



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:08 PM UTC

PDB ID : 2BQ1 / pdb_00002bq1
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

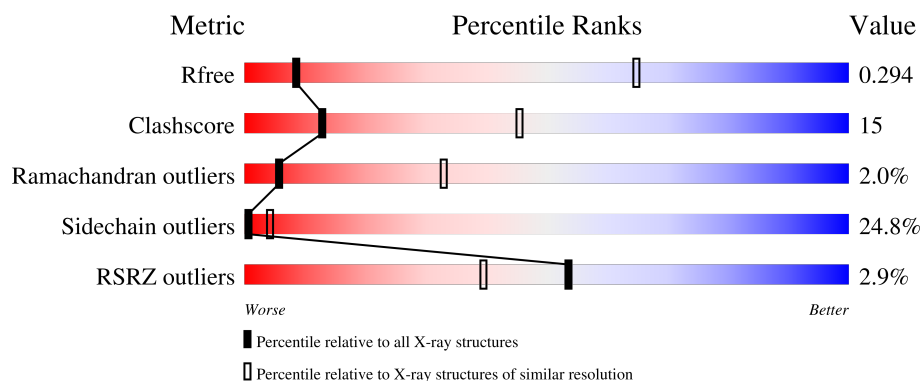
1 Overall quality at a glance

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}	180053	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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 $\leq 5\%$. 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	10% 52% 35% 7% 5%
1	F	714	2% 52% 37% 7% •
2	I	319	47% 35% 9% • 8%
2	J	319	10% 38% 41% 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.

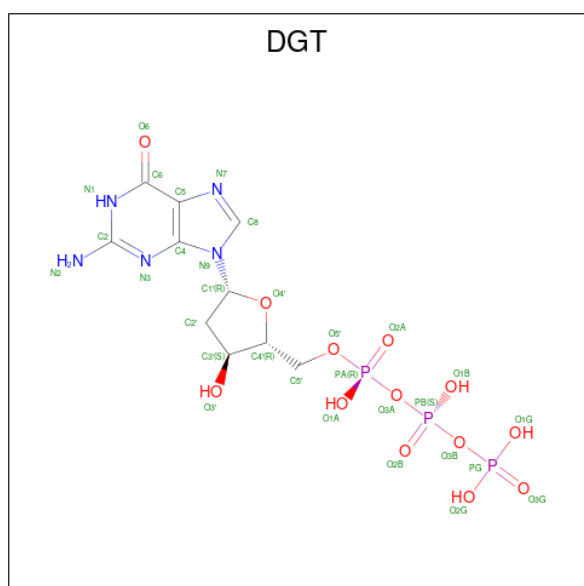
- Molecule 1 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 ALPHA SUBUNIT.

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

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

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

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



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

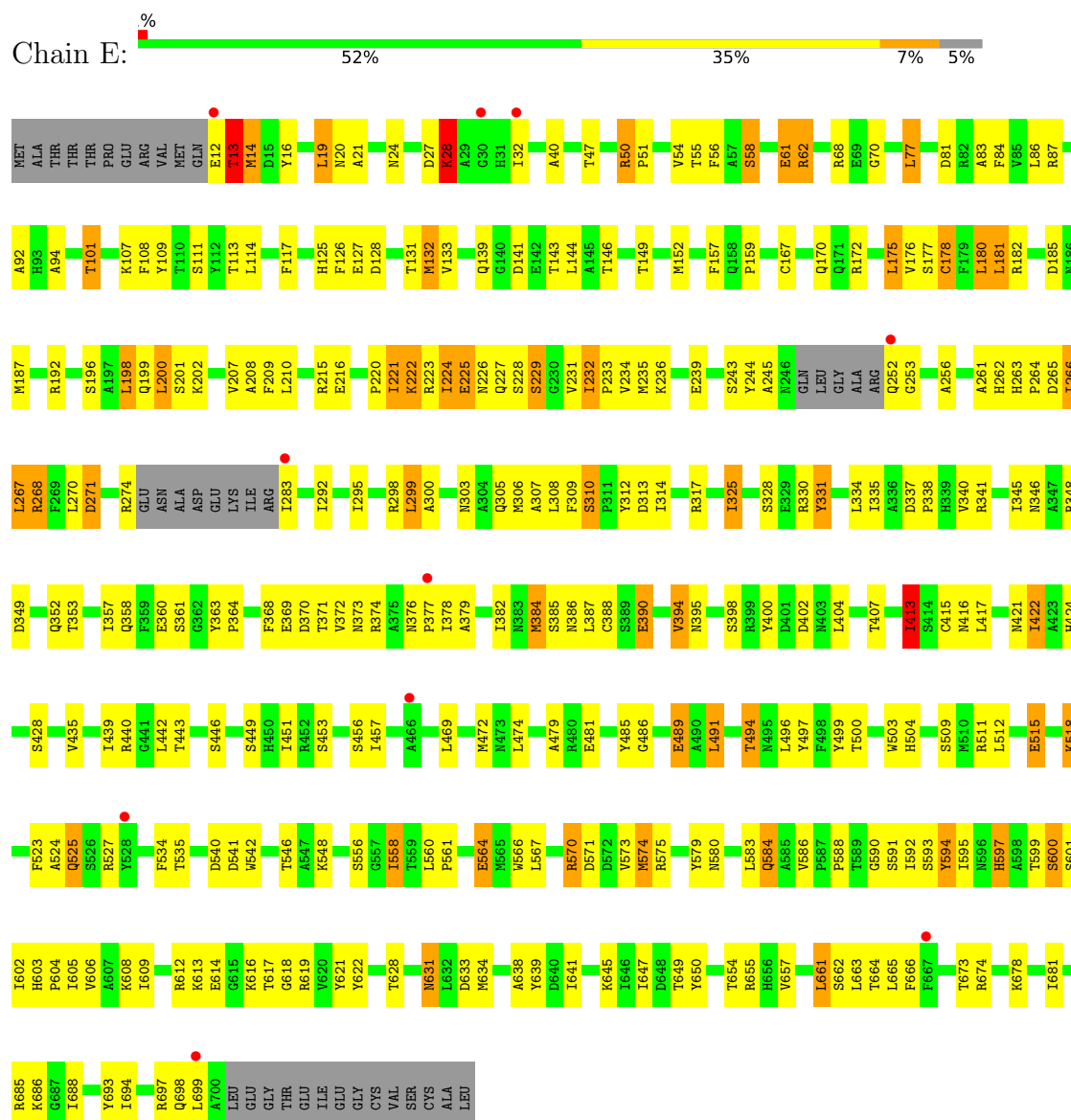
- Molecule 5 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

