



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:02 PM UTC

PDB ID : 5IZK / pdb_00005izk
Title : The crystal structure of human eEFSec in complex with GDP
Authors : Dobosz-Bartoszek, M.; Simonovic, M.
Deposited on : 2016-03-25
Resolution : 3.25 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

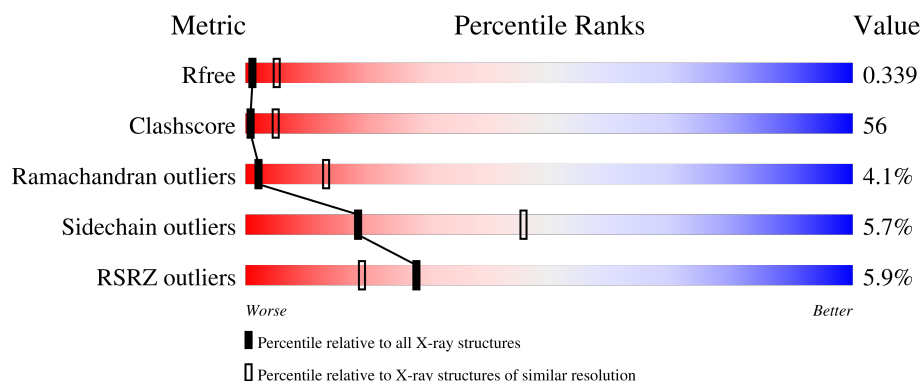
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

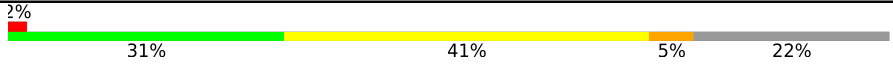
The reported resolution of this entry is 3.25 Å.

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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	A	616	
1	B	616	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6060 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 Selenocysteine-specific elongation factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	1	0
			3216	2046	566	585	19			
1	B	451	Total	C	N	O	S	0	1	0
			2767	1746	499	514	8			

There are 40 discrepancies between the modelled and reference sequences:

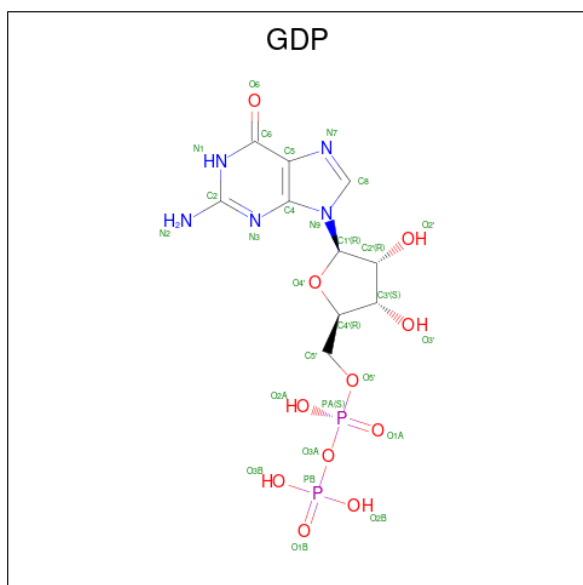
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P57772
A	-18	GLY	-	expression tag	UNP P57772
A	-17	SER	-	expression tag	UNP P57772
A	-16	SER	-	expression tag	UNP P57772
A	-15	HIS	-	expression tag	UNP P57772
A	-14	HIS	-	expression tag	UNP P57772
A	-13	HIS	-	expression tag	UNP P57772
A	-12	HIS	-	expression tag	UNP P57772
A	-11	HIS	-	expression tag	UNP P57772
A	-10	HIS	-	expression tag	UNP P57772
A	-9	SER	-	expression tag	UNP P57772
A	-8	SER	-	expression tag	UNP P57772
A	-7	GLY	-	expression tag	UNP P57772
A	-6	LEU	-	expression tag	UNP P57772
A	-5	VAL	-	expression tag	UNP P57772
A	-4	PRO	-	expression tag	UNP P57772
A	-3	ARG	-	expression tag	UNP P57772
A	-2	GLY	-	expression tag	UNP P57772
A	-1	SER	-	expression tag	UNP P57772
A	0	HIS	-	expression tag	UNP P57772
B	-19	MET	-	initiating methionine	UNP P57772
B	-18	GLY	-	expression tag	UNP P57772
B	-17	SER	-	expression tag	UNP P57772
B	-16	SER	-	expression tag	UNP P57772
B	-15	HIS	-	expression tag	UNP P57772

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P57772
B	-13	HIS	-	expression tag	UNP P57772
B	-12	HIS	-	expression tag	UNP P57772
B	-11	HIS	-	expression tag	UNP P57772
B	-10	HIS	-	expression tag	UNP P57772
B	-9	SER	-	expression tag	UNP P57772
B	-8	SER	-	expression tag	UNP P57772
B	-7	GLY	-	expression tag	UNP P57772
B	-6	LEU	-	expression tag	UNP P57772
B	-5	VAL	-	expression tag	UNP P57772
B	-4	PRO	-	expression tag	UNP P57772
B	-3	ARG	-	expression tag	UNP P57772
B	-2	GLY	-	expression tag	UNP P57772
B	-1	SER	-	expression tag	UNP P57772
B	0	HIS	-	expression tag	UNP P57772

