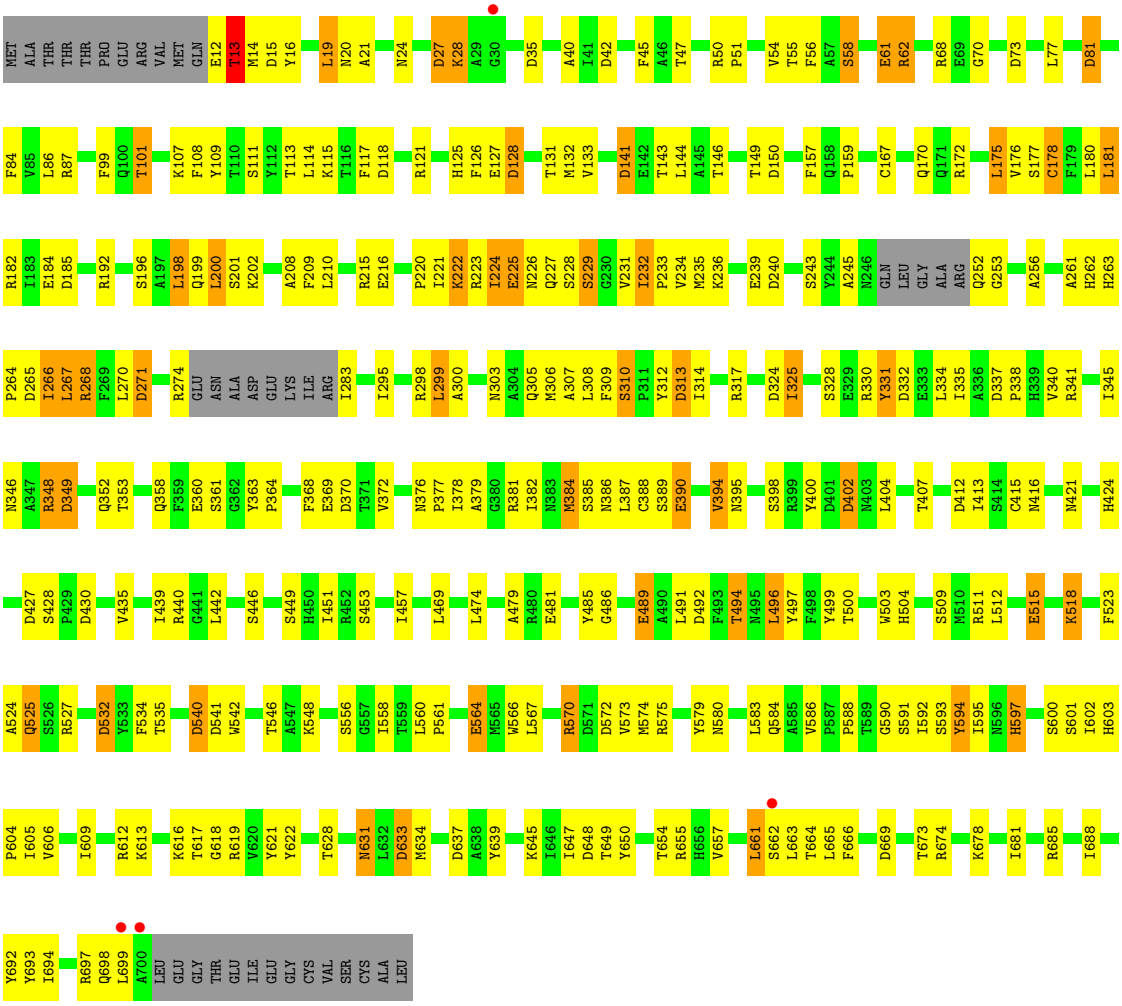
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Fe		
5	I	2	2	2	0	0
5	J	2	2	2	0	0

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.

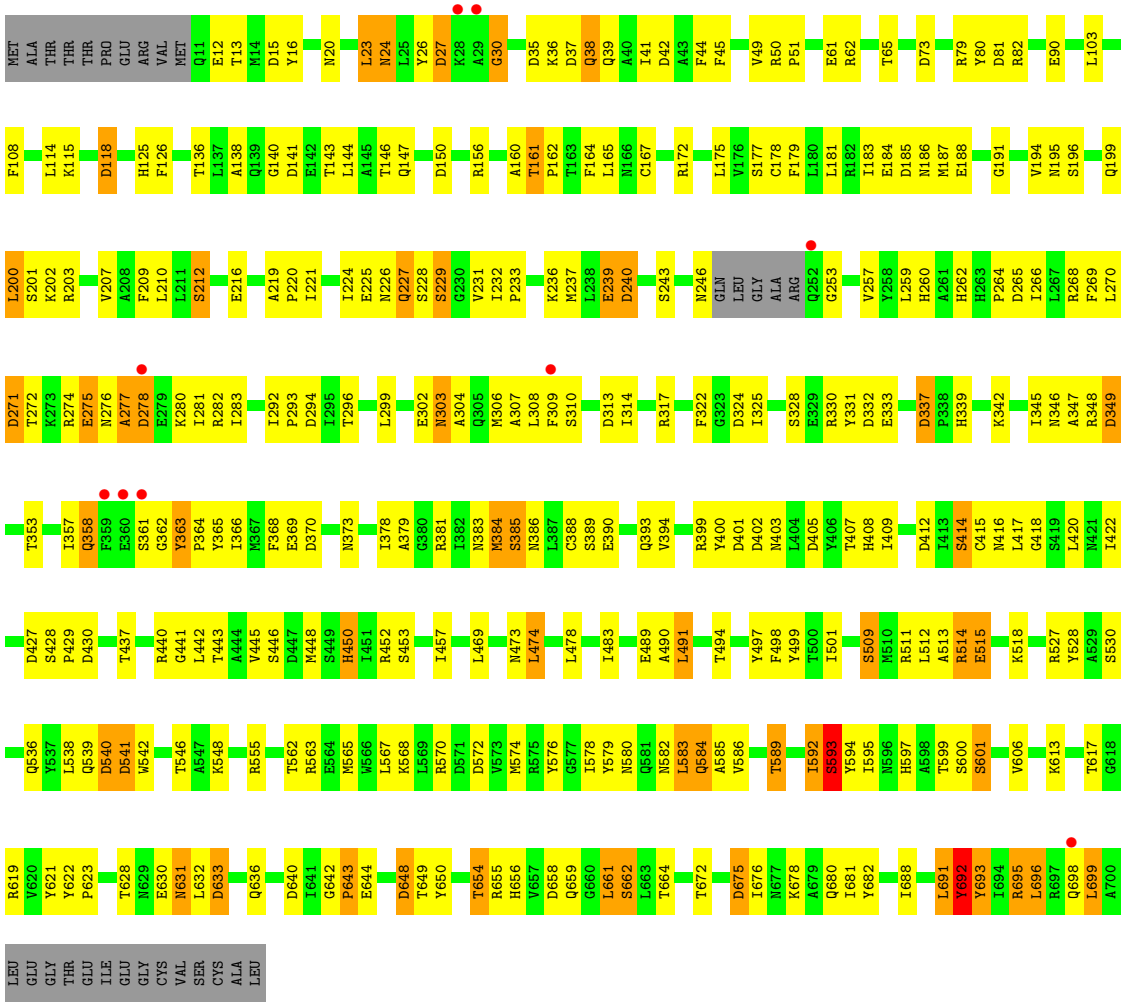
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 ALPHA SUBUNIT

Chain E:



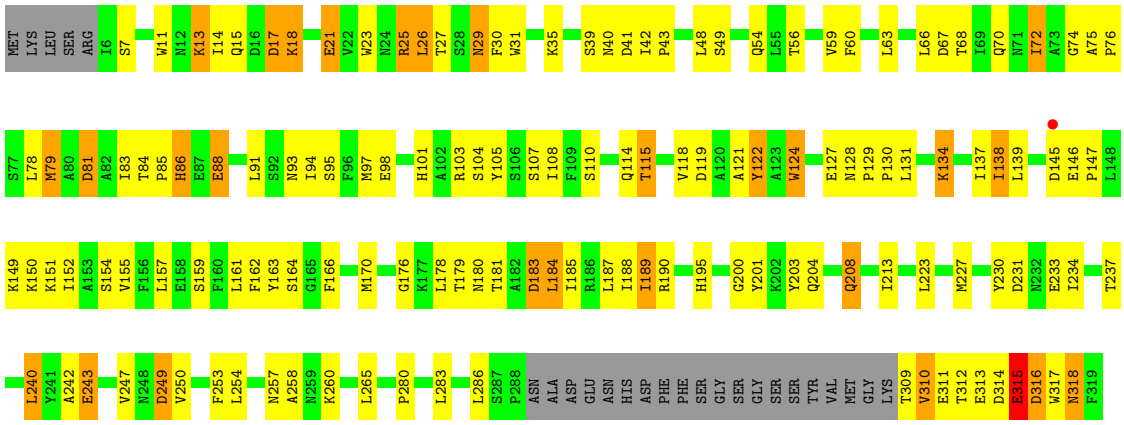
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 ALPHA SUBUNIT

Chain F:



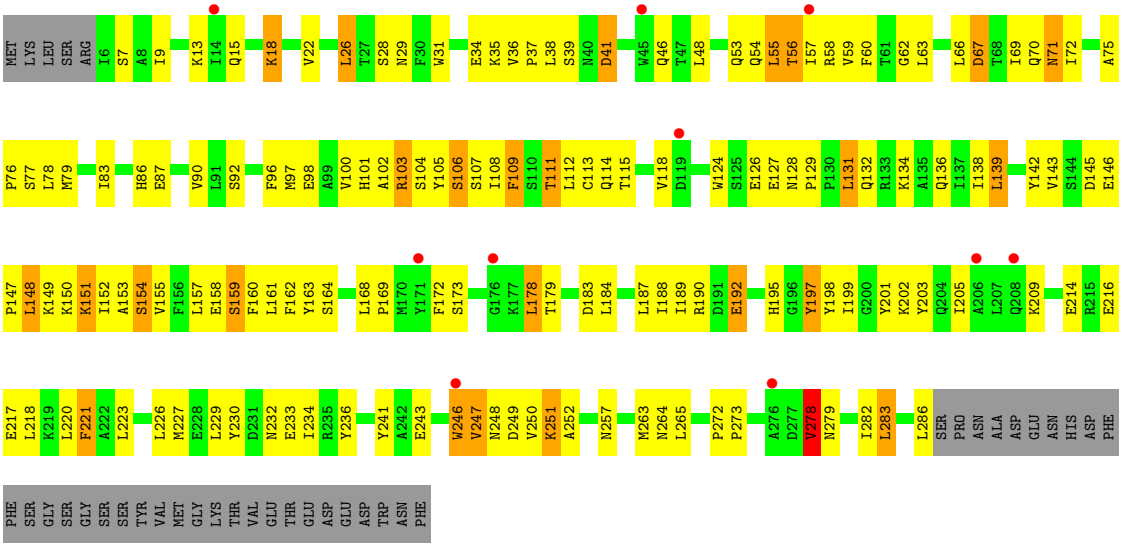
- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 BETA SUBUNIT