3 Residue-property plots

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.

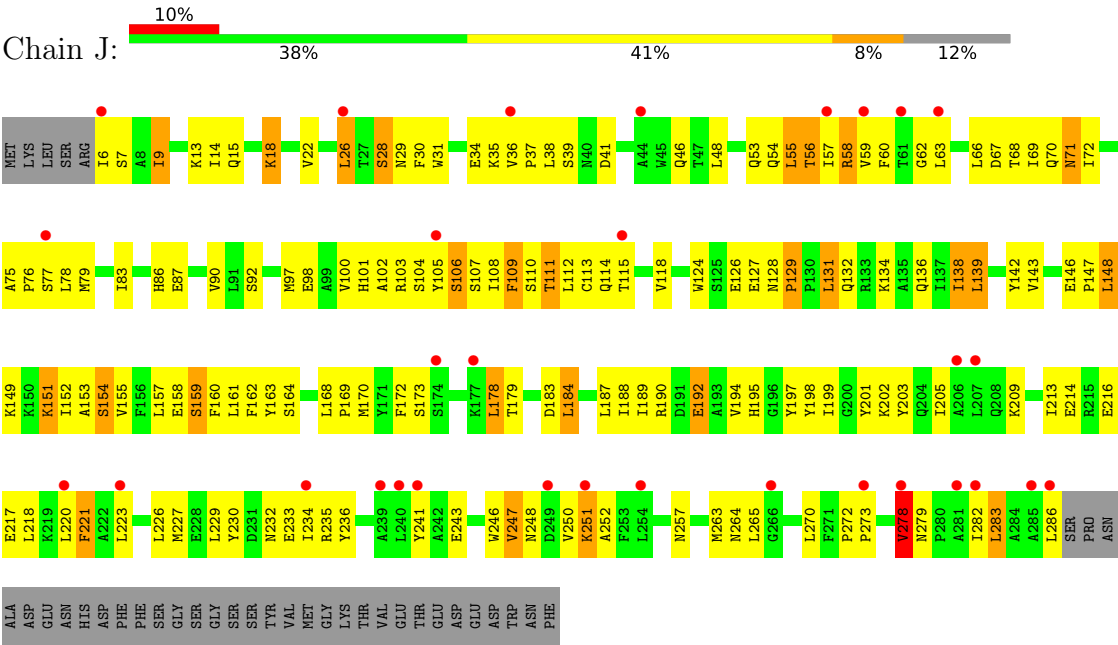
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 ALPHA SUBUNIT



• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 ALPHA SUBUNIT



● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 2 BETA SUBUNIT



4 Data and refinement statistics

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 – 3.99 182.57 – 3.99	Depositor EDS
% Data completeness (in resolution range)	99.7 (182.57-3.99) 99.7 (182.57-3.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.29 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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, FE, MG

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	0.45	1/5513 (0.0%)	0.89	4/7465 (0.1%)
1	F	0.46	2/5590 (0.0%)	0.89	1/7569 (0.0%)
2	I	0.49	0/2401	0.96	2/3273 (0.1%)
2	J	0.58	0/2310	0.97	1/3146 (0.0%)
All	All	0.48	3/15814 (0.0%)	0.92	8/21453 (0.0%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	699	LEU	C-N	-6.77	1.23	1.33
1	E	699	LEU	C-N	-6.42	1.24	1.33
1	F	281	ILE	CA-CB	5.02	1.61	1.54

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	315	GLU	N-CA-C	-8.52	92.64	110.80
1	E	292	ILE	N-CA-C	6.88	114.36	107.55
2	I	129	PRO	N-CA-C	6.21	118.27	110.70
1	E	699	LEU	O-C-N	-6.08	113.27	123.00
2	J	129	PRO	N-CA-C	5.95	117.96	110.70
1	E	28	LYS	N-CA-C	5.62	118.13	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	413	ILE	N-CA-C	5.61	115.96	108.11
1	F	699	LEU	O-C-N	-5.46	114.27	123.00

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 ⓘ

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	154	0
1	F	5465	0	5344	150	0
2	I	2343	0	2300	85	0
2	J	2255	0	2235	92	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
All	All	15520	0	15174	464	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 15.