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

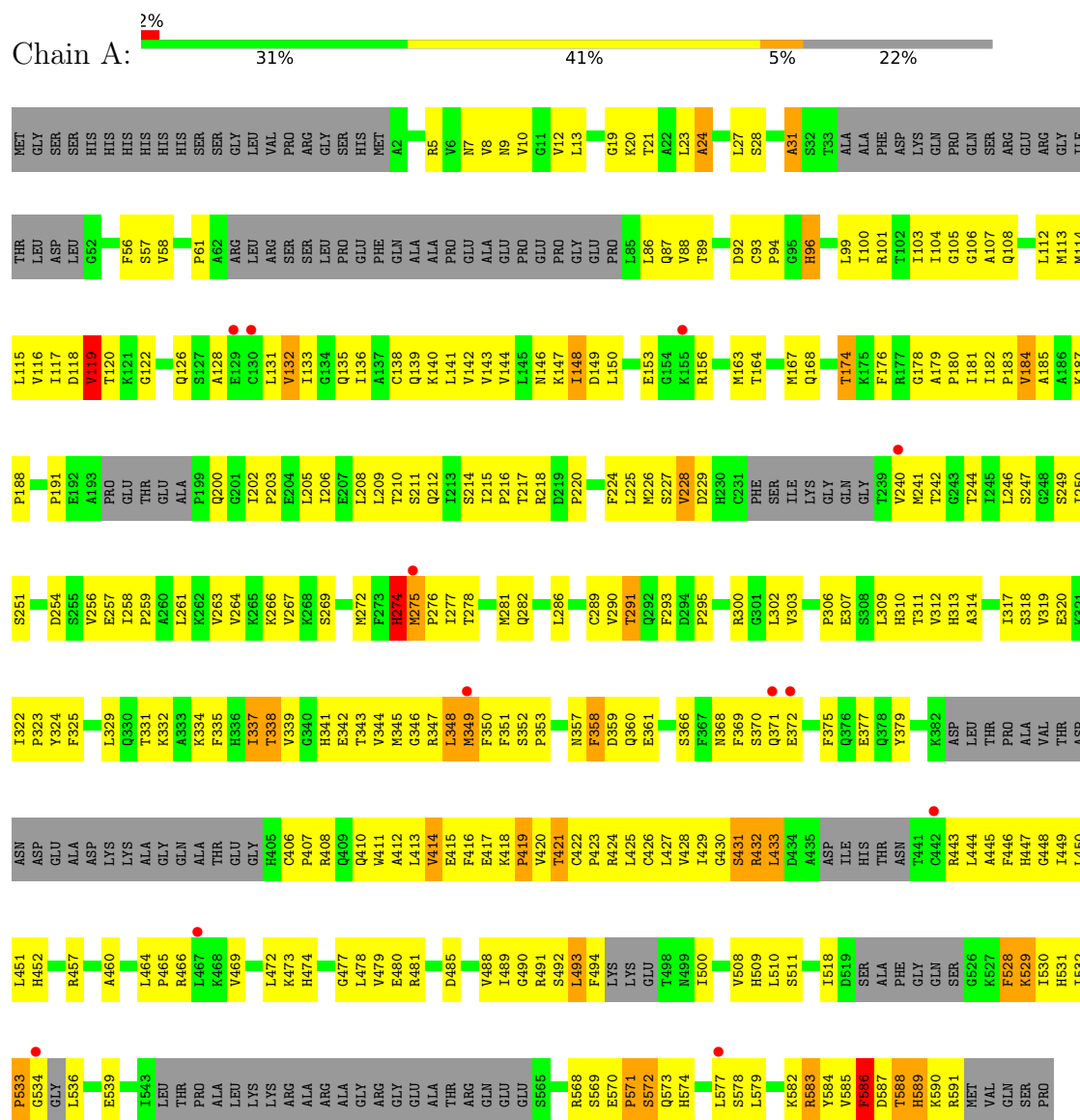


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	15	Total 15	O 15	0	0
3	B	6	Total 6	O 6	0	0

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: Selenocysteine-specific elongation factor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	58.69Å 96.86Å 125.41Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	42.94 – 3.25 42.94 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.0 (42.94-3.25) 99.1 (42.94-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.296 , 0.338 0.297 , 0.339	Depositor DCC
R_{free} test set	1286 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	89.2	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 96.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	1/3276 (0.0%)	0.81	18/4477 (0.4%)
1	B	0.35	0/2816	0.81	20/3868 (0.5%)
All	All	0.38	1/6092 (0.0%)	0.81	38/8345 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	HIS	CA-C	-5.05	1.48	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	588	THR	N-CA-C	16.08	128.71	108.45
1	B	588	THR	N-CA-C	16.08	128.71	108.45
1	A	464	LEU	N-CA-C	13.86	132.84	113.16
1	B	341	HIS	N-CA-C	11.65	130.53	113.40
1	B	582	LYS	N-CA-C	-11.42	94.40	110.50
1	A	274	HIS	CB-CA-C	-10.57	94.93	110.16
1	B	534	GLY	N-CA-C	-8.78	105.02	114.67
1	A	275	MET	N-CA-C	8.40	128.38	109.81
1	B	583	ARG	N-CA-C	7.93	122.21	112.54
1	A	215	ILE	N-CA-C	7.85	125.83	108.88
1	A	338	THR	N-CA-C	-7.79	95.71	108.41
1	A	583	ARG	N-CA-C	7.50	120.41	111.33
1	B	586	PHE	N-CA-C	7.32	119.34	111.36
1	B	565	SER	CB-CA-C	-7.32	96.19	110.10
1	A	586	PHE	N-CA-C	7.31	119.33	111.36
1	B	569	SER	N-CA-C	7.03	121.34	111.92
1	A	572	SER	N-CA-C	6.78	120.75	111.39
1	A	349	MET	N-CA-C	-6.76	96.40	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	LEU	CA-C-N	-6.67	112.43	122.29
1	B	536	LEU	C-N-CA	-6.67	112.43	122.29
1	B	536	LEU	N-CA-C	-6.29	102.19	110.43
1	B	262	LYS	N-CA-C	6.07	120.24	111.56
1	B	491	ARG	CB-CA-C	6.05	122.46	110.42
1	B	491	ARG	N-CA-C	-5.76	98.53	110.80
1	B	300	ARG	N-CA-C	-5.73	98.59	110.80
1	A	433	LEU	N-CA-CB	-5.71	100.58	110.17
1	A	432	ARG	N-CA-C	5.69	122.92	110.80
1	A	337	ILE	N-CA-C	5.60	116.30	109.30
1	A	431	SER	N-CA-CB	-5.46	102.46	111.69
1	B	529	LYS	CB-CA-C	5.43	121.23	110.42
1	B	533	PRO	CB-CA-C	-5.42	102.61	111.56
1	B	566	ALA	N-CA-CB	-5.41	101.34	110.49
1	B	533	PRO	N-CA-C	5.24	123.26	112.47
1	B	492	SER	N-CA-CB	5.23	119.33	110.49
1	A	214	SER	CB-CA-C	5.22	121.57	110.19
1	A	349	MET	CB-CA-C	5.22	120.80	110.42
1	A	431	SER	N-CA-C	5.18	116.31	108.07
1	A	571	PRO	N-CA-C	-5.12	101.92	112.47

There are no chirality outliers.