Chain I:



- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 BETA SUBUNIT

Chain J:


MET LYS LEU SER ARG I6 S7 A8 I9 K13 I14 Q15 K18 V22 L26 T27 S28 N29 F30 W31 E34 K35 V36 P37 L38 S39 N40 D41 W45 Q46 T47 L48 Q53 Q54 L55 T56 I57 R58 V59 F60 T61 G62 L63 L66 D67 T68 I69 Q70 N71 I72 A75
P76 S77 L78 M79 I83 H86 E87 V90 L91 S92 F96 M97 E98 A99 V100 H101 A102 R103 S104 Y105 S106 S107 I108 F109 S110 T111 L112 C113 Q114 T115 V118 D119 W124 S125 E126 E127 N128 P129 P130 L131 Q132 R133 K134 A135 Q136 I137 I138 L139 Y142 V143 S144 D145 E146
P147 L148 K149 K150 K151 I152 A153 S154 V155 F156 L157 E158 S159 F160 L161 F162 Y163 S164 L168 P169 M170 Y171 F172 S173 G176 K177 L178 T179 D183 L184 L187 I188 I189 R190 D191 E192 H195 G196 Y197 Y198 I199 G200 Y201 K202 Y203 Q204 I205 A206 L207 Q208 K209 E214 R215 E216
E217 L218 K219 L220 F221 A222 L223 L226 M227 E228 L229 Y230 D231 N232 E233 I234 R235 Y236 Y241 A242 E243 W246 V247 N248 D249 V250 K251 A252 N257 M263 N264 L265 P272 P273 A276 D277 V278 N279 I282 L283 L286 SER PRO ASN ALA ASP GLU ASN HIS ASP PHE
PHE SER GLY SER GLY SER SER TYR VAL MET GLY LYS THR VAL GLU THR GLU ASP GLU ASP TRP ASN PHE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α, β, γ	270.37Å 270.37Å 270.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	182.57 – 3.99 39.86 – 3.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (182.57-3.99) 99.9 (39.86-3.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.39 (at 4.00Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.262 , 0.310 0.241 , 0.294	Depositor DCC
R_{free} test set	1485 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	90.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 73.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	15520	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: DGT, MG, FE

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	E	0.35	0/5513	0.74	30/7465 (0.4%)
1	F	0.37	0/5590	0.74	30/7569 (0.4%)
2	I	0.40	0/2401	0.68	6/3273 (0.2%)
2	J	0.45	0/2310	0.70	4/3146 (0.1%)
All	All	0.38	0/15814	0.72	70/21453 (0.3%)

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
2	I	0	1

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	315	GLU	N-CA-C	-6.80	92.64	111.00
1	F	332	ASP	CB-CG-OD2	6.73	124.36	118.30
1	E	572	ASP	CB-CG-OD2	6.64	124.28	118.30
1	F	240	ASP	CB-CG-OD2	6.40	124.06	118.30
1	F	37	ASP	CB-CG-OD2	6.40	124.06	118.30
1	F	648	ASP	CB-CG-OD2	6.33	124.00	118.30
1	F	572	ASP	CB-CG-OD2	6.24	123.92	118.30
1	E	240	ASP	CB-CG-OD2	6.21	123.89	118.30
1	F	324	ASP	CB-CG-OD2	6.21	123.88	118.30
1	F	73	ASP	CB-CG-OD2	6.20	123.88	118.30
1	E	430	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	313	ASP	CB-CG-OD2	6.01	123.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	540	ASP	CB-CG-OD2	5.97	123.68	118.30
1	E	699	LEU	O-C-N	-5.90	113.27	122.70
1	E	141	ASP	CB-CG-OD2	5.88	123.59	118.30
1	E	81	ASP	CB-CG-OD2	5.85	123.57	118.30
1	E	73	ASP	CB-CG-OD2	5.82	123.54	118.30
1	E	370	ASP	CB-CG-OD2	5.80	123.52	118.30
1	E	427	ASP	CB-CG-OD2	5.80	123.52	118.30
1	E	349	ASP	CB-CG-OD2	5.74	123.47	118.30
1	F	427	ASP	CB-CG-OD2	5.73	123.46	118.30
1	E	633	ASP	CB-CG-OD2	5.73	123.45	118.30
2	I	67	ASP	CB-CG-OD2	5.62	123.36	118.30
2	J	145	ASP	CB-CG-OD2	5.62	123.36	118.30
2	I	145	ASP	CB-CG-OD2	5.59	123.33	118.30
1	F	27	ASP	CB-CG-OD2	5.58	123.32	118.30
1	F	633	ASP	CB-CG-OD2	5.58	123.32	118.30
2	J	67	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	412	ASP	CB-CG-OD2	5.56	123.31	118.30
1	F	349	ASP	CB-CG-OD2	5.54	123.28	118.30
1	E	648	ASP	CB-CG-OD2	5.51	123.26	118.30
2	I	17	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	637	ASP	CB-CG-OD2	5.50	123.25	118.30
1	E	332	ASP	CB-CG-OD2	5.45	123.21	118.30
1	F	42	ASP	CB-CG-OD2	5.43	123.19	118.30
1	F	430	ASP	CB-CG-OD2	5.43	123.19	118.30
1	F	150	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	81	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	405	ASP	CB-CG-OD2	5.39	123.15	118.30
1	F	313	ASP	CB-CG-OD2	5.38	123.14	118.30
1	F	370	ASP	CB-CG-OD2	5.37	123.14	118.30
1	E	492	ASP	CB-CG-OD2	5.32	123.09	118.30
1	E	35	ASP	CB-CG-OD2	5.32	123.09	118.30
1	F	675	ASP	CB-CG-OD2	5.32	123.09	118.30
2	I	231	ASP	CB-CG-OD2	5.31	123.08	118.30
1	E	128	ASP	CB-CG-OD2	5.30	123.07	118.30
2	J	249	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	324	ASP	CB-CG-OD2	5.29	123.06	118.30
1	F	278	ASP	CB-CG-OD2	5.28	123.05	118.30
1	F	699	LEU	O-C-N	-5.27	114.27	122.70
1	E	15	ASP	CB-CG-OD2	5.25	123.03	118.30
1	F	185	ASP	CB-CG-OD2	5.24	123.02	118.30
1	E	42	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	496	LEU	CA-CB-CG	5.21	127.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	669	ASP	CB-CG-OD2	5.18	122.96	118.30
1	E	532	ASP	CB-CG-OD2	5.18	122.96	118.30
2	I	119	ASP	CB-CG-OD2	5.18	122.96	118.30
1	F	118	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	35	ASP	CB-CG-OD2	5.15	122.93	118.30
1	F	658	ASP	CB-CG-OD2	5.14	122.93	118.30
1	E	150	ASP	CB-CG-OD2	5.14	122.92	118.30
1	E	402	ASP	CB-CG-OD2	5.12	122.91	118.30
2	J	41	ASP	CB-CG-OD2	5.09	122.88	118.30
1	F	294	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	540	ASP	CB-CG-OD2	5.06	122.85	118.30
1	F	271	ASP	CB-CG-OD2	5.05	122.84	118.30
1	E	27	ASP	CB-CG-OD2	5.04	122.84	118.30
1	E	118	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	412	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	337	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	314	ASP	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	E	5389	0	5271	137	0
1	F	5465	0	5344	139	0
2	I	2343	0	2300	82	0
2	J	2255	0	2235	89	0
3	E	31	0	12	6	0
3	F	31	0	12	1	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	I	2	0	0	0	0
5	J	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15520	0	15174	433	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 14.