All (464) 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
2:I:227:MET:HE2	2:I:227:MET:HA	1.49	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:564:GLU:CD	1:E:564:GLU:H	1.89	0.78
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: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:608:LYS:HG2	1:F:627:MET:HE1	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:227:MET:HA	2:I:227:MET:CE	2.28	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
1:F:592:ILE:C	1:F:594:TYR:H	2.13	0.56
2:J:151:LYS:HB3	2:J:203:TYR:HD1	1.71	0.56
2:J:197:TYR:CD1	2:J:197:TYR:C	2.83	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:77:LEU:HD21	1:E:132:MET:HE1	1.88	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:E:27:ASP:CG	1:E:28:LYS:H	2.15	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
2:I:242:ALA:O	2:I:243:GLU:HB2	2.06	0.55
1:E:573:VAL:C	1:E:575:ARG:H	2.15	0.54
1:E:133:VAL:HB	1:E:152:MET:HE1	1.88	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:244:TYR:CE1	1:F:187:MET:HE1	2.43	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
1:F:231:VAL:C	1:F:233:PRO:HD2	2.34	0.52
2:J:129:PRO:HA	2:J:132:GLN:HB2	1.91	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:277:ALA:O	1:F:278:ASP:HB2	2.09	0.51
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
1:E:220:PRO:HG2	1:E:312:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
1:E:187:MET:HE1	1:F:244:TYR:CE1	2.47	0.49
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
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:E:198:LEU:HD21	1:F:237:MET:HE1	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:160:ALA:O	1:F:161:THR:C	2.56	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
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
1:F:138:ALA:C	1:F:140:GLY:H	2.23	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:180:LEU:HD21	1:E:385:SER:C	2.40	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:I:315:GLU:O	2:I:316:ASP:C	2.58	0.46
2:J:164:SER:CB	2:J:236:TYR:HE2	2.28	0.46
1:E:503:TRP:HD1	1:E:566:TRP:CE2	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:509:SER:OG	1:F:580:ASN:ND2	2.48	0.46
1:F:592:ILE:C	1:F:594:TYR:N	2.74	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
1:E:235:MET:O	1:E:236:LYS:C	2.58	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: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:302:GLU:C	1:F:304:ALA:H	2.24	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:E:523:PHE:C	1:E:525:GLN:H	2.23	0.45
1:F:108:PHE:CZ	1:F:126:PHE:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:E:499:TYR:C	1:E:499:TYR:CD2	2.95	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
1:F:125:HIS:O	1:F:126:PHE:C	2.59	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
1:E:523:PHE:C	1:E:525:GLN:N	2.76	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
1:F:58:SER:C	1:F:60:HIS:N	2.75	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
1:E:373:ASN:O	1:E:374:ARG:C	2.61	0.43
1:E:27:ASP:CG	1:E:28:LYS:N	2.76	0.43
2:J:197:TYR:O	2:J:197:TYR:CD1	2.70	0.43
1:E:599:THR:O	1:E:600:SER:C	2.61	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:499:TYR:CE2	1:E:561:PRO:HD2	2.53	0.43
1:F:426:MET:HE2	1:F:493:PHE:HE1	1.84	0.43
1:F:585:ALA:HB2	1:F:659:GLN:HB2	2.00	0.43
2:I:246:TRP:O	2:I:247:VAL:C	2.61	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:E:92:ALA:C	1:E:94:ALA:H	2.27	0.43
1:F:216:GLU:O	1:F:228:SER:OG	2.37	0.43
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
1:F:502:THR:O	1:F:503:TRP:C	2.60	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:132:MET:O	1:F:133:VAL:C	2.63	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
2:J:108:ILE:C	2:J:110:SER:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:490:ALA:O	1:F:491:LEU:C	2.63	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
2:J:28:SER:C	2:J:30:PHE:H	2.28	0.42
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
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
2:I:188:ILE:O	2:I:189:ILE:C	2.62	0.41
1:E:348:ARG:HE	1:E:348:ARG:HB2	1.73	0.41
1:E:370:ASP:O	1:E:371:THR:C	2.62	0.41
1:E:421:ASN:O	1:E:422:ILE:C	2.63	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: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
2:J:169:PRO:HG2	2:J:170:MET:HE2	2.02	0.41
1:F:278:ASP:H	1:F:282:ARG:HD2	1.86	0.41
1:F:487:SER:O	1:F:488:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:81:ASP:C	1:E:83:ALA:N	2.77	0.41
1:F:368:PHE:O	1:F:369:GLU:C	2.63	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:638:ALA:O	1:E:639:TYR:C	2.62	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:44:ALA:O	2:I:47:THR:OG1	2.38	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
1:E:313:ASP:HB3	1:E:340:VAL:HA	2.02	0.41
1:E:613:LYS:C	1:E:614:GLU:HG2	2.46	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:E:346:ASN:HD22	1:E:349:ASP:CG	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:ASN:O	1:F:199:GLN:HG2	2.21	0.40
1:F:235:MET:HE2	1:F:283:ILE:HD13	2.04	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%)	6	34
1	F	681/714 (95%)	585 (86%)	79 (12%)	17 (2%)	4	29
2	I	290/319 (91%)	261 (90%)	23 (8%)	6 (2%)	5	32
2	J	279/319 (88%)	251 (90%)	25 (9%)	3 (1%)	11	44
All	All	1920/2066 (93%)	1676 (87%)	205 (11%)	39 (2%)	6	33

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	430 (76%)	135 (24%)	1	5
1	F	573/596 (96%)	438 (76%)	135 (24%)	1	5
2	I	248/275 (90%)	188 (76%)	60 (24%)	1	5
2	J	241/275 (88%)	168 (70%)	73 (30%)	0	3
All	All	1627/1742 (93%)	1224 (75%)	403 (25%)	1	4