There are no planarity outliers.

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	A	3216	0	2771	349	0
1	B	2767	0	2027	267	0
2	A	28	0	12	4	0
2	B	28	0	12	7	0
3	A	15	0	0	19	0
3	B	6	0	0	10	0
All	All	6060	0	4822	610	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 56.

All (610) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:GLY:HA2	1:B:492:SER:CB	1.25	1.59
1:B:477:GLY:CA	1:B:492:SER:CB	2.02	1.36
1:B:476:HIS:O	1:B:492:SER:CB	1.79	1.31
1:B:490:GLY:O	1:B:528:PHE:CD2	1.84	1.30
1:B:311:THR:CA	1:B:421:THR:HG22	1.65	1.24
1:A:588:THR:CG2	1:A:589:HIS:H	1.39	1.24
1:B:473:LYS:CD	1:B:579:LEU:HD21	1.71	1.20
1:B:473:LYS:HG2	1:B:579:LEU:CD1	1.72	1.19
1:B:473:LYS:CG	1:B:579:LEU:HD21	1.71	1.19
1:B:473:LYS:HG2	1:B:579:LEU:HD11	1.17	1.16
1:B:580:THR:HG23	1:B:590:LYS:HD3	1.18	1.16
1:B:372:GLU:CD	1:B:582:LYS:NZ	2.04	1.16
1:B:205:LEU:O	1:B:209:LEU:HB2	1.48	1.14
1:B:20:LYS:N	2:B:1001:GDP:O1A	1.81	1.13
1:B:490:GLY:O	1:B:528:PHE:HD2	1.20	1.12
1:B:311:THR:CB	1:B:421:THR:HG22	1.79	1.12
1:A:432:ARG:CB	1:A:443:ARG:O	1.99	1.11
1:B:311:THR:HA	1:B:421:THR:HG22	1.10	1.09
1:A:490:GLY:O	1:A:528:PHE:HB2	1.53	1.08
1:B:473:LYS:HG2	1:B:579:LEU:CG	1.83	1.07
1:A:588:THR:HG22	1:A:589:HIS:N	1.64	1.05
1:A:588:THR:HG22	1:A:589:HIS:H	0.95	1.05
1:B:580:THR:HG23	1:B:590:LYS:CD	1.87	1.03
1:A:433:LEU:HD12	1:A:433:LEU:O	1.59	1.01
1:B:347:ARG:HB2	1:B:415:GLU:HB2	1.43	1.00
1:A:583:ARG:N	3:A:1101:HOH:O	1.82	0.99
1:B:473:LYS:CG	1:B:579:LEU:CD2	2.40	0.99
1:A:469:VAL:O	3:A:1101:HOH:O	1.81	0.97
1:B:311:THR:HA	1:B:421:THR:CG2	1.95	0.96
1:B:187:LYS:O	2:B:1001:GDP:C6	2.17	0.96
1:B:543:ILE:HD13	1:B:571:PRO:HD2	1.48	0.96
1:A:113:MET:O	1:A:141:LEU:HG	1.66	0.95
1:B:322:ILE:HD13	1:B:444:LEU:HB3	1.47	0.95
1:B:476:HIS:C	1:B:492:SER:CB	2.39	0.95
1:A:226:MET:O	3:A:1102:HOH:O	1.85	0.93
1:B:311:THR:CB	1:B:421:THR:CG2	2.46	0.92
1:A:372:GLU:OE2	1:A:582:LYS:NZ	2.02	0.92
1:B:491:ARG:HA	1:B:528:PHE:CE2	2.05	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LEU:HA	3:A:1102:HOH:O	1.70	0.91
1:B:473:LYS:CG	1:B:579:LEU:CG	2.49	0.91
1:A:153[B]:GLU:OE2	3:A:1103:HOH:O	1.88	0.90
1:A:478:LEU:O	3:A:1104:HOH:O	1.89	0.90
1:A:224:PHE:CD1	1:A:250:ILE:HD11	2.05	0.90
1:B:475:LYS:HD3	1:B:493:LEU:CB	2.02	0.90
1:A:220:PRO:HD3	1:A:281:MET:HE2	1.54	0.90
1:B:471:LYS:N	1:B:581:PHE:O	2.05	0.90
1:B:428:VAL:N	1:B:448:GLY:O	2.05	0.89
1:B:491:ARG:HA	1:B:528:PHE:HE2	1.34	0.89
1:A:422:CYS:SG	3:A:1114:HOH:O	2.32	0.88
1:B:110:ILE:O	3:B:1101:HOH:O	1.92	0.88
1:B:431:SER:OG	1:B:445:ALA:N	2.07	0.88
1:A:250:ILE:HG22	1:A:251:SER:H	1.36	0.87
1:B:473:LYS:HG2	1:B:579:LEU:CD2	2.02	0.87
1:A:148:ILE:HG22	1:A:185:ALA:HB2	1.56	0.87
1:B:362:PRO:HA	1:B:409:GLN:NE2	1.90	0.86
1:A:144:VAL:HG12	1:A:182:ILE:HB	1.57	0.86
1:A:229:ASP:OD1	1:A:242:THR:O	1.95	0.85
1:A:224:PHE:CE1	1:A:250:ILE:HD11	2.12	0.84
1:B:473:LYS:HG2	1:B:579:LEU:HD21	1.58	0.84
1:A:359:ASP:HA	1:A:408:ARG:HG3	1.58	0.84
1:A:588:THR:HG23	1:A:589:HIS:H	1.40	0.84
1:A:588:THR:CG2	1:A:589:HIS:N	2.17	0.84