All (433) 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)
2:J:128:ASN:HD22	2:J:131:LEU:HB2	1.27	1.00
1:E:220:PRO:HB3	1:E:225:GLU:HA	1.53	0.89
1:F:363:TYR:HB3	1:F:364:PRO:HA	1.55	0.87
1:E:603:HIS:HB2	1:E:604:PRO:HD2	1.59	0.85
1:E:363:TYR:HB2	1:E:364:PRO:HA	1.57	0.84
1:F:589:THR:HB	1:F:593:SER:HB3	1.59	0.82
1:E:20:ASN:HD21	1:E:621:TYR:H	1.29	0.81
1:E:584:GLN:HB2	1:E:657:VAL:HG13	1.63	0.80
2:I:70:GLN:HG2	2:I:157:LEU:HD21	1.65	0.79
2:I:315:GLU:O	2:I:317:TRP:N	2.15	0.79
2:J:22:VAL:O	2:J:26:LEU:HB2	1.82	0.78
2:I:155:VAL:HG21	2:I:265:LEU:HD21	1.65	0.78
1:E:564:GLU:CD	1:E:564:GLU:H	1.89	0.75
1:F:363:TYR:CB	1:F:364:PRO:HA	2.15	0.74
2:I:185:ILE:HA	2:I:188:ILE:HD12	1.69	0.74
1:F:20:ASN:HD21	1:F:621:TYR:H	1.33	0.73
1:F:644:GLU:HG2	1:F:682:TYR:CE2	2.24	0.73
1:E:256:ALA:HB2	1:E:387:LEU:HD13	1.71	0.73
2:J:173:SER:HA	2:J:179:THR:HG22	1.70	0.72
1:F:540:ASP:O	1:F:541:ASP:HB2	1.89	0.71
1:E:201:SER:HB3	1:E:245:ALA:HB3	1.72	0.71
1:E:16:TYR:HE2	1:E:47:THR:HB	1.55	0.70
2:J:248:ASN:HA	2:J:251:LYS:HB2	1.73	0.70
2:I:151:LYS:O	2:I:155:VAL:HG23	1.92	0.69
1:E:256:ALA:HB2	1:E:387:LEU:CD1	2.23	0.69
2:J:158:GLU:OE2	2:J:195:HIS:HB3	1.93	0.69
1:E:133:VAL:HG22	1:E:167:CYS:HB2	1.75	0.68
2:J:128:ASN:ND2	2:J:131:LEU:HB2	2.07	0.68
2:J:22:VAL:HG21	2:J:198:TYR:CD1	2.30	0.67
1:F:509:SER:HA	1:F:512:LEU:HD12	1.77	0.67
1:E:262:HIS:ND1	1:E:307:ALA:O	2.26	0.66
2:I:31:TRP:CZ2	2:I:188:ILE:HG13	2.30	0.66
1:F:388:CYS:HA	1:F:692:TYR:CE2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:70:GLN:HA	2:I:74:GLY:HA3	1.75	0.66
1:E:379:ALA:HB2	1:E:525:GLN:HB3	1.76	0.66
2:J:60:PHE:HD1	2:J:63:LEU:HD12	1.61	0.66
2:J:155:VAL:HG11	2:J:265:LEU:HG	1.78	0.66
1:E:216:GLU:OE1	1:E:310:SER:HB2	1.97	0.65
2:J:31:TRP:HZ2	2:J:101:HIS:CD2	2.14	0.65
1:E:486:GLY:HA3	1:E:645:LYS:HG2	1.77	0.65
2:J:252:ALA:HB3	2:J:278:VAL:HG13	1.77	0.65
2:I:315:GLU:O	2:I:318:ASN:N	2.30	0.65
1:E:628:THR:H	1:E:631:ASN:HD21	1.44	0.64
1:F:278:ASP:HA	1:F:282:ARG:HD2	1.80	0.64
1:F:161:THR:HB	1:F:162:PRO:CD	2.28	0.64
1:E:16:TYR:CE2	1:E:47:THR:HB	2.33	0.63
2:I:227:MET:HA	2:I:227:MET:CE	2.28	0.63
1:E:639:TYR:CD2	1:E:666:PHE:HB3	2.33	0.63
1:F:491:LEU:HD11	1:F:648:ASP:HB3	1.81	0.62
1:F:414:SER:HB3	1:F:457:ILE:HG22	1.81	0.62
2:J:184:LEU:HA	2:J:187:LEU:HD12	1.81	0.62
2:J:154:SER:HB3	2:J:199:ILE:HG21	1.80	0.62
2:I:180:ASN:HA	2:I:183:ASP:HB2	1.81	0.62
2:I:75:ALA:N	2:I:76:PRO:HD2	2.14	0.62
2:J:104:SER:HB3	2:J:184:LEU:HD21	1.81	0.62
1:E:485:TYR:CE2	1:E:604:PRO:HD3	2.35	0.61
1:F:346:ASN:HB3	1:F:349:ASP:HB2	1.81	0.61
2:I:157:LEU:HA	2:I:161:LEU:HD12	1.82	0.61
1:E:229:SER:HB3	1:E:233:PRO:HG2	1.81	0.61
1:E:108:PHE:CZ	1:E:126:PHE:HA	2.36	0.61
1:E:50:ARG:N	1:E:51:PRO:HD2	2.15	0.61
1:F:586:VAL:HB	1:F:661:LEU:HG	1.82	0.61
2:J:138:ILE:HD13	2:J:161:LEU:HD11	1.83	0.61
2:J:187:LEU:HD23	2:J:190:ARG:HH12	1.66	0.61
1:E:673:THR:HG23	2:I:309:THR:HA	1.83	0.61
1:F:580:ASN:HB2	1:F:583:LEU:CD1	2.31	0.60
2:I:41:ASP:HB3	2:I:178:LEU:HD23	1.83	0.60
2:J:105:TYR:HA	2:J:108:ILE:HD12	1.83	0.60
2:J:227:MET:HA	2:J:230:TYR:HB2	1.84	0.60
1:F:644:GLU:HG2	1:F:682:TYR:HE2	1.66	0.60
2:I:310:VAL:HG22	2:I:311:GLU:H	1.67	0.60
1:E:215:ARG:NH1	1:E:220:PRO:O	2.35	0.59
1:F:229:SER:HB3	1:F:233:PRO:HG3	1.83	0.59
1:F:161:THR:HB	1:F:162:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:511:ARG:O	1:F:515:GLU:HG2	2.02	0.59
1:E:180:LEU:HD11	1:E:386:ASN:HB3	1.84	0.59
1:F:239:GLU:HG3	1:F:240:ASP:N	2.17	0.59
1:F:441:GLY:O	1:F:445:VAL:HG23	2.01	0.59
1:E:176:VAL:HG11	1:E:416:ASN:HA	1.83	0.59
1:E:404:LEU:HD11	1:F:195:ASN:HD21	1.67	0.59
1:E:512:LEU:HA	1:E:515:GLU:HG3	1.84	0.59
1:F:420:LEU:HD13	1:F:469:LEU:HD11	1.85	0.59
1:E:177:SER:O	1:E:178:CYS:CB	2.50	0.58
1:E:421:ASN:HB3	1:E:424:HIS:HB2	1.85	0.58
1:F:399:ARG:HB2	1:F:408:HIS:HB3	1.86	0.58
2:I:23:TRP:O	2:I:27:THR:OG1	2.19	0.57
2:I:31:TRP:HZ2	2:I:188:ILE:HG13	1.69	0.57
2:J:197:TYR:HD1	2:J:197:TYR:O	1.86	0.57
2:J:227:MET:HA	2:J:230:TYR:CB	2.34	0.57
2:J:241:TYR:O	2:J:247:VAL:HG22	2.04	0.57
2:I:115:THR:HA	2:I:118:VAL:HB	1.87	0.57
1:E:192:ARG:HG2	1:E:404:LEU:HD23	1.86	0.57
1:F:418:GLY:HA3	1:F:442:LEU:HD21	1.86	0.57
1:E:497:TYR:O	1:E:500:THR:HG22	2.05	0.56
2:J:75:ALA:HA	2:J:78:LEU:HD12	1.87	0.56
1:F:201:SER:OG	1:F:253:GLY:HA2	2.04	0.56
2:J:158:GLU:HA	2:J:162:PHE:HD2	1.70	0.56
1:F:221:ILE:HD12	1:F:227:GLN:HB3	1.87	0.56
2:J:151:LYS:HB3	2:J:203:TYR:HD1	1.71	0.56
1:F:584:GLN:O	1:F:659:GLN:HB2	2.05	0.56
2:J:159:SER:HA	2:J:163:TYR:HE1	1.69	0.56
1:E:665:LEU:HB2	1:E:694:ILE:HG22	1.88	0.55
2:J:63:LEU:HD23	2:J:66:LEU:HD12	1.88	0.55
1:E:594:TYR:N	1:E:594:TYR:CD2	2.74	0.55
1:E:509:SER:OG	1:E:580:ASN:ND2	2.35	0.55
2:J:201:TYR:CE2	2:J:205:ILE:HD11	2.42	0.55
1:E:358:GLN:HG3	1:E:364:PRO:HD2	1.89	0.55
2:J:48:LEU:HB2	2:J:53:GLN:HG3	1.89	0.55
1:E:390:GLU:HG2	1:E:588:PRO:HD3	1.89	0.55
1:F:628:THR:H	1:F:631:ASN:HD21	1.54	0.55
1:F:216:GLU:HB3	1:F:264:PRO:HG2	1.89	0.55
1:F:299:LEU:HD23	1:F:306:MET:HA	1.87	0.55
1:F:592:ILE:HA	1:F:595:ILE:HD12	1.87	0.55
2:J:55:LEU:O	2:J:55:LEU:HG	2.06	0.55
1:F:292:ILE:HD12	1:F:366:ILE:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:242:ALA:O	2:I:243:GLU:HB2	2.06	0.55
1:E:518:LYS:HD2	1:E:579:TYR:HE1	1.73	0.54
1:E:601:SER:HB3	1:E:603:HIS:CD2	2.42	0.54
2:I:128:ASN:HD22	2:I:131:LEU:HB3	1.71	0.54
2:J:138:ILE:HG13	2:J:153:ALA:HB1	1.90	0.54
1:F:45:PHE:HA	1:F:49:VAL:HB	1.88	0.54
2:J:272:PRO:HB2	2:J:273:PRO:HD2	1.89	0.54
1:E:180:LEU:HB2	1:E:413:ILE:HB	1.90	0.54
1:E:377:PRO:HA	1:E:527:ARG:HD2	1.88	0.54
1:E:603:HIS:HB3	1:E:650:TYR:HE1	1.73	0.54
2:J:71:ASN:ND2	2:J:72:ILE:HG13	2.22	0.54
1:F:303:ASN:HD22	1:F:348:ARG:HH11	1.56	0.54
1:F:26:TYR:HD1	1:F:30:GLY:CA	2.21	0.53
2:I:312:THR:HG22	2:I:313:GLU:N	2.23	0.53
2:J:18:LYS:O	2:J:22:VAL:HG23	2.08	0.53
1:E:177:SER:O	1:E:178:CYS:HB3	2.07	0.53
2:I:25:ARG:HG3	2:I:29:ASN:HD21	1.72	0.53
2:J:283:LEU:O	2:J:286:LEU:HB2	2.09	0.53
1:E:612:ARG:O	1:E:619:ARG:HA	2.08	0.53
1:F:16:TYR:CD2	1:F:44:PHE:HA	2.43	0.53
2:J:142:TYR:OH	2:J:157:LEU:HD23	2.08	0.53
2:J:188:ILE:O	2:J:192:GLU:HG2	2.09	0.53
3:F:1700:DGT:O5'	3:F:1700:DGT:H8	2.08	0.53
2:I:134:LYS:O	2:I:138:ILE:HG12	2.09	0.53
2:J:164:SER:HB2	2:J:236:TYR:HE2	1.73	0.53
2:J:248:ASN:HA	2:J:251:LYS:HD2	1.91	0.53
1:E:306:MET:HB2	1:E:345:ILE:HG13	1.91	0.53
3:E:1700:DGT:H8	3:E:1700:DGT:O5'	2.08	0.52
1:E:469:LEU:H	1:E:584:GLN:HA	1.75	0.52
1:F:156:ARG:HD3	1:F:428:SER:HB2	1.92	0.52
1:E:58:SER:O	1:E:61:GLU:HG2	2.10	0.52
1:E:586:VAL:HB	1:E:661:LEU:HG	1.91	0.52
2:J:202:LYS:HA	2:J:205:ILE:HD12	1.92	0.52
1:F:281:ILE:O	1:F:281:ILE:HG23	2.10	0.52
2:J:87:GLU:HG3	2:J:198:TYR:OH	2.10	0.52
2:J:158:GLU:HA	2:J:162:PHE:CD2	2.45	0.52
2:J:129:PRO:HA	2:J:132:GLN:HB2	1.91	0.52
1:F:277:ALA:O	1:F:278:ASP:HB2	2.09	0.52
2:J:41:ASP:HB3	2:J:178:LEU:HD23	1.91	0.52
1:E:215:ARG:NH2	3:E:1700:DGT:O3G	2.43	0.52
1:F:592:ILE:C	1:F:594:TYR:H	2.13	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:78:LEU:HA	2:I:81:ASP:OD2	2.09	0.51
1:E:639:TYR:HD2	1:E:666:PHE:HB3	1.75	0.51
2:J:197:TYR:CD1	2:J:197:TYR:C	2.83	0.51
1:E:220:PRO:HG2	1:E:312:TYR:CE2	2.45	0.51
1:E:19:LEU:HB3	1:E:40:ALA:HB2	1.92	0.51
1:F:216:GLU:HG2	1:F:219:ALA:HB2	1.92	0.51
1:F:275:GLU:HA	1:F:282:ARG:HH22	1.76	0.51
1:F:309:PHE:HZ	1:F:331:TYR:CD1	2.28	0.51
1:F:365:TYR:O	1:F:366:ILE:HG13	2.11	0.51
2:I:94:ILE:O	2:I:98:GLU:HG2	2.11	0.51
1:F:260:HIS:O	1:F:266:ILE:HD13	2.11	0.51
1:E:534:PHE:CE1	1:E:570:ARG:HA	2.46	0.51
1:E:221:ILE:HG21	3:E:1700:DGT:C8	2.40	0.50
1:F:401:ASP:OD1	1:F:402:ASP:N	2.44	0.50
2:J:226:LEU:O	2:J:230:TYR:HB2	2.11	0.50
1:E:348:ARG:HD3	2:I:312:THR:HB	1.93	0.50
1:F:478:LEU:HD22	1:F:483:ILE:HG21	1.93	0.50
1:E:27:ASP:CG	1:E:28:LYS:H	2.15	0.50
1:E:192:ARG:HG3	1:E:400:TYR:CE1	2.47	0.50
1:E:268:ARG:HA	1:E:271:ASP:HB2	1.94	0.50
1:E:616:LYS:HE3	2:I:43:PRO:HB3	1.92	0.50
1:F:260:HIS:HE1	1:F:293:PRO:HG3	1.75	0.50
2:J:164:SER:HB2	2:J:236:TYR:CE2	2.46	0.50
1:F:216:GLU:OE1	1:F:310:SER:HB2	2.10	0.50
1:F:280:LYS:O	1:F:281:ILE:HG22	2.11	0.50
2:I:162:PHE:HB3	2:I:166:PHE:CE2	2.46	0.50
1:E:221:ILE:HD11	1:E:228:SER:HA	1.93	0.50
1:F:386:ASN:ND2	1:F:388:CYS:H	2.09	0.50
1:E:573:VAL:C	1:E:575:ARG:H	2.15	0.50
1:E:363:TYR:HB2	1:E:364:PRO:CA	2.36	0.50
1:F:416:ASN:ND2	1:F:446:SER:HB2	2.27	0.50
2:I:163:TYR:HA	2:I:166:PHE:HB2	1.92	0.50
2:J:230:TYR:O	2:J:234:ILE:HG12	2.11	0.49
1:E:299:LEU:HG	1:E:305:GLN:O	2.12	0.49
2:I:104:SER:HB3	2:I:184:LEU:HD11	1.95	0.49
2:I:149:LYS:HA	2:I:152:ILE:HD12	1.94	0.49
2:I:70:GLN:HG2	2:I:157:LEU:CD2	2.40	0.49
2:I:105:TYR:HA	2:I:108:ILE:HD12	1.95	0.49
2:I:128:ASN:HD22	2:I:131:LEU:CB	2.26	0.49
2:I:204:GLN:O	2:I:208:GLN:HG3	2.13	0.49
2:I:56:THR:HG22	2:I:60:PHE:CE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:513:ALA:HB2	1:F:579:TYR:N	2.28	0.48
2:I:230:TYR:CE1	2:I:234:ILE:HD11	2.48	0.48
1:F:221:ILE:O	1:F:224:ILE:HG12	2.13	0.48
2:J:22:VAL:HG12	2:J:90:VAL:HG11	1.95	0.48
1:E:594:TYR:H	1:E:594:TYR:HD2	1.61	0.48
2:I:88:GLU:HA	2:I:91:LEU:HD12	1.95	0.48
2:I:164:SER:HB3	2:I:254:LEU:HD21	1.95	0.48
2:I:98:GLU:O	2:I:101:HIS:HB2	2.14	0.48
1:E:84:PHE:HA	1:E:87:ARG:HB2	1.96	0.48
2:I:68:THR:HG22	2:I:72:ILE:HD11	1.95	0.48
2:I:200:GLY:O	2:I:203:TYR:HB3	2.13	0.48
1:E:20:ASN:ND2	1:E:621:TYR:H	2.05	0.48
1:E:479:ALA:HB1	1:E:634:MET:HB3	1.94	0.48
1:F:147:GLN:HG3	1:F:437:THR:OG1	2.14	0.48
1:F:186:ASN:OD1	1:F:188:GLU:HB2	2.13	0.48
2:I:18:LYS:HD2	2:I:201:TYR:CE2	2.49	0.48
2:J:179:THR:O	2:J:183:ASP:N	2.45	0.48
1:E:185:ASP:O	3:E:1700:DGT:H5'A	2.13	0.47
1:F:363:TYR:CB	1:F:364:PRO:CA	2.90	0.47
1:E:647:ILE:HG23	1:E:688:ILE:HD11	1.95	0.47
1:F:196:SER:O	1:F:200:LEU:HB2	2.15	0.47