All (403) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	12	GLU
1	E	13	THR
1	E	14	MET
1	E	19	LEU
1	E	24	ASN
1	E	28	LYS
1	E	32	ILE
1	E	50	ARG
1	E	54	VAL
1	E	55	THR
1	E	58	SER
1	E	61	GLU
1	E	62	ARG
1	E	68	ARG
1	E	77	LEU
1	E	86	LEU
1	E	101	THR
1	E	107	LYS
1	E	111	SER
1	E	114	LEU
1	E	127	GLU
1	E	131	THR
1	E	132	MET
1	E	139	GLN
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	180	LEU
1	E	181	LEU
1	E	198	LEU

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Mol	Chain	Res	Type
1	E	200	LEU
1	E	202	LYS
1	E	207	VAL
1	E	221	ILE
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
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	352	GLN
1	E	353	THR
1	E	357	ILE
1	E	360	GLU
1	E	361	SER
1	E	384	MET
1	E	390	GLU
1	E	394	VAL
1	E	398	SER
1	E	407	THR
1	E	413	ILE

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Mol	Chain	Res	Type
1	E	415	CYS
1	E	417	LEU
1	E	422	ILE
1	E	428	SER
1	E	440	ARG
1	E	442	LEU
1	E	443	THR
1	E	446	SER
1	E	449	SER
1	E	451	ILE
1	E	453	SER
1	E	456	SER
1	E	457	ILE
1	E	472	MET
1	E	474	LEU
1	E	481	GLU
1	E	489	GLU
1	E	491	LEU
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	535	THR
1	E	548	LYS
1	E	558	ILE
1	E	560	LEU
1	E	564	GLU
1	E	567	LEU
1	E	570	ARG
1	E	571	ASP
1	E	574	MET
1	E	583	LEU
1	E	584	GLN
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

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Mol	Chain	Res	Type
1	E	606	VAL
1	E	608	LYS
1	E	609	ILE
1	E	617	THR
1	E	631	ASN
1	E	633	ASP
1	E	641	ILE
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	686	LYS
1	E	693	TYR
1	E	697	ARG
1	E	698	GLN
1	F	12	GLU
1	F	15	ASP
1	F	23	LEU
1	F	24	ASN
1	F	27	ASP
1	F	36	LYS
1	F	39	GLN
1	F	50	ARG
1	F	76	VAL
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	127	GLU
1	F	136	THR
1	F	142	GLU
1	F	143	THR
1	F	146	THR
1	F	153	LEU
1	F	164	PHE
1	F	165	LEU

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Mol	Chain	Res	Type
1	F	167	CYS
1	F	172	ARG
1	F	175	LEU
1	F	178	CYS
1	F	183	ILE
1	F	184	GLU
1	F	194	VAL
1	F	198	LEU
1	F	200	LEU
1	F	202	LYS
1	F	212	SER
1	F	227	GLN
1	F	229	SER
1	F	232	ILE
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	284	LYS
1	F	288	LEU
1	F	295	ILE
1	F	308	LEU
1	F	317	ARG
1	F	320	LYS
1	F	325	ILE
1	F	328	SER
1	F	329	GLU
1	F	330	ARG
1	F	333	GLU
1	F	345	ILE
1	F	353	THR
1	F	357	ILE
1	F	358	GLN
1	F	361	SER
1	F	363	TYR

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Mol	Chain	Res	Type
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	413	ILE
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	491	LEU
1	F	494	THR
1	F	501	ILE
1	F	509	SER
1	F	511	ARG
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	558	ILE
1	F	563	ARG
1	F	567	LEU
1	F	568	LYS
1	F	574	MET
1	F	583	LEU
1	F	584	GLN
1	F	589	THR
1	F	592	ILE
1	F	593	SER
1	F	597	HIS

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Mol	Chain	Res	Type
1	F	601	SER
1	F	606	VAL
1	F	613	LYS
1	F	617	THR
1	F	619	ARG
1	F	627	MET
1	F	630	GLU
1	F	631	ASN
1	F	632	LEU
1	F	633	ASP
1	F	636	GLN
1	F	649	THR
1	F	654	THR
1	F	655	ARG
1	F	661	LEU
1	F	664	THR
1	F	678	LYS
1	F	680	GLN
1	F	681	ILE
1	F	689	LYS
1	F	691	LEU
1	F	693	TYR
1	F	694	ILE
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	49	SER
2	I	53	GLN
2	I	54	GLN

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Mol	Chain	Res	Type
2	I	59	VAL
2	I	66	LEU
2	I	72	ILE
2	I	79	MET
2	I	81	ASP
2	I	83	ILE
2	I	84	THR
2	I	86	HIS
2	I	88	GLU
2	I	95	SER
2	I	97	MET
2	I	107	SER
2	I	110	SER
2	I	114	GLN
2	I	115	THR
2	I	127	GLU
2	I	134	LYS
2	I	138	ILE
2	I	139	LEU
2	I	146	GLU
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	192	GLU
2	I	204	GLN
2	I	205	ILE
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	250	VAL
2	I	260	LYS
2	I	264	ASN

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Mol	Chain	Res	Type
2	I	268	GLU
2	I	275	MET
2	I	286	LEU
2	J	6	ILE
2	J	7	SER
2	J	9	ILE
2	J	13	LYS
2	J	14	ILE
2	J	15	GLN
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	58	ARG
2	J	59	VAL
2	J	68	THR
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	97	MET
2	J	100	VAL
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