1:B:119:VAL:HA	1:B:163:MET:HE1	1.58	0.84
1:B:322:ILE:CD1	1:B:444:LEU:HB3	2.07	0.84
1:B:148:ILE:HD11	1:B:183:PRO:HB2	1.59	0.84
1:A:149:ASP:OD2	1:A:188:PRO:HA	1.79	0.83
1:B:480:GLU:HG2	1:B:481:ARG:HG2	1.58	0.83
1:B:57:SER:HA	1:B:86:LEU:O	1.78	0.83
1:B:473:LYS:CG	1:B:579:LEU:HD11	2.06	0.83
1:A:579:LEU:HA	1:A:590:LYS:HB2	1.60	0.82
1:A:114:MET:HE2	1:A:209:LEU:HD21	1.61	0.82
1:B:16:ILE:O	3:B:1102:HOH:O	1.98	0.81
1:A:148:ILE:HG22	1:A:185:ALA:CB	2.11	0.81
1:A:488:VAL:HG12	1:A:489:ILE:H	1.45	0.81
1:A:335:PHE:HD1	1:A:431:SER:HA	1.46	0.81
1:B:372:GLU:CD	1:B:582:LYS:HZ1	1.78	0.81
1:A:205:LEU:O	1:A:209:LEU:HG	1.80	0.80
1:B:148:ILE:CD1	1:B:183:PRO:HB2	2.10	0.80
1:A:337:ILE:HA	1:A:430:GLY:HA3	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:GLU:OE1	3:A:1105:HOH:O	2.00	0.80
1:A:511:SER:N	1:A:574:HIS:O	2.16	0.79
1:A:258:ILE:HD12	1:A:261:LEU:HD21	1.64	0.79
1:B:224:PHE:CD2	1:B:304:CYS:HA	2.18	0.79
1:A:490:GLY:O	1:A:528:PHE:CB	2.31	0.78
1:B:479:VAL:HB	1:B:573:GLN:CB	2.12	0.78
1:A:331:THR:HG23	1:A:349:MET:HA	1.66	0.78
1:A:510:LEU:O	3:A:1106:HOH:O	2.01	0.78
1:A:465:PRO:HA	1:A:584:TYR:HB2	1.65	0.78
1:B:372:GLU:CD	1:B:582:LYS:HZ2	1.90	0.77
1:B:329:LEU:HD12	1:B:379:TYR:HD2	1.50	0.77
1:A:212:GLN:N	1:A:212:GLN:OE1	2.18	0.77
1:A:13:LEU:HD11	1:A:113:MET:HE3	1.67	0.77
1:A:138:CYS:SG	1:A:139:GLN:N	2.58	0.76
1:A:587:ASP:O	1:A:588:THR:OG1	2.02	0.76
1:A:119:VAL:HG23	1:A:146:ASN:O	1.85	0.76
1:A:338:THR:O	1:A:429:ILE:O	2.02	0.76
1:A:342:GLU:OE1	1:A:418:LYS:NZ	2.15	0.76
1:B:485:ASP:OD1	1:B:536:LEU:HB2	1.86	0.75
1:A:153[A]:GLU:OE1	1:A:156:ARG:NH2	2.18	0.75
1:B:136:ILE:HD13	1:B:447:HIS:HB3	1.68	0.75
1:B:319:VAL:HG22	1:B:410:GLN:O	1.86	0.74
1:A:112:LEU:HD11	1:A:212:GLN:HB3	1.68	0.74
1:A:148:ILE:HG22	1:A:185:ALA:N	2.03	0.74
1:B:490:GLY:C	1:B:528:PHE:CD2	2.66	0.74
1:A:225:LEU:HD11	1:A:302:LEU:HD22	1.69	0.73
1:A:351:PHE:CE1	1:A:411:TRP:HB2	2.22	0.73
1:B:317:ILE:HG22	1:B:450:LEU:HA	1.71	0.73
1:A:5:ARG:HH12	1:A:272:MET:C	1.96	0.73
1:A:528:PHE:C	1:A:529:LYS:HG3	2.14	0.73
1:B:274:HIS:C	1:B:276:PRO:HD2	2.14	0.73
1:B:187:LYS:O	2:B:1001:GDP:N1	2.21	0.73
1:A:114:MET:HE2	1:A:209:LEU:CD2	2.19	0.73
1:B:148:ILE:HG13	1:B:184:VAL:O	1.89	0.73
1:B:570:GLU:O	1:B:572:SER:N	2.21	0.73
1:A:266:LYS:O	1:A:290:VAL:HG13	1.88	0.72
1:A:112:LEU:HA	1:A:138:CYS:SG	2.30	0.72
1:A:413:LEU:HD23	1:A:413:LEU:O	1.90	0.72
1:A:310:HIS:CD2	1:A:312:VAL:CG2	2.72	0.72
1:A:13:LEU:HD21	1:A:113:MET:CE	2.20	0.72
1:B:431:SER:HB3	1:B:443:ARG:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:THR:CG2	1:B:590:LYS:HD3	2.10	0.72
1:A:113:MET:HB2	1:A:141:LEU:HD12	1.72	0.71
1:A:274:HIS:C	1:A:276:PRO:HD2	2.15	0.71
1:A:302:LEU:HD23	3:A:1102:HOH:O	1.90	0.71
1:B:477:GLY:N	1:B:492:SER:CB	2.52	0.71
1:B:588:THR:OG1	1:B:589:HIS:N	2.23	0.71
1:A:349:MET:O	1:A:412:ALA:HB1	1.90	0.71
1:B:10:VAL:HG13	1:B:112:LEU:O	1.91	0.71
1:A:105:GLY:HA3	1:A:341:HIS:CE1	2.26	0.70
1:A:101:ARG:HD2	1:A:341:HIS:O	1.90	0.70
1:A:246:LEU:O	1:A:282:GLN:NE2	2.19	0.70