1:F:246:ASN:OD1	1:F:253:GLY:HA3	2.13	0.47
2:I:48:LEU:HD11	2:I:178:LEU:HD11	1.96	0.47
2:J:114:GLN:O	2:J:118:VAL:HG23	2.14	0.47
2:I:15:GLN:H	2:I:86:HIS:CE1	2.32	0.47
2:J:246:TRP:O	2:J:250:VAL:HG23	2.13	0.47
1:F:103:LEU:HD22	1:F:622:TYR:HB2	1.95	0.47
1:F:231:VAL:C	1:F:233:PRO:HD2	2.34	0.47
2:J:31:TRP:CZ2	2:J:101:HIS:CD2	2.99	0.47
1:E:303:ASN:HD22	1:E:348:ARG:CZ	2.27	0.47
1:E:494:THR:HG21	1:E:649:THR:HG23	1.97	0.47
2:I:41:ASP:OD2	2:I:181:THR:N	2.48	0.47
2:I:60:PHE:HD1	2:I:63:LEU:HD12	1.78	0.47
1:E:56:PHE:CG	1:E:62:ARG:HG3	2.50	0.47
1:E:314:ILE:HG21	1:E:325:ILE:HD11	1.96	0.47
1:F:589:THR:CB	1:F:593:SER:HB3	2.38	0.47
2:J:124:TRP:HH2	2:J:236:TYR:HE1	1.63	0.47
2:J:138:ILE:HD13	2:J:161:LEU:CD1	2.45	0.47
1:E:181:LEU:CD1	1:E:209:PHE:CE2	2.98	0.46
1:E:499:TYR:HE2	1:E:561:PRO:HD2	1.79	0.46
2:J:164:SER:CB	2:J:236:TYR:HE2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:503:TRP:HD1	1:E:566:TRP:CE2	2.33	0.46
1:F:509:SER:OG	1:F:580:ASN:ND2	2.48	0.46
1:F:383:ASN:OD1	1:F:383:ASN:N	2.47	0.46
1:F:514:ARG:HD2	1:F:576:TYR:CD1	2.50	0.46
1:E:185:ASP:OD2	1:E:215:ARG:HG2	2.15	0.46
1:E:674:ARG:H	2:I:310:VAL:CG1	2.29	0.46
1:F:362:GLY:O	1:F:693:TYR:HB2	2.16	0.46
2:I:253:PHE:O	2:I:257:ASN:ND2	2.47	0.46
1:E:215:ARG:HH21	3:E:1700:DGT:H5'	1.81	0.46
2:J:149:LYS:HG2	2:J:221:PHE:CZ	2.51	0.46
1:E:300:ALA:HB1	2:I:317:TRP:CH2	2.50	0.46
1:F:209:PHE:HB2	1:F:257:VAL:HG12	1.98	0.46
1:F:275:GLU:HA	1:F:282:ARG:NH2	2.31	0.46
2:I:121:ALA:O	2:I:124:TRP:HE3	1.98	0.46
2:I:13:LYS:HE3	2:I:13:LYS:HB3	1.81	0.46
1:F:303:ASN:ND2	1:F:348:ARG:HD2	2.31	0.46
2:I:18:LYS:HA	2:I:21:GLU:HG3	1.98	0.46
1:F:499:TYR:CE1	1:F:542:TRP:CD2	3.04	0.46
2:I:124:TRP:HZ2	2:I:240:LEU:HD11	1.81	0.46
1:F:448:MET:HA	1:F:450:HIS:CE1	2.50	0.45
2:I:63:LEU:HA	2:I:66:LEU:HD12	1.97	0.45
1:F:26:TYR:HB3	1:F:30:GLY:HA2	1.97	0.45
2:I:223:LEU:O	2:I:227:MET:HG2	2.17	0.45
2:I:227:MET:HA	2:I:227:MET:HE1	1.98	0.45
2:J:67:ASP:HB3	2:J:98:GLU:O	2.15	0.45
1:E:232:ILE:O	1:E:235:MET:HB2	2.16	0.45
1:F:368:PHE:HD2	1:F:688:ILE:O	1.99	0.45
2:I:122:TYR:OH	2:J:9:ILE:O	2.33	0.45
1:E:125:HIS:O	1:E:128:ASP:HB2	2.17	0.45
1:E:208:ALA:HA	1:E:256:ALA:O	2.17	0.45
1:F:306:MET:HG3	1:F:347:ALA:HB2	1.99	0.45
2:J:217:GLU:O	2:J:221:PHE:HB3	2.16	0.45
1:E:439:ILE:HD11	1:E:469:LEU:HD22	1.98	0.45
1:F:292:ILE:HG23	1:F:296:THR:HB	1.98	0.45
1:F:473:ASN:HA	1:F:599:THR:H	1.82	0.45
1:F:695:ARG:HG3	1:F:696:LEU:N	2.32	0.45
1:E:435:VAL:HG11	1:E:504:HIS:HB3	1.99	0.45
1:E:489:GLU:HB3	1:E:546:THR:HG21	1.98	0.45
1:F:108:PHE:CZ	1:F:126:PHE:HA	2.52	0.45
1:F:232:ILE:N	1:F:233:PRO:HD2	2.32	0.45
2:I:11:TRP:CD1	2:J:103:ARG:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:67:ASP:O	2:J:71:ASN:HB3	2.17	0.45
1:E:222:LYS:O	1:E:224:ILE:HG22	2.17	0.45
1:F:393:GLN:HG2	1:F:582:ASN:ND2	2.32	0.45
2:I:42:ILE:HB	2:I:43:PRO:HD3	1.98	0.45
1:F:220:PRO:HB3	1:F:225:GLU:HA	1.97	0.44
2:I:146:GLU:HA	2:I:147:PRO:HD3	1.82	0.44
2:J:63:LEU:HB3	2:J:105:TYR:CZ	2.52	0.44
1:E:368:PHE:O	1:E:372:VAL:HG23	2.17	0.44
1:E:556:SER:HB3	1:E:558:ILE:HD13	1.99	0.44
2:J:31:TRP:HZ2	2:J:101:HIS:HD2	1.63	0.44
2:J:38:LEU:HB2	2:J:111:THR:HG21	1.99	0.44
1:E:542:TRP:HA	1:E:542:TRP:CE3	2.53	0.44
1:E:673:THR:CG2	2:I:309:THR:HA	2.47	0.44
2:J:164:SER:HB3	2:J:233:GLU:OE2	2.18	0.44
1:E:70:GLY:O	1:E:117:PHE:HZ	1.99	0.44
1:E:125:HIS:H	1:E:128:ASP:HB2	1.82	0.44
1:E:295:ILE:HG13	1:E:295:ILE:O	2.16	0.44
1:E:402:ASP:O	1:F:453:SER:HA	2.17	0.44
2:J:147:PRO:HG2	2:J:148:LEU:HD23	1.99	0.44
1:E:261:ALA:HA	1:E:266:ILE:HD13	2.00	0.44
2:I:31:TRP:CZ3	2:I:184:LEU:HD12	2.53	0.44
1:F:38:GLN:HA	1:F:41:ILE:HD12	2.00	0.44
1:F:224:ILE:O	1:F:224:ILE:HG13	2.18	0.44
1:E:491:LEU:HA	1:E:494:THR:HG23	1.99	0.44
1:F:61:GLU:O	1:F:65:THR:N	2.51	0.44
2:I:237:THR:HG21	2:I:250:VAL:HB	2.00	0.44
1:E:199:GLN:OE1	1:F:187:MET:HG3	2.18	0.43
1:F:269:PHE:O	1:F:272:THR:HG23	2.18	0.43
2:I:15:GLN:OE1	2:I:85:PRO:HD2	2.18	0.43
2:J:197:TYR:O	2:J:197:TYR:CD1	2.70	0.43
2:J:169:PRO:HA	2:J:172:PHE:HB2	1.99	0.43
1:E:50:ARG:N	1:E:51:PRO:CD	2.81	0.43
1:E:499:TYR:CE2	1:E:561:PRO:HD2	2.53	0.43
1:F:585:ALA:HB2	1:F:659:GLN:HB2	2.00	0.43
1:F:160:ALA:O	1:F:161:THR:C	2.56	0.43
1:F:212:SER:HA	1:F:259:LEU:HD12	2.00	0.43
2:I:249:ASP:OD1	2:I:249:ASP:N	2.51	0.43
1:F:422:ILE:HG12	1:F:497:TYR:CZ	2.53	0.43
2:I:79:MET:HA	2:I:91:LEU:HD13	2.00	0.43
1:E:21:ALA:HB3	2:I:176:GLY:HA3	2.01	0.43
1:F:216:GLU:O	1:F:228:SER:OG	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:GLU:O	1:F:304:ALA:N	2.51	0.43
1:F:307:ALA:HB3	1:F:331:TYR:CE1	2.54	0.43
2:J:168:LEU:N	2:J:169:PRO:HD2	2.33	0.43
1:E:262:HIS:HA	1:E:308:LEU:HD23	2.01	0.42
1:E:346:ASN:HB3	1:E:349:ASP:HB2	2.01	0.42
2:J:60:PHE:HA	2:J:63:LEU:HD12	2.01	0.42
1:E:141:ASP:HB3	1:E:144:LEU:HB3	2.00	0.42
1:E:540:ASP:O	1:E:541:ASP:HB3	2.19	0.42
1:F:24:ASN:HD22	1:F:24:ASN:HA	1.54	0.42
1:F:210:LEU:HD13	1:F:384:MET:HB3	2.01	0.42
2:J:160:PHE:CZ	2:J:230:TYR:HA	2.54	0.42
2:J:192:GLU:HA	2:J:195:HIS:HB2	2.01	0.42
1:E:299:LEU:HD21	1:E:331:TYR:OH	2.19	0.42
1:F:309:PHE:HB2	1:F:314:ILE:HD11	2.00	0.42
1:F:358:GLN:NE2	1:F:364:PRO:O	2.52	0.42
1:F:528:TYR:CD1	1:F:578:ILE:HD11	2.54	0.42
2:J:218:LEU:HA	2:J:221:PHE:HD2	1.84	0.42
1:F:26:TYR:HD1	1:F:30:GLY:HA2	1.84	0.42
1:F:562:THR:OG1	1:F:565:MET:HG3	2.20	0.42
2:I:11:TRP:HB2	2:J:106:SER:HB3	2.01	0.42
2:J:109:PHE:HA	2:J:113:CYS:HB2	2.00	0.42
1:F:337:ASP:OD1	1:F:339:HIS:HB2	2.18	0.42
2:I:84:THR:HA	2:I:85:PRO:HD2	1.77	0.42
2:J:18:LYS:HA	2:J:18:LYS:HD3	1.82	0.42
2:J:31:TRP:CZ2	2:J:101:HIS:HD2	2.37	0.42
1:E:180:LEU:HD21	1:E:385:SER:C	2.40	0.42
1:F:179:PHE:HB2	1:F:207:VAL:HG22	2.02	0.42
1:F:262:HIS:CE1	1:F:306:MET:HG2	2.55	0.42
1:E:157:PHE:CE2	1:E:159:PRO:HG3	2.55	0.42
1:E:175:LEU:HD12	1:E:175:LEU:HA	1.85	0.42
1:E:196:SER:O	1:E:200:LEU:HB2	2.20	0.42
1:F:422:ILE:HG12	1:F:497:TYR:CE2	2.54	0.42
1:E:101:THR:HG21	1:E:622:TYR:CE1	2.55	0.42
2:I:315:GLU:O	2:I:316:ASP:C	2.58	0.42
2:J:62:GLY:O	2:J:66:LEU:HG	2.20	0.42
2:J:139:LEU:O	2:J:143:VAL:HG22	2.20	0.42
1:E:681:ILE:HD11	2:I:317:TRP:CZ3	2.55	0.42
1:F:181:LEU:CD1	1:F:196:SER:HB3	2.50	0.42
1:F:138:ALA:C	1:F:140:GLY:H	2.23	0.41
1:F:141:ASP:HB3	1:F:144:LEU:HB3	2.02	0.41
1:F:474:LEU:HD22	1:F:478:LEU:HG	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:592:ILE:C	1:F:594:TYR:N	2.74	0.41
1:F:622:TYR:HA	1:F:623:PRO:HD3	1.89	0.41
2:I:75:ALA:HA	2:I:78:LEU:HD12	2.02	0.41
2:I:134:LYS:HA	2:I:137:ILE:HD12	2.02	0.41
1:E:109:TYR:O	1:E:113:THR:HG22	2.20	0.41
1:E:182:ARG:NH1	1:E:395:ASN:OD1	2.52	0.41
1:E:386:ASN:ND2	1:E:388:CYS:H	2.18	0.41
1:F:378:ILE:HG22	1:F:379:ALA:N	2.35	0.41
1:F:628:THR:H	1:F:631:ASN:ND2	2.18	0.41
1:E:309:PHE:CE2	1:E:334:LEU:HB3	2.55	0.41
1:E:663:LEU:HD23	1:E:688:ILE:HG21	2.01	0.41
1:F:642:GLY:O	1:F:644:GLU:N	2.54	0.41
1:E:235:MET:O	1:E:236:LYS:C	2.58	0.41
1:E:348:ARG:HE	1:E:348:ARG:HB2	1.73	0.41
1:E:603:HIS:HB3	1:E:650:TYR:CE1	2.54	0.41
1:F:23:LEU:HD11	1:F:623:PRO:HG3	2.02	0.41
1:F:125:HIS:O	1:F:126:PHE:C	2.59	0.41
1:F:388:CYS:O	1:F:662:SER:OG	2.28	0.41
1:F:592:ILE:HD13	1:F:592:ILE:H	1.84	0.41
2:I:128:ASN:HA	2:I:129:PRO:HD2	1.95	0.41
2:J:67:ASP:HB2	2:J:102:ALA:HB2	2.02	0.41
1:E:210:LEU:HD13	1:E:384:MET:HB3	2.02	0.41
1:E:268:ARG:H	1:E:268:ARG:HG3	1.60	0.41
1:E:337:ASP:OD1	1:E:338:PRO:HD2	2.20	0.41
1:F:672:THR:O	1:F:676:ILE:HD12	2.21	0.41
2:I:128:ASN:ND2	2:I:130:PRO:HD2	2.36	0.41
1:F:278:ASP:H	1:F:282:ARG:HD2	1.86	0.41
1:F:650:TYR:O	1:F:654:THR:OG1	2.37	0.41
2:J:124:TRP:O	2:J:128:ASN:HB2	2.20	0.41
2:J:155:VAL:HG23	2:J:199:ILE:HG22	2.03	0.41
1:F:498:PHE:CB	1:F:656:HIS:HD2	2.33	0.41
1:E:263:HIS:HA	1:E:264:PRO:HD3	1.91	0.41
1:E:523:PHE:C	1:E:525:GLN:H	2.23	0.41
1:F:498:PHE:HB2	1:F:656:HIS:HD2	1.86	0.41
1:F:642:GLY:HA2	1:F:643:PRO:HD2	1.74	0.41
1:E:201:SER:HB3	1:E:245:ALA:CB	2.48	0.41
1:E:376:ASN:ND2	1:E:378:ILE:O	2.50	0.41
1:E:613:LYS:HA	1:E:618:GLY:O	2.21	0.41
1:F:369:GLU:O	1:F:373:ASN:ND2	2.54	0.41
2:I:88:GLU:H	2:I:88:GLU:HG2	1.61	0.41
2:I:280:PRO:HA	2:I:283:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:ASP:HB3	1:E:340:VAL:HA	2.02	0.41
1:F:357:ILE:HG22	1:F:363:TYR:O	2.21	0.41
1:F:385:SER:OG	1:F:389:SER:HA	2.21	0.41
2:I:26:LEU:HD21	2:I:195:HIS:HE2	1.84	0.41
2:J:72:ILE:O	2:J:76:PRO:HG2	2.21	0.41
2:J:146:GLU:HA	2:J:147:PRO:HD3	1.98	0.41
1:E:382:ILE:HG13	1:E:394:VAL:HG13	2.03	0.40
1:E:523:PHE:O	1:E:525:GLN:N	2.54	0.40
1:F:358:GLN:HA	1:F:363:TYR:O	2.21	0.40
2:J:53:GLN:O	2:J:56:THR:HB	2.21	0.40
2:J:227:MET:HA	2:J:230:TYR:HB3	2.03	0.40
2:I:26:LEU:HD22	2:I:93:ASN:OD1	2.22	0.40
2:J:58:ARG:HG2	2:J:124:TRP:CE3	2.56	0.40
1:E:81:ASP:O	1:E:84:PHE:N	2.52	0.40
1:E:198:LEU:HD23	1:F:191:GLY:HA2	2.02	0.40
1:E:215:ARG:NH2	3:E:1700:DGT:H5'	2.36	0.40
1:E:265:ASP:O	1:E:267:LEU:N	2.55	0.40
1:F:50:ARG:N	1:F:51:PRO:CD	2.84	0.40
1:F:388:CYS:HA	1:F:692:TYR:HE2	1.82	0.40
1:F:401:ASP:HB3	1:F:403:ASN:OD1	2.22	0.40
2:J:22:VAL:HG12	2:J:26:LEU:HD12	2.03	0.40
1:E:348:ARG:NE	2:I:317:TRP:HE1	2.18	0.40
1:F:195:ASN:O	1:F:199:GLN:HG2	2.21	0.40
1:F:302:GLU:C	1:F:304:ALA:H	2.24	0.40
1:F:366:ILE:HB	1:F:691:LEU:HB2	2.03	0.40
1:F:414:SER:HB3	1:F:457:ILE:CG2	2.48	0.40
1:F:672:THR:H	1:F:675:ASP:HB2	1.85	0.40
2:I:254:LEU:O	2:I:258:ALA:N	2.54	0.40
2:J:36:VAL:HA	2:J:37:PRO:HD3	1.95	0.40
1:E:13:THR:O	1:E:14:MET:HG2	2.21	0.40
1:F:200:LEU:HD12	1:F:200:LEU:HA	1.85	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	E	670/714 (94%)	579 (86%)	78 (12%)	13 (2%)	8 40
1	F	681/714 (95%)	585 (86%)	79 (12%)	17 (2%)	5 35
2	I	290/319 (91%)	261 (90%)	23 (8%)	6 (2%)	7 39
2	J	279/319 (88%)	251 (90%)	25 (9%)	3 (1%)	14 51
All	All	1920/2066 (93%)	1676 (87%)	205 (11%)	39 (2%)	7 40