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Mol	Chain	Res	Type
2	J	136	GLN
2	J	138	ILE
2	J	139	LEU
2	J	148	LEU
2	J	151	LYS
2	J	152	ILE
2	J	154	SER
2	J	159	SER
2	J	178	LEU
2	J	184	LEU
2	J	189	ILE
2	J	192	GLU
2	J	194	VAL
2	J	209	LYS
2	J	213	ILE
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	235	ARG
2	J	243	GLU
2	J	247	VAL
2	J	251	LYS
2	J	257	ASN
2	J	263	MET
2	J	264	ASN
2	J	270	LEU
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 (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	20	ASN
1	E	24	ASN
1	E	33	GLN
1	E	38	GLN

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Mol	Chain	Res	Type
1	E	39	GLN
1	E	48	HIS
1	E	100	GLN
1	E	139	GLN
1	E	158	GLN
1	E	195	ASN
1	E	227	GLN
1	E	252	GLN
1	E	303	ASN
1	E	305	GLN
1	E	315	GLN
1	E	339	HIS
1	E	346	ASN
1	E	507	HIS
1	E	597	HIS
1	E	631	ASN
1	F	20	ASN
1	F	24	ASN
1	F	31	HIS
1	F	52	HIS
1	F	59	GLN
1	F	125	HIS
1	F	158	GLN
1	F	195	ASN
1	F	199	GLN
1	F	213	ASN
1	F	252	GLN
1	F	303	ASN
1	F	315	GLN
1	F	424	HIS
1	F	450	HIS
1	F	539	GLN
1	F	580	ASN
1	F	582	ASN
1	F	631	ASN
1	F	698	GLN
2	I	12	ASN
2	I	29	ASN
2	I	53	GLN
2	I	70	GLN
2	I	86	HIS
2	I	114	GLN

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Mol	Chain	Res	Type
2	I	128	ASN
2	I	232	ASN
2	I	264	ASN
2	J	29	ASN
2	J	40	ASN
2	J	53	GLN
2	J	54	GLN
2	J	70	GLN
2	J	71	ASN
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 oligosaccharides 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	F	1700	4	32,33,33	1.88	9 (28%)	48,52,52	1.61	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	DGT	E	1700	4	32,33,33	1.89	9 (28%)	48,52,52	1.67	10 (20%)

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	F	1700	4	-	0/22/34/34	0/3/3/3
3	DGT	E	1700	4	-	0/22/34/34	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1700	DGT	PB-O3A	5.69	1.65	1.59
3	F	1700	DGT	PB-O3A	5.35	1.65	1.59
3	E	1700	DGT	C4-N3	4.55	1.44	1.34
3	F	1700	DGT	C4-N3	4.54	1.44	1.34
3	E	1700	DGT	PG-O3G	2.89	1.59	1.50
3	F	1700	DGT	PG-O3G	2.82	1.59	1.50
3	F	1700	DGT	PB-O3B	2.82	1.62	1.59
3	F	1700	DGT	PB-O2B	2.63	1.59	1.50
3	E	1700	DGT	C6-N1	-2.60	1.34	1.38
3	F	1700	DGT	C6-N1	-2.59	1.34	1.38
3	E	1700	DGT	PB-O2B	2.50	1.59	1.50
3	E	1700	DGT	C4-N9	-2.37	1.32	1.38
3	F	1700	DGT	C4-N9	-2.33	1.32	1.38
3	F	1700	DGT	C5-C4	2.24	1.44	1.38
3	E	1700	DGT	C5-C4	2.14	1.44	1.38
3	E	1700	DGT	PB-O3B	2.12	1.61	1.59
3	E	1700	DGT	PA-O2A	2.07	1.58	1.50
3	F	1700	DGT	C8-N7	2.03	1.38	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1700	DGT	C6-C5-N7	5.44	140.19	130.29
3	F	1700	DGT	C6-C5-N7	5.16	139.68	130.29
3	E	1700	DGT	C5-C4-N3	-4.11	121.85	128.39
3	F	1700	DGT	C5-C4-N3	-3.98	122.06	128.39
3	F	1700	DGT	C6-C5-C4	-3.67	113.31	118.83
3	E	1700	DGT	C6-C5-C4	-3.46	113.62	118.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1700	DGT	C2-N3-C4	3.43	118.20	112.30
3	F	1700	DGT	C2-N3-C4	3.30	117.99	112.30
3	F	1700	DGT	C5-C6-N1	3.15	121.27	113.25
3	F	1700	DGT	O6-C6-C5	-3.02	118.56	126.53
3	E	1700	DGT	C5-C6-N1	2.99	120.86	113.25
3	E	1700	DGT	C4-C5-N7	-2.83	106.19	110.67
3	E	1700	DGT	O6-C6-C5	-2.61	119.64	126.53
3	E	1700	DGT	C5-C4-N9	2.33	109.83	105.66
3	F	1700	DGT	C4-C5-N7	-2.30	107.02	110.67
3	F	1700	DGT	C3'-C2'-C1'	2.21	108.01	102.60
3	E	1700	DGT	C2'-C3'-C4'	2.08	107.01	102.80
3	F	1700	DGT	C5-C4-N9	2.07	109.36	105.66
3	E	1700	DGT	C3'-C2'-C1'	2.04	107.58	102.60

There are no chirality outliers.