1:B:473:LYS:CG	1:B:579:LEU:HG	2.22	0.70
1:B:570:GLU:OE2	3:B:1103:HOH:O	2.10	0.70
1:A:322:ILE:N	1:A:445:ALA:O	2.20	0.70
1:A:313:HIS:CD2	1:A:419:PRO:HB3	2.27	0.69
1:A:220:PRO:CD	1:A:281:MET:HE2	2.22	0.69
1:A:148:ILE:CG2	1:A:185:ALA:HB2	2.21	0.69
1:A:366:SER:O	1:A:451:LEU:HD13	1.92	0.69
1:A:249:SER:O	1:A:250:ILE:HD13	1.92	0.69
1:B:293:PHE:O	1:B:295:PRO:HD3	1.93	0.69
1:B:275:MET:N	1:B:276:PRO:HD2	2.08	0.68
1:A:310:HIS:CD2	1:A:312:VAL:HG23	2.27	0.68
1:A:117:ILE:O	1:A:146:ASN:N	2.26	0.68
1:A:228:VAL:HG12	1:A:300:ARG:HA	1.73	0.67
1:A:23:LEU:HD23	1:A:23:LEU:O	1.95	0.67
1:A:348:LEU:HD23	1:A:350:PHE:CZ	2.29	0.67
1:A:317:ILE:HD11	1:A:319:VAL:HG22	1.76	0.67
1:B:148:ILE:H	1:B:185:ALA:HB2	1.60	0.67
1:A:293:PHE:O	1:A:295:PRO:HD3	1.95	0.67
1:A:372:GLU:CD	1:A:582:LYS:NZ	2.53	0.67
1:B:187:LYS:N	2:B:1001:GDP:O6	2.27	0.67
1:B:149:ASP:OD2	1:B:188:PRO:HA	1.95	0.67
1:B:580:THR:O	1:B:588:THR:HG23	1.95	0.67
1:B:338:THR:HA	1:B:342:GLU:O	1.94	0.67
1:B:354:ALA:O	1:B:358:PHE:N	2.28	0.67
1:A:250:ILE:HG22	1:A:251:SER:N	2.09	0.66
1:A:224:PHE:HA	1:A:247:SER:O	1.95	0.66
1:B:501:GLN:C	1:B:502:LEU:HD12	2.19	0.66
1:A:480:GLU:HG3	1:A:481:ARG:H	1.61	0.66
1:B:373:TYR:O	1:B:469:VAL:HA	1.96	0.65
1:A:570:GLU:HG3	1:A:570:GLU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:TYR:HD1	1:B:535:GLY:HA2	1.61	0.65
1:A:310:HIS:CE1	1:A:424:ARG:HG2	2.32	0.65
1:B:322:ILE:HG13	1:B:446:PHE:HA	1.79	0.65
1:B:224:PHE:O	1:B:304:CYS:HB2	1.97	0.65
1:B:473:LYS:HG3	1:B:579:LEU:HG	1.78	0.64
1:A:335:PHE:CD1	1:A:431:SER:HA	2.31	0.64
1:A:122:GLY:HA2	1:A:163:MET:CE	2.28	0.64
1:A:417:GLU:HG3	1:A:418:LYS:N	2.11	0.64
1:A:13:LEU:HD11	1:A:113:MET:CE	2.27	0.64
1:A:431:SER:HB2	1:A:445:ALA:CB	2.28	0.64
1:A:491:ARG:N	3:A:1104:HOH:O	2.06	0.64
1:B:245:ILE:O	1:B:283:GLY:N	2.26	0.64
1:B:312:VAL:HG13	1:B:454:LEU:O	1.98	0.64
1:B:133:ILE:HG13	1:B:444:LEU:HD11	1.80	0.64
1:A:585:VAL:HG22	1:A:586:PHE:N	2.11	0.63
1:B:372:GLU:HA	1:B:468:LYS:O	1.98	0.63
1:B:580:THR:CG2	1:B:590:LYS:CD	2.69	0.63
1:A:578:SER:O	1:A:590:LYS:HG2	1.97	0.63
1:B:148:ILE:HG22	1:B:148:ILE:O	1.98	0.63
1:A:335:PHE:O	1:A:345:MET:HG3	1.99	0.63
1:A:570:GLU:O	1:A:572:SER:N	2.31	0.63
1:B:321:LYS:H	1:B:379:TYR:HE2	1.46	0.63
1:B:585:VAL:HG22	1:B:586:PHE:N	2.11	0.63
1:A:428:VAL:O	1:A:429:ILE:HG13	1.99	0.62
1:A:112:LEU:CD1	1:A:212:GLN:HB3	2.27	0.62
1:A:20:LYS:N	2:A:1001:GDP:O2A	2.32	0.62
1:A:92:ASP:OD1	1:A:93:CYS:N	2.24	0.62
1:A:274:HIS:HB3	1:A:276:PRO:HD2	1.81	0.62
1:B:220:PRO:HB2	1:B:249:SER:HB2	1.82	0.62
1:A:359:ASP:HA	1:A:408:ARG:CG	2.27	0.62
1:B:224:PHE:HD2	1:B:304:CYS:HA	1.62	0.62
1:B:372:GLU:OE1	1:B:582:LYS:NZ	2.32	0.62
1:B:570:GLU:CD	3:B:1103:HOH:O	2.43	0.62
1:A:57:SER:HA	1:A:86:LEU:O	1.99	0.62
1:A:431:SER:OG	1:A:444:LEU:HA	1.98	0.62
1:A:257:GLU:OE2	1:A:306:PRO:HA	2.00	0.61
1:B:372:GLU:OE2	1:B:582:LYS:NZ	2.15	0.61
1:A:450:LEU:HD23	1:A:452:HIS:H	1.64	0.61
1:A:539:GLU:N	1:A:539:GLU:OE1	2.32	0.61
1:B:338:THR:CB	1:B:343:THR:HG22	2.30	0.61