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	178	CYS
1	E	331	TYR
1	E	600	SER
1	F	13	THR
1	F	541	ASP
2	I	310	VAL
2	I	315	GLU
2	I	316	ASP
1	E	226	ASN
1	E	266	ILE
1	F	303	ASN
1	F	490	ALA
1	E	13	THR
1	E	369	GLU
1	E	574	MET
1	E	597	HIS
1	F	12	GLU
1	F	62	ARG
1	F	226	ASN
1	F	429	PRO
1	F	593	SER
1	F	161	THR
1	F	277	ALA
1	F	322	PHE
1	F	600	SER
1	F	692	TYR
2	I	318	ASN
1	E	590	GLY
1	E	524	ALA
1	F	601	SER

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Mol	Chain	Res	Type
2	I	243	GLU
2	J	29	ASN
2	J	109	PHE
1	E	253	GLY
1	F	643	PRO
2	I	189	ILE
2	J	278	VAL
1	E	602	ILE
1	F	30	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	E	565/596 (95%)	442 (78%)	123 (22%)	1 6
1	F	573/596 (96%)	446 (78%)	127 (22%)	1 6
2	I	248/275 (90%)	195 (79%)	53 (21%)	1 6
2	J	241/275 (88%)	174 (72%)	67 (28%)	0 3
All	All	1627/1742 (93%)	1257 (77%)	370 (23%)	1 5