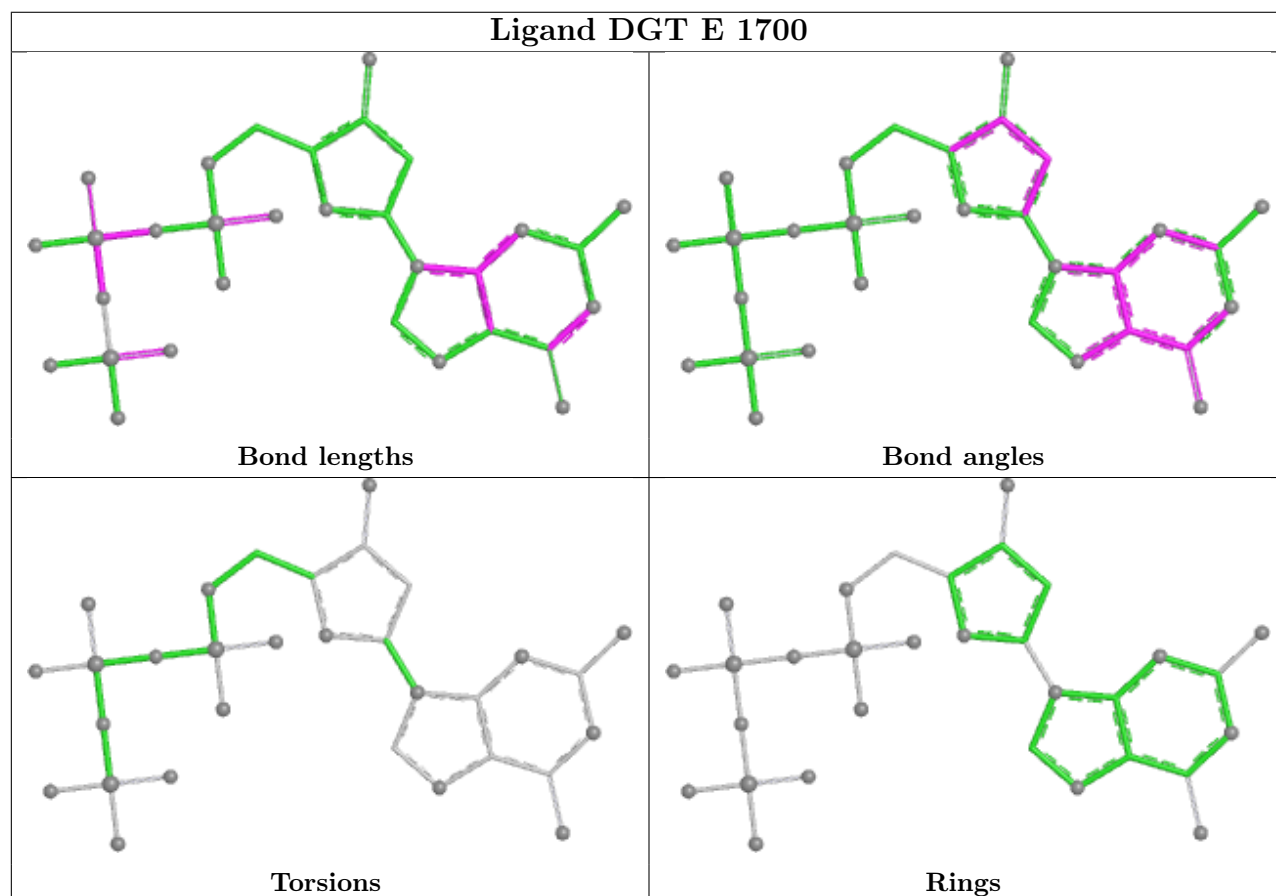
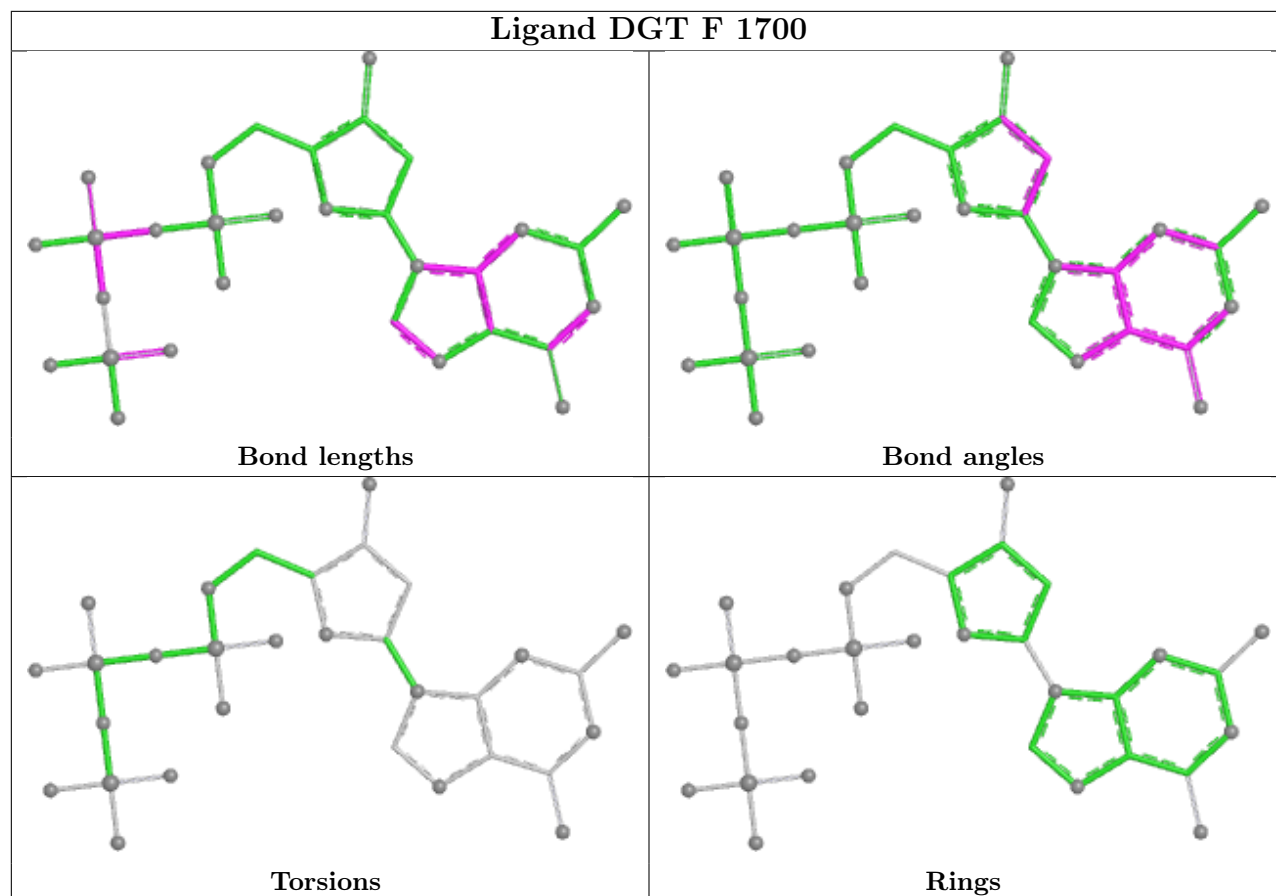
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