1:A:21:THR:HB	2:A:1001:GDP:O1A	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:PRO:O	1:B:206:ILE:N	2.34	0.61
1:A:488:VAL:HG12	1:A:489:ILE:N	2.16	0.61
1:B:472:LEU:HD23	1:B:472:LEU:O	2.01	0.61
1:B:117:ILE:HG13	1:B:167:MET:HE1	1.82	0.61
1:B:456:ASP:OD2	1:B:462:SER:CB	2.48	0.60
1:A:251:SER:HA	1:A:278:THR:O	2.00	0.60
1:B:491:ARG:CA	1:B:528:PHE:CE2	2.80	0.60
1:A:258:ILE:CG2	1:A:261:LEU:HG	2.31	0.60
1:B:570:GLU:O	1:B:570:GLU:HG2	2.00	0.60
1:A:258:ILE:HG12	1:A:303:VAL:HG22	1.84	0.60
1:A:13:LEU:HD21	1:A:113:MET:HE1	1.83	0.60
1:A:583:ARG:CB	3:A:1101:HOH:O	2.49	0.60
1:B:97:ALA:N	3:B:1105:HOH:O	2.26	0.60
1:B:409:GLN:OE1	1:B:411:TRP:NE1	2.35	0.60
1:A:183:PRO:O	1:A:184:VAL:HG23	2.02	0.60
1:A:174:THR:CG2	1:A:176:PHE:H	2.15	0.59
1:A:420:VAL:HG22	1:A:421:THR:N	2.17	0.59
1:B:136:ILE:HD13	1:B:447:HIS:CB	2.33	0.59
1:A:420:VAL:HG22	1:A:421:THR:H	1.66	0.59
1:B:357:ASN:O	1:B:360:GLN:N	2.26	0.59
1:B:472:LEU:HA	1:B:579:LEU:O	2.03	0.59
1:B:490:GLY:O	1:B:528:PHE:CG	2.53	0.59
1:B:532:ILE:HD12	1:B:532:ILE:N	2.16	0.59
1:A:310:HIS:HD2	1:A:312:VAL:CG2	2.15	0.59
1:A:334:LYS:CE	1:A:345:MET:HG2	2.33	0.59
1:A:431:SER:HB2	1:A:445:ALA:HB3	1.85	0.59
1:A:103:ILE:CD1	1:A:113:MET:HE1	2.33	0.59
1:B:117:ILE:HG22	1:B:118:ASP:H	1.68	0.59
1:B:543:ILE:HD13	1:B:571:PRO:CD	2.29	0.59
1:A:259:PRO:HG2	1:A:309:LEU:HD12	1.83	0.59
1:B:138:CYS:SG	1:B:139:GLN:N	2.75	0.59
1:B:515:LEU:HD12	1:B:516:GLY:H	1.67	0.59
1:A:24:ALA:O	1:A:27:LEU:N	2.36	0.59
1:A:589:HIS:NE2	3:A:1112:HOH:O	2.32	0.58
1:B:473:LYS:HG3	1:B:579:LEU:CD2	2.29	0.58
1:A:313:HIS:NE2	1:A:419:PRO:HB3	2.17	0.58
1:B:311:THR:CA	1:B:421:THR:CG2	2.58	0.58
1:B:491:ARG:CB	1:B:528:PHE:HD2	2.17	0.58
1:A:269:SER:O	1:A:289:CYS:N	2.37	0.58
1:A:258:ILE:HB	1:A:261:LEU:HG	1.86	0.58
1:A:579:LEU:O	1:A:579:LEU:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:SER:CB	1:A:410:GLN:NE2	2.67	0.57
1:A:174:THR:HG22	1:A:176:PHE:H	1.69	0.57
1:B:7:ASN:OD1	1:B:8:VAL:N	2.38	0.57
1:B:148:ILE:N	1:B:185:ALA:HB2	2.19	0.57
1:B:578:SER:O	1:B:590:LYS:HG2	2.05	0.57
1:A:108:GLN:N	3:A:1107:HOH:O	2.06	0.57
1:A:472:LEU:HG	1:A:474:HIS:NE2	2.19	0.57
1:A:530:ILE:HG22	1:A:531:HIS:O	2.04	0.57
1:A:120:THR:HG21	1:A:150:LEU:HD23	1.87	0.57
1:A:590:LYS:HG3	1:A:591:ARG:N	2.20	0.57
1:B:364:LEU:O	1:B:451:LEU:HD21	2.04	0.57
1:B:485:ASP:HA	1:B:536:LEU:HD12	1.87	0.57
1:A:115:LEU:HD22	1:A:131:LEU:HD13	1.85	0.57
1:A:422:CYS:HB3	1:A:423:PRO:HD2	1.86	0.57
1:A:13:LEU:HD21	1:A:113:MET:HE3	1.85	0.57
1:A:508:VAL:C	1:A:509:HIS:CD2	2.83	0.57
1:B:590:LYS:HG3	1:B:591:ARG:N	2.20	0.57
1:A:290:VAL:HG12	1:A:291:THR:H	1.69	0.56
1:A:148:ILE:HG23	1:A:148:ILE:O	2.04	0.56
1:B:140:LYS:HE2	1:B:179:ALA:HA	1.88	0.56
1:A:113:MET:O	1:A:141:LEU:HA	2.05	0.56
1:A:358:PHE:CE1	1:A:407:PRO:HB3	2.41	0.56
1:A:577:LEU:HD21	1:A:579:LEU:HG	1.87	0.56
1:B:317:ILE:HG21	1:B:428:VAL:HG21	1.86	0.56
1:A:103:ILE:HD12	1:A:113:MET:HE1	1.88	0.56
1:A:143:VAL:O	1:A:181:ILE:HA	2.06	0.56
1:B:163:MET:O	1:B:166:LYS:HB3	2.06	0.56
1:B:317:ILE:O	1:B:411:TRP:HB3	2.06	0.56
1:A:257:GLU:HB2	1:A:306:PRO:HA	1.87	0.56