All (370) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	12	GLU
1	E	13	THR
1	E	19	LEU
1	E	24	ASN
1	E	28	LYS
1	E	45	PHE
1	E	54	VAL
1	E	55	THR
1	E	58	SER
1	E	61	GLU
1	E	62	ARG
1	E	68	ARG

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Mol	Chain	Res	Type
1	E	77	LEU
1	E	86	LEU
1	E	99	PHE
1	E	101	THR
1	E	107	LYS
1	E	111	SER
1	E	114	LEU
1	E	115	LYS
1	E	121	ARG
1	E	127	GLU
1	E	131	THR
1	E	132	MET
1	E	143	THR
1	E	146	THR
1	E	149	THR
1	E	170	GLN
1	E	172	ARG
1	E	175	LEU
1	E	181	LEU
1	E	184	GLU
1	E	198	LEU
1	E	200	LEU
1	E	202	LYS
1	E	222	LYS
1	E	223	ARG
1	E	224	ILE
1	E	225	GLU
1	E	227	GLN
1	E	229	SER
1	E	231	VAL
1	E	232	ILE
1	E	234	VAL
1	E	239	GLU
1	E	243	SER
1	E	252	GLN
1	E	267	LEU
1	E	268	ARG
1	E	270	LEU
1	E	271	ASP
1	E	274	ARG
1	E	283	ILE
1	E	298	ARG

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Mol	Chain	Res	Type
1	E	299	LEU
1	E	310	SER
1	E	317	ARG
1	E	325	ILE
1	E	328	SER
1	E	330	ARG
1	E	335	ILE
1	E	341	ARG
1	E	348	ARG
1	E	352	GLN
1	E	353	THR
1	E	360	GLU
1	E	361	SER
1	E	381	ARG
1	E	384	MET
1	E	389	SER
1	E	390	GLU
1	E	394	VAL
1	E	398	SER
1	E	407	THR
1	E	415	CYS
1	E	428	SER
1	E	440	ARG
1	E	442	LEU
1	E	446	SER
1	E	449	SER
1	E	451	ILE
1	E	453	SER
1	E	457	ILE
1	E	474	LEU
1	E	481	GLU
1	E	489	GLU
1	E	494	THR
1	E	496	LEU
1	E	511	ARG
1	E	515	GLU
1	E	518	LYS
1	E	525	GLN
1	E	532	ASP
1	E	535	THR
1	E	548	LYS
1	E	560	LEU

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Mol	Chain	Res	Type
1	E	564	GLU
1	E	567	LEU
1	E	570	ARG
1	E	583	LEU
1	E	591	SER
1	E	592	ILE
1	E	593	SER
1	E	594	TYR
1	E	595	ILE
1	E	597	HIS
1	E	605	ILE
1	E	606	VAL
1	E	609	ILE
1	E	617	THR
1	E	631	ASN
1	E	633	ASP
1	E	654	THR
1	E	655	ARG
1	E	661	LEU
1	E	662	SER
1	E	664	THR
1	E	678	LYS
1	E	685	ARG
1	E	692	TYR
1	E	693	TYR
1	E	697	ARG
1	E	698	GLN
1	F	15	ASP
1	F	23	LEU
1	F	24	ASN
1	F	27	ASP
1	F	36	LYS
1	F	38	GLN
1	F	39	GLN
1	F	79	ARG
1	F	80	TYR
1	F	82	ARG
1	F	90	GLU
1	F	114	LEU
1	F	115	LYS
1	F	118	ASP
1	F	136	THR

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Mol	Chain	Res	Type
1	F	143	THR
1	F	146	THR
1	F	164	PHE
1	F	165	LEU
1	F	167	CYS
1	F	172	ARG
1	F	175	LEU
1	F	177	SER
1	F	178	CYS
1	F	183	ILE
1	F	184	GLU
1	F	194	VAL
1	F	200	LEU
1	F	202	LYS
1	F	203	ARG
1	F	212	SER
1	F	227	GLN
1	F	229	SER
1	F	236	LYS
1	F	237	MET
1	F	239	GLU
1	F	243	SER
1	F	265	ASP
1	F	268	ARG
1	F	270	LEU
1	F	271	ASP
1	F	274	ARG
1	F	275	GLU
1	F	276	ASN
1	F	283	ILE
1	F	308	LEU
1	F	317	ARG
1	F	325	ILE
1	F	328	SER
1	F	330	ARG
1	F	333	GLU
1	F	342	LYS
1	F	345	ILE
1	F	353	THR
1	F	358	GLN
1	F	361	SER
1	F	363	TYR