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



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, 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%)	0.02	10 (1%) 72 54	38, 57, 71, 89	0
1	F	685/714 (95%)	0.09	15 (2%) 62 46	40, 62, 81, 100	0
2	I	294/319 (92%)	-0.02	1 (0%) 90 78	8, 65, 84, 90	0
2	J	281/319 (88%)	0.87	31 (11%) 10 13	69, 91, 103, 105	0
All	All	1936/2066 (93%)	0.16	57 (2%) 53 39	8, 62, 95, 105	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	309	PHE	5.4
1	E	12	GLU	4.5
1	E	528	TYR	4.3
1	E	667	PHE	4.1
2	J	239	ALA	3.7
1	F	12	GLU	3.6
2	J	273	PRO	3.1
2	J	286	LEU	3.1
1	F	281	ILE	3.0
1	F	252	GLN	2.9
2	J	6	ILE	2.9
2	J	281	ALA	2.8
2	J	251	LYS	2.7
1	E	30	GLY	2.7
1	F	29	ALA	2.7
1	F	638	ALA	2.6
2	J	115	THR	2.6
2	J	207	LEU	2.6
1	F	699	LEU	2.6
2	J	206	ALA	2.6
2	J	105	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	234	ILE	2.5
2	J	241	TYR	2.5
1	F	234	VAL	2.5
2	J	57	ILE	2.5
2	J	254	LEU	2.5
1	F	237	MET	2.5
1	F	666	PHE	2.5
1	F	680	GLN	2.5
2	J	282	ILE	2.4
1	F	602	ILE	2.4
1	E	466	ALA	2.4
2	J	278	VAL	2.3
2	J	266	GLY	2.3
2	J	36	VAL	2.3
2	J	26	LEU	2.3
1	F	307	ALA	2.3
2	J	59	VAL	2.3
1	E	252	GLN	2.3
2	J	240	LEU	2.2
2	J	220	LEU	2.2
1	E	32	ILE	2.2
1	F	700	ALA	2.2
2	J	223	LEU	2.2
2	I	288	PRO	2.2
1	E	699	LEU	2.2
2	J	63	LEU	2.2
2	J	285	ALA	2.1
1	F	33	GLN	2.1
1	E	283	ILE	2.1
2	J	77	SER	2.1
2	J	249	ASP	2.1
2	J	61	THR	2.1
2	J	177	LYS	2.1
2	J	44	ALA	2.1
2	J	174	SER	2.0
1	E	377	PRO	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

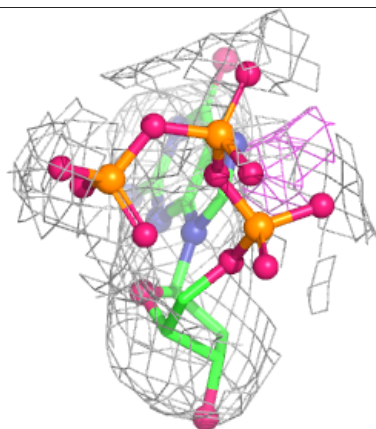
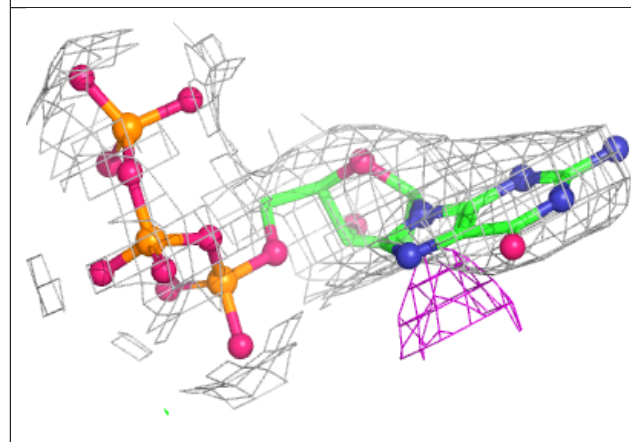
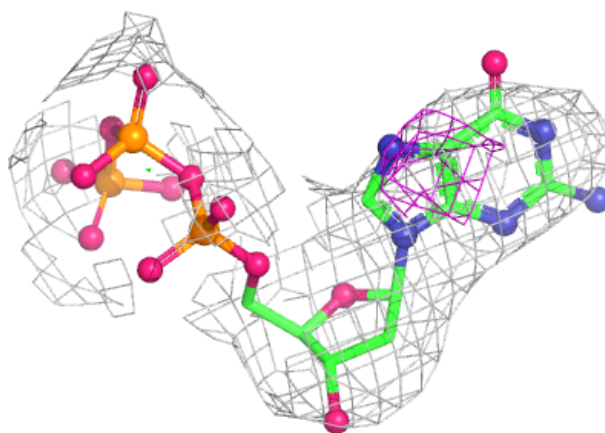
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