1:A:479:VAL:N	1:A:573:GLN:O	2.32	0.56
1:B:322:ILE:HD12	1:B:444:LEU:C	2.31	0.56
1:A:533:PRO:HG2	1:A:534:GLY:H	1.71	0.56
1:A:349:MET:O	1:A:412:ALA:CB	2.53	0.56
1:B:251:SER:HA	1:B:278:THR:O	2.05	0.56
1:B:471:LYS:HE3	1:B:581:PHE:CD2	2.41	0.56
1:B:486:TYR:CD1	1:B:535:GLY:HA2	2.40	0.56
1:A:429:ILE:HG12	1:A:447:HIS:CB	2.36	0.55
1:B:337:ILE:HA	1:B:430:GLY:HA3	1.89	0.55
1:B:475:LYS:HB2	1:B:577:LEU:HD23	1.88	0.55
1:A:430:GLY:O	1:A:431:SER:HB3	2.05	0.55
1:A:141:LEU:HD23	1:A:142:VAL:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:ALA:O	1:A:465:PRO:HD3	2.07	0.55
1:B:349:MET:O	1:B:412:ALA:HB1	2.07	0.55
1:A:586:PHE:N	1:A:586:PHE:CD2	2.72	0.55
1:B:510:LEU:HA	1:B:574:HIS:O	2.07	0.55
1:B:325:PHE:CD1	1:B:445:ALA:HA	2.42	0.55
1:A:136:ILE:HD13	1:A:429:ILE:HD11	1.89	0.55
1:A:465:PRO:HA	1:A:584:TYR:CB	2.36	0.55
1:A:577:LEU:C	1:A:577:LEU:HD23	2.31	0.55
1:A:317:ILE:CD1	1:A:319:VAL:HG22	2.37	0.55
1:B:117:ILE:HG22	1:B:118:ASP:N	2.22	0.55
1:A:20:LYS:HG3	2:A:1001:GDP:O3B	2.07	0.55
1:B:491:ARG:CB	1:B:528:PHE:CD2	2.90	0.55
1:A:56:PHE:O	1:A:87:GLN:HA	2.07	0.54
1:A:319:VAL:HG21	1:A:412:ALA:CB	2.37	0.54
1:A:368:ASN:O	1:A:370:SER:N	2.40	0.54
1:B:545:THR:CB	1:B:546:PRO:CD	2.85	0.54
1:A:422:CYS:HB3	1:A:423:PRO:CD	2.37	0.54
1:A:334:LYS:HE2	1:A:345:MET:HG2	1.90	0.54
1:B:347:ARG:NH1	1:B:417:GLU:OE2	2.40	0.54
1:A:220:PRO:CG	1:A:281:MET:HE2	2.38	0.54
1:A:531:HIS:CG	1:A:532:ILE:H	2.25	0.54
1:B:508:VAL:HG12	1:B:509:HIS:N	2.23	0.54
1:B:579:LEU:HD12	1:B:579:LEU:C	2.33	0.54
1:A:135:GLN:HA	1:A:176:PHE:CZ	2.43	0.54
1:A:187:LYS:O	2:A:1001:GDP:C6	2.61	0.54
1:A:335:PHE:CA	1:A:433:LEU:HD23	2.38	0.54
1:B:425:LEU:HA	1:B:450:LEU:O	2.08	0.54
1:B:329:LEU:HD12	1:B:379:TYR:CD2	2.36	0.54
1:A:348:LEU:HD23	1:A:350:PHE:CE1	2.43	0.54
1:B:205:LEU:O	1:B:209:LEU:CB	2.40	0.54
1:B:227:SER:O	1:B:243:GLY:HA3	2.08	0.54
1:B:490:GLY:C	1:B:528:PHE:HD2	2.06	0.54
1:A:28:SER:O	1:A:31:ALA:HB2	2.08	0.53
1:B:140:LYS:CE	1:B:179:ALA:HA	2.38	0.53
1:B:473:LYS:O	1:B:579:LEU:HG	2.08	0.53
1:B:491:ARG:CA	1:B:528:PHE:CD2	2.91	0.53
1:B:508:VAL:HG12	1:B:509:HIS:H	1.71	0.53
1:B:226:MET:O	1:B:303:VAL:N	2.37	0.53
1:A:508:VAL:C	1:A:509:HIS:HD2	2.15	0.53
1:B:485:ASP:C	1:B:536:LEU:HG	2.33	0.53
1:A:23:LEU:HD23	1:A:27:LEU:HG	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LYS:HD2	1:A:141:LEU:H	1.73	0.53
1:A:250:ILE:CG2	1:A:251:SER:H	2.16	0.53
1:B:479:VAL:HG13	1:B:489:ILE:O	2.07	0.53
1:A:208:LEU:O	1:A:211:SER:N	2.41	0.53
1:B:15:HIS:ND1	1:B:126:GLN:HB3	2.23	0.53
1:B:316:LEU:HD21	1:B:367:PHE:CZ	2.43	0.53
1:A:290:VAL:HG12	1:A:291:THR:N	2.24	0.53
1:A:353:PRO:HG2	1:A:358:PHE:CD1	2.44	0.53
1:A:433:LEU:HD12	1:A:433:LEU:C	2.31	0.53
1:B:245:ILE:CD1	1:B:280:ALA:HB3	2.39	0.53
1:B:372:GLU:CD	1:B:582:LYS:HZ3	2.12	0.53
1:A:120:THR:HG21	1:A:150:LEU:CD2	2.39	0.53
1:A:96:HIS:O	1:A:99:LEU:N	2.42	0.53
1:A:217:THR:C	1:A:218:ARG:HG2	2.34	0.53
1:A:227:SER:HA	3:A:1102:HOH:O	2.09	0.53
1:A:334:LYS:HD2	1:A:347:ARG:HG2	1.91	0.53
1:B:477:GLY:N	1:B:575:VAL:O	2.42	0.52