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Mol	Chain	Res	Type
1	F	381	ARG
1	F	384	MET
1	F	385	SER
1	F	390	GLU
1	F	394	VAL
1	F	400	TYR
1	F	407	THR
1	F	409	ILE
1	F	414	SER
1	F	415	CYS
1	F	417	LEU
1	F	440	ARG
1	F	443	THR
1	F	450	HIS
1	F	452	ARG
1	F	474	LEU
1	F	489	GLU
1	F	491	LEU
1	F	494	THR
1	F	501	ILE
1	F	509	SER
1	F	514	ARG
1	F	515	GLU
1	F	518	LYS
1	F	527	ARG
1	F	530	SER
1	F	536	GLN
1	F	538	LEU
1	F	539	GLN
1	F	546	THR
1	F	548	LYS
1	F	555	ARG
1	F	563	ARG
1	F	567	LEU
1	F	568	LYS
1	F	570	ARG
1	F	574	MET
1	F	583	LEU
1	F	584	GLN
1	F	589	THR
1	F	592	ILE
1	F	593	SER

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Mol	Chain	Res	Type
1	F	597	HIS
1	F	601	SER
1	F	606	VAL
1	F	613	LYS
1	F	617	THR
1	F	619	ARG
1	F	630	GLU
1	F	631	ASN
1	F	632	LEU
1	F	633	ASP
1	F	636	GLN
1	F	640	ASP
1	F	649	THR
1	F	654	THR
1	F	655	ARG
1	F	661	LEU
1	F	662	SER
1	F	664	THR
1	F	678	LYS
1	F	680	GLN
1	F	681	ILE
1	F	691	LEU
1	F	692	TYR
1	F	693	TYR
1	F	695	ARG
1	F	696	LEU
1	F	698	GLN
1	F	699	LEU
2	I	7	SER
2	I	13	LYS
2	I	14	ILE
2	I	17	ASP
2	I	18	LYS
2	I	21	GLU
2	I	25	ARG
2	I	26	LEU
2	I	29	ASN
2	I	30	PHE
2	I	35	LYS
2	I	39	SER
2	I	40	ASN
2	I	49	SER

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Mol	Chain	Res	Type
2	I	54	GLN
2	I	59	VAL
2	I	72	ILE
2	I	79	MET
2	I	81	ASP
2	I	83	ILE
2	I	86	HIS
2	I	88	GLU
2	I	95	SER
2	I	97	MET
2	I	103	ARG
2	I	107	SER
2	I	110	SER
2	I	114	GLN
2	I	115	THR
2	I	122	TYR
2	I	124	TRP
2	I	127	GLU
2	I	134	LYS
2	I	138	ILE
2	I	139	LEU
2	I	150	LYS
2	I	154	SER
2	I	159	SER
2	I	170	MET
2	I	179	THR
2	I	183	ASP
2	I	184	LEU
2	I	187	LEU
2	I	189	ILE
2	I	190	ARG
2	I	208	GLN
2	I	213	ILE
2	I	233	GLU
2	I	240	LEU
2	I	247	VAL
2	I	249	ASP
2	I	260	LYS
2	I	286	LEU
2	J	7	SER
2	J	13	LYS
2	J	15	GLN

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Mol	Chain	Res	Type
2	J	18	LYS
2	J	26	LEU
2	J	28	SER
2	J	34	GLU
2	J	35	LYS
2	J	39	SER
2	J	46	GLN
2	J	54	GLN
2	J	55	LEU
2	J	56	THR
2	J	57	ILE
2	J	59	VAL
2	J	69	ILE
2	J	70	GLN
2	J	71	ASN
2	J	77	SER
2	J	79	MET
2	J	83	ILE
2	J	86	HIS
2	J	92	SER
2	J	96	PHE
2	J	97	MET
2	J	100	VAL
2	J	103	ARG
2	J	106	SER
2	J	107	SER
2	J	111	THR
2	J	112	LEU
2	J	115	THR
2	J	126	GLU
2	J	127	GLU
2	J	131	LEU
2	J	134	LYS
2	J	136	GLN
2	J	139	LEU
2	J	148	LEU
2	J	150	LYS
2	J	151	LYS
2	J	152	ILE
2	J	154	SER
2	J	159	SER
2	J	178	LEU

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Mol	Chain	Res	Type
2	J	189	ILE
2	J	192	GLU
2	J	197	TYR
2	J	209	LYS
2	J	214	GLU
2	J	216	GLU
2	J	220	LEU
2	J	221	PHE
2	J	223	LEU
2	J	229	LEU
2	J	232	ASN
2	J	243	GLU
2	J	246	TRP
2	J	247	VAL
2	J	251	LYS
2	J	257	ASN
2	J	263	MET
2	J	264	ASN
2	J	278	VAL
2	J	279	ASN
2	J	282	ILE
2	J	283	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	ASN
1	E	38	GLN
1	E	39	GLN
1	E	171	GLN
1	E	195	ASN
1	E	252	GLN
1	E	303	ASN
1	E	346	ASN
1	E	507	HIS
1	E	580	ASN
1	E	597	HIS
1	E	631	ASN
1	F	20	ASN
1	F	24	ASN
1	F	31	HIS
1	F	52	HIS

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Mol	Chain	Res	Type
1	F	125	HIS
1	F	158	GLN
1	F	195	ASN
1	F	199	GLN
1	F	252	GLN
1	F	303	ASN
1	F	346	ASN
1	F	450	HIS
1	F	507	HIS
1	F	580	ASN
1	F	581	GLN
1	F	582	ASN
2	I	29	ASN
2	I	53	GLN
2	I	71	ASN
2	I	86	HIS
2	I	128	ASN
2	I	208	GLN
2	I	232	ASN
2	I	264	ASN
2	J	29	ASN
2	J	53	GLN
2	J	54	GLN
2	J	70	GLN
2	J	71	ASN
2	J	101	HIS
2	J	128	ASN
2	J	180	ASN
2	J	259	ASN
2	J	264	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	DGT	E	1700	4	26,33,33	1.38	4 (15%)	32,52,52	1.47	5 (15%)
3	DGT	F	1700	4	26,33,33	1.39	4 (15%)	32,52,52	1.46	5 (15%)

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
3	DGT	E	1700	4	-	0/18/34/34	0/3/3/3
3	DGT	F	1700	4	-	0/18/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1700	DGT	C4-N3	3.01	1.44	1.37
3	F	1700	DGT	C4-N3	3.00	1.44	1.37
3	E	1700	DGT	PG-O3G	2.77	1.59	1.50
3	F	1700	DGT	PG-O3G	2.69	1.59	1.50
3	E	1700	DGT	C6-N1	-2.61	1.34	1.37
3	F	1700	DGT	C6-N1	-2.60	1.34	1.37
3	F	1700	DGT	PB-O2B	2.55	1.59	1.50
3	E	1700	DGT	PB-O2B	2.42	1.59	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	1700	DGT	C5-C6-N1	4.14	121.27	113.95
3	E	1700	DGT	PB-O3B-PG	-4.07	118.86	132.83
3	E	1700	DGT	C5-C6-N1	3.91	120.86	113.95
3	F	1700	DGT	PB-O3B-PG	-3.61	120.43	132.83
3	F	1700	DGT	O6-C6-C5	-2.98	118.56	124.37
3	F	1700	DGT	PA-O3A-PB	-2.49	124.27	132.83
3	E	1700	DGT	O6-C6-C5	-2.42	119.64	124.37
3	F	1700	DGT	C3'-C2'-C1'	2.19	108.01	102.54
3	E	1700	DGT	C2'-C3'-C4'	2.04	107.01	102.76
3	E	1700	DGT	C3'-C2'-C1'	2.02	107.58	102.54

There are no chirality outliers.

There are no torsion outliers.

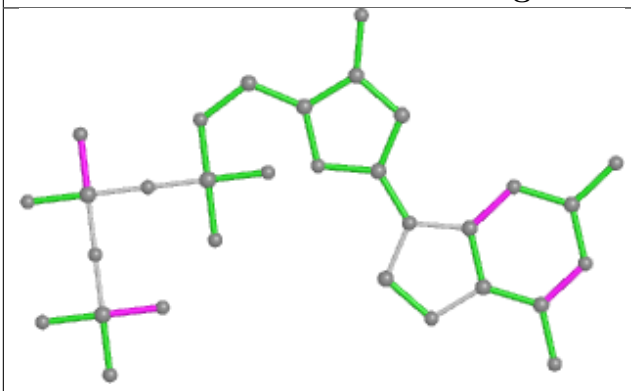
There are no ring outliers.

2 monomers are involved in 7 short contacts:

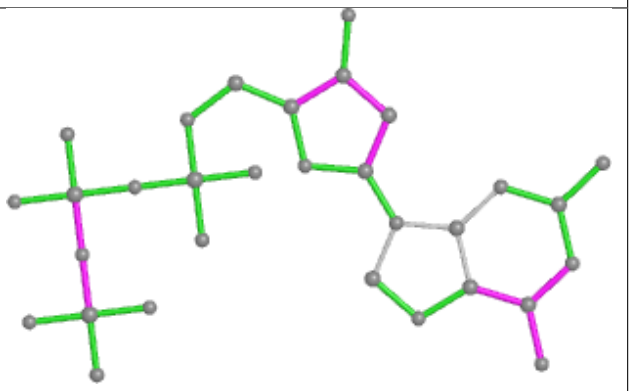
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1700	DGT	6	0
3	F	1700	DGT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