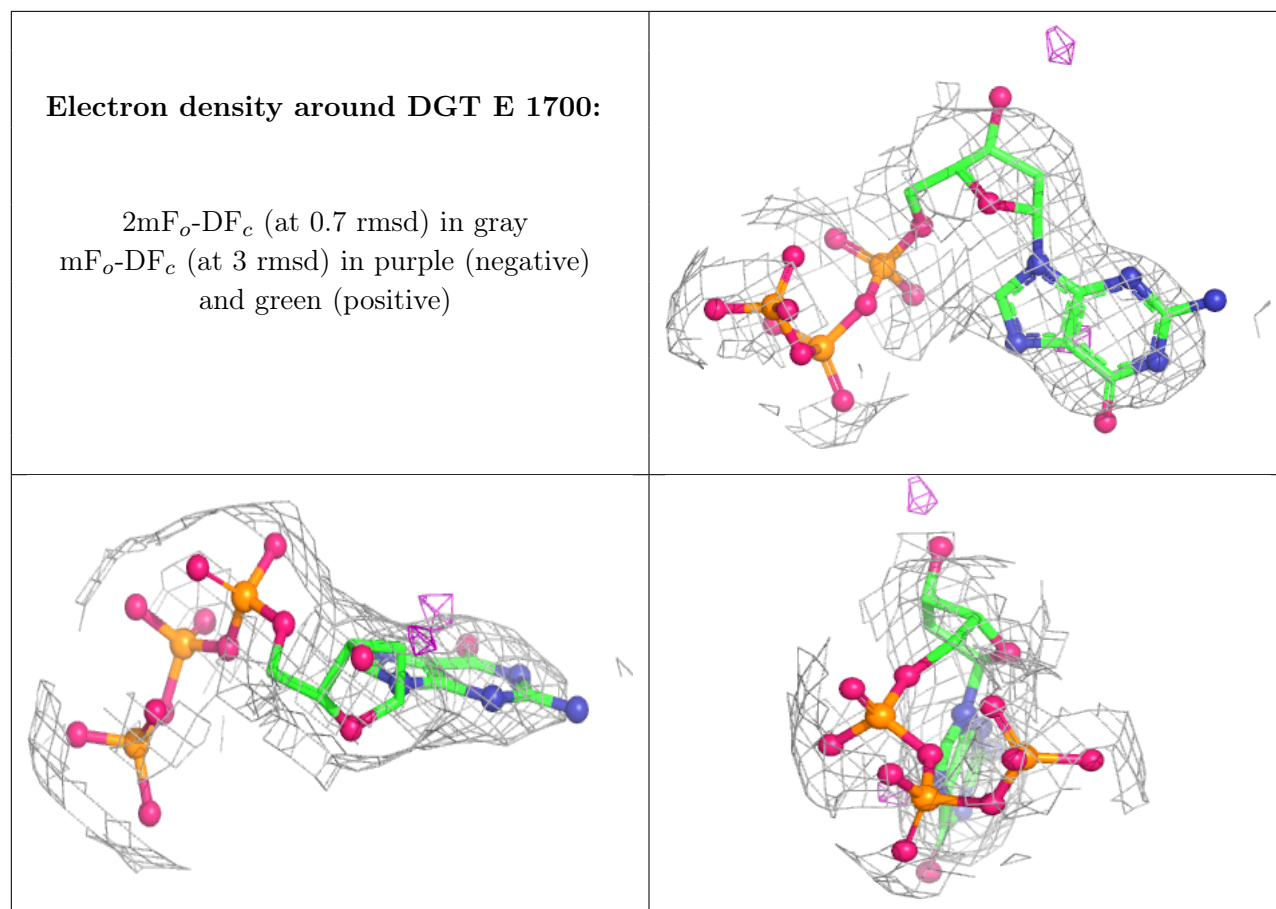
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	F	1701	1/1	0.91	0.18	33,33,33,33	0
3	DGT	F	1700	31/31	0.94	0.10	43,44,51,51	1
3	DGT	E	1700	31/31	0.95	0.09	29,35,40,41	1
4	MG	E	1701	1/1	0.96	0.13	12,12,12,12	0
5	FE	I	1320	1/1	0.99	0.07	47,47,47,47	0
5	FE	J	1288	1/1	0.99	0.06	68,68,68,68	0
5	FE	J	1287	1/1	1.00	0.03	59,59,59,59	1
5	FE	I	1321	1/1	1.00	0.03	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)





6.5 Other polymers [i](#)

There are no such residues in this entry.