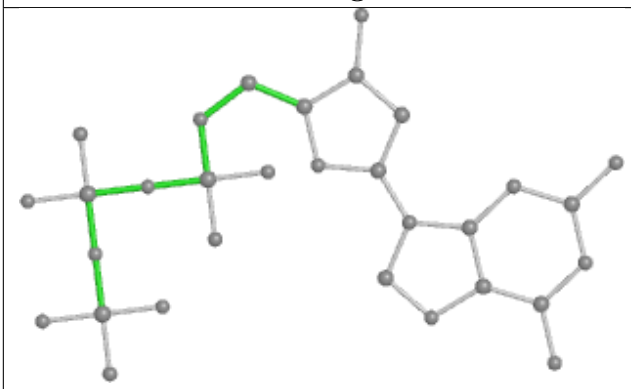
Ligand DGT E 1700



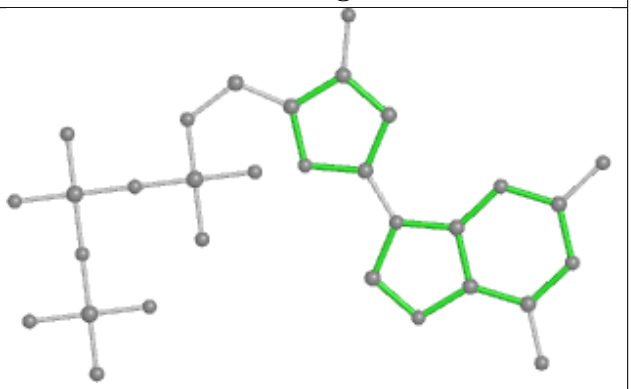
Bond lengths



Bond angles

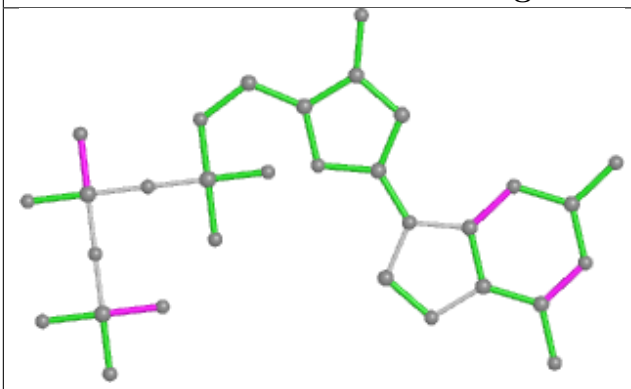


Torsions

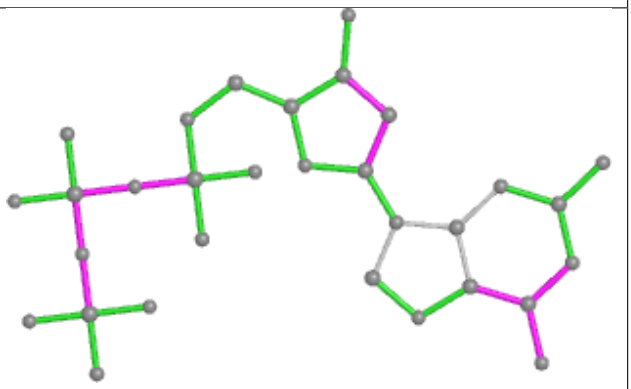


Rings

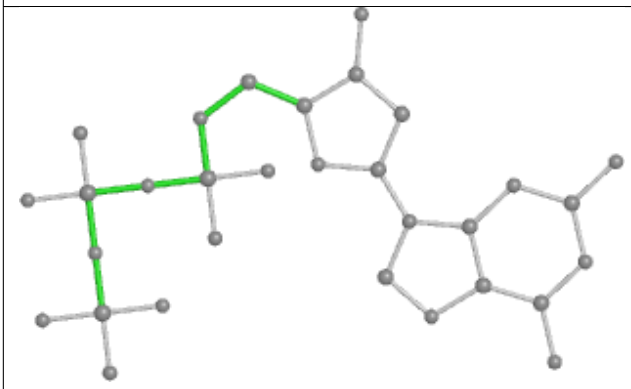
Ligand DGT F 1700



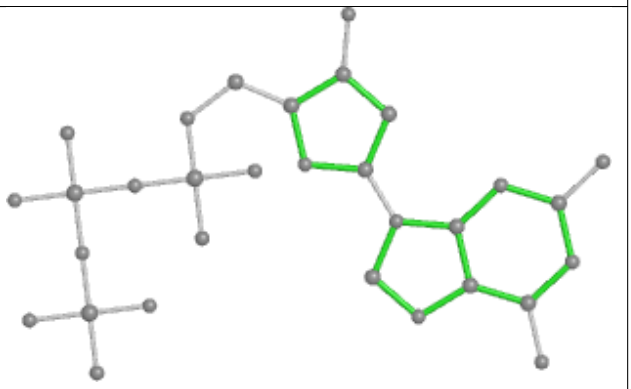
Bond lengths



Bond angles



Torsions



Rings

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	E	676/714 (94%)	-0.38	4 (0%)	89	84	38, 57, 71, 89	0
1	F	685/714 (95%)	-0.36	9 (1%)	77	68	40, 62, 81, 100	0
2	I	294/319 (92%)	-0.54	1 (0%)	94	90	8, 65, 84, 90	0
2	J	281/319 (88%)	0.25	10 (3%)	42	34	69, 91, 103, 105	0
All	All	1936/2066 (93%)	-0.30	24 (1%)	79	70	8, 62, 95, 105	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	700	ALA	3.3
2	J	119	ASP	3.0
2	J	45	TRP	2.9
2	J	176	GLY	2.6
1	E	699	LEU	2.6
1	F	698	GLN	2.6
2	J	246	TRP	2.5
1	E	662	SER	2.5
2	J	14	ILE	2.4
1	F	309	PHE	2.4
1	F	278	ASP	2.4
2	J	57	ILE	2.3
1	F	29	ALA	2.3
2	J	276	ALA	2.3
2	I	145	ASP	2.2
1	E	30	GLY	2.2
1	F	360	GLU	2.2
1	F	361	SER	2.2
2	J	206	ALA	2.1
1	F	359	PHE	2.1
2	J	171	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	28	LYS	2.1
1	F	252	GLN	2.1
2	J	208	GLN	2.1

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)

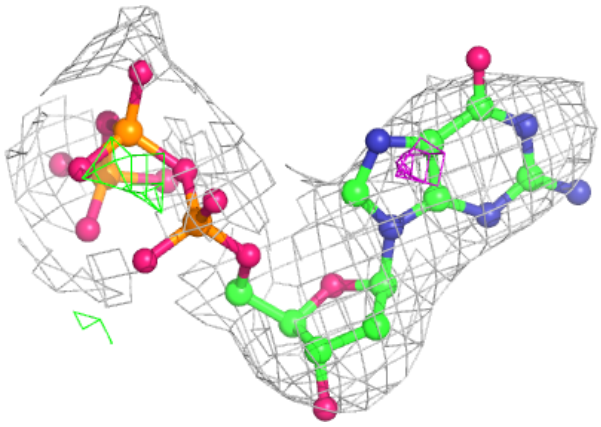
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

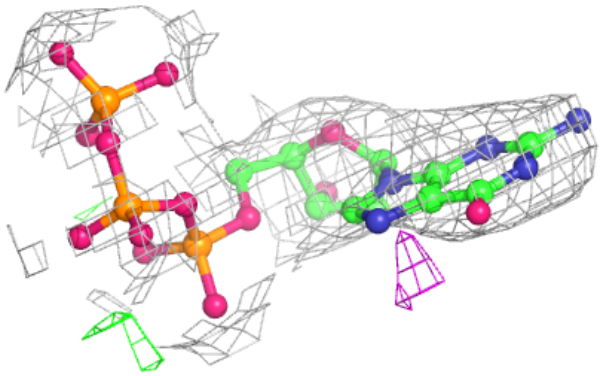
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DGT	F	1700	31/31	0.94	0.19	43,44,51,51	1
3	DGT	E	1700	31/31	0.95	0.20	29,35,40,41	1
5	FE	J	1287	1/1	0.95	0.10	59,59,59,59	1
5	FE	I	1320	1/1	0.97	0.07	47,47,47,47	0
5	FE	J	1288	1/1	0.97	0.05	68,68,68,68	0
4	MG	E	1701	1/1	0.98	0.14	12,12,12,12	0
4	MG	F	1701	1/1	0.99	0.22	33,33,33,33	0
5	FE	I	1321	1/1	0.99	0.07	41,41,41,41	0

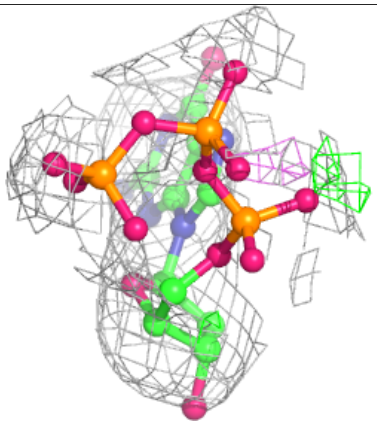
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DGT F 1700:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

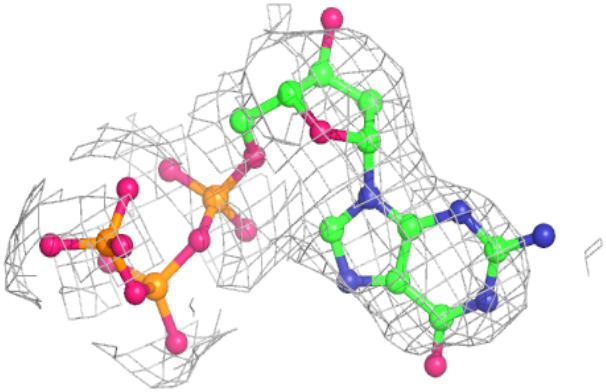


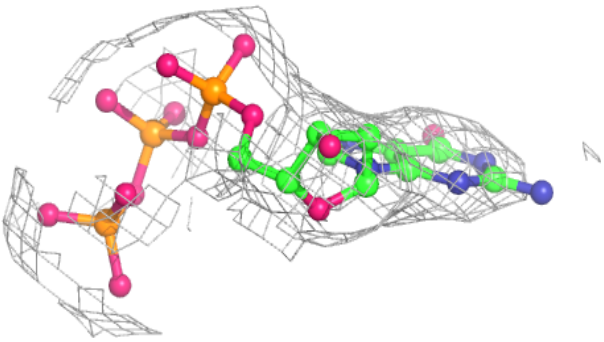


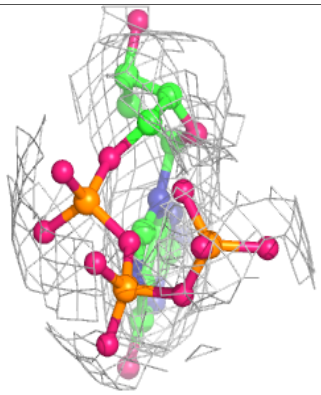


Electron density around DGT E 1700:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.