1:A:148:ILE:HG22	1:A:185:ALA:CA	2.39	0.52
1:A:174:THR:HG22	1:A:176:PHE:N	2.24	0.52
1:A:257:GLU:OE2	1:A:307:GLU:N	2.40	0.52
1:B:570:GLU:OE1	3:B:1103:HOH:O	2.19	0.52
1:B:148:ILE:HD11	1:B:183:PRO:CB	2.33	0.52
1:B:346:GLY:HA2	1:B:417:GLU:OE1	2.09	0.52
1:A:100:ILE:HG22	1:A:101:ARG:N	2.25	0.52
1:A:101:ARG:CD	1:A:341:HIS:O	2.58	0.52
1:A:319:VAL:HG21	1:A:412:ALA:HB2	1.91	0.52
1:A:220:PRO:HB3	1:A:281:MET:CG	2.40	0.51
1:A:274:HIS:O	1:A:276:PRO:HD2	2.09	0.51
1:B:348:LEU:HD21	1:B:350:PHE:CE1	2.45	0.51
1:B:317:ILE:CG2	1:B:428:VAL:HG21	2.40	0.51
1:B:487:SER:O	1:B:536:LEU:HD21	2.10	0.51
1:A:206:ILE:O	1:A:210:THR:HG23	2.09	0.51
1:A:58:VAL:O	1:A:86:LEU:HB3	2.11	0.51
1:A:220:PRO:HG3	1:A:281:MET:HE2	1.92	0.51
1:A:477:GLY:HA2	1:A:492:SER:CB	2.40	0.51
1:A:490:GLY:HA3	1:A:528:PHE:HD2	1.74	0.51
1:A:577:LEU:HD23	1:A:578:SER:N	2.26	0.51
1:B:205:LEU:HG	1:B:209:LEU:HD12	1.93	0.51
1:B:515:LEU:HD12	1:B:516:GLY:N	2.26	0.51
1:A:425:LEU:HD23	1:A:425:LEU:N	2.24	0.51
1:A:589:HIS:CD2	3:A:1112:HOH:O	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ILE:O	1:B:136:ILE:HB	2.11	0.51
1:B:330:GLN:N	3:B:1104:HOH:O	2.26	0.51
1:A:122:GLY:HA2	1:A:163:MET:HE1	1.92	0.51
1:A:153[B]:GLU:CD	3:A:1103:HOH:O	2.46	0.51
1:A:568:ARG:O	1:A:569:SER:OG	2.24	0.51
1:A:258:ILE:CD1	1:A:261:LEU:HD21	2.39	0.50
1:A:132:VAL:O	1:A:135:GLN:N	2.43	0.50
1:A:345:MET:O	1:A:417:GLU:HG2	2.11	0.50
1:B:473:LYS:CG	1:B:579:LEU:CD1	2.66	0.50
1:A:220:PRO:HB3	1:A:281:MET:HG2	1.94	0.50
1:B:9:ASN:HB2	1:B:109:ILE:O	2.11	0.49
1:A:493:LEU:O	1:A:494:PHE:C	2.54	0.49
1:A:346:GLY:HA2	1:A:416:PHE:HA	1.94	0.49
1:A:433:LEU:O	1:A:433:LEU:CD1	2.46	0.49
1:A:587:ASP:C	1:A:588:THR:HG1	2.10	0.49
1:B:203:PRO:O	1:B:204:GLU:C	2.55	0.49
1:A:341:HIS:N	3:A:1114:HOH:O	2.45	0.49
1:A:585:VAL:CG2	1:A:586:PHE:N	2.76	0.49
1:A:320:GLU:O	1:A:446:PHE:HB2	2.12	0.49
1:B:187:LYS:C	2:B:1001:GDP:C6	2.90	0.49
1:B:329:LEU:HA	3:B:1104:HOH:O	2.12	0.49
1:B:585:VAL:CG2	1:B:586:PHE:N	2.76	0.49
1:A:261:LEU:HD12	1:A:261:LEU:C	2.38	0.49
1:A:334:LYS:HE3	1:A:345:MET:HG2	1.94	0.48
1:A:490:GLY:H	1:A:528:PHE:HB3	1.77	0.48
1:A:531:HIS:CG	1:A:532:ILE:N	2.81	0.48
1:B:311:THR:CB	1:B:421:THR:HG21	2.39	0.48
1:B:580:THR:OG1	1:B:589:HIS:O	2.30	0.48
1:A:338:THR:N	1:A:429:ILE:O	2.32	0.48
1:B:329:LEU:HB2	1:B:379:TYR:HB3	1.93	0.48
1:B:422:CYS:HB2	1:B:423:PRO:CD	2.44	0.48
1:B:117:ILE:CD1	1:B:167:MET:HE1	2.42	0.48
1:B:471:LYS:CB	1:B:581:PHE:HB3	2.43	0.48
1:A:101:ARG:HG3	1:A:341:HIS:C	2.39	0.48
1:B:584:TYR:C	1:B:585:VAL:O	2.51	0.48
1:A:272:MET:HB3	1:A:286:LEU:CB	2.44	0.48
1:B:212:GLN:C	1:B:214:SER:H	2.22	0.48
1:B:519:ASP:O	1:B:520:SER:CB	2.61	0.48
1:A:466:ARG:HG3	1:B:505:GLY:HA3	1.95	0.48
1:B:329:LEU:O	1:B:378:GLN:HA	2.14	0.48
1:A:582:LYS:HB2	1:A:585:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HG23	1:B:123:MET:HA	1.95	0.48
1:A:164:THR:O	1:A:168:GLN:HG3	2.14	0.47
1:A:335:PHE:HA	1:A:433:LEU:HD23	1.96	0.47
1:B:311:THR:HA	1:B:421:THR:CB	2.44	0.47
1:B:317:ILE:HD12	1:B:317:ILE:C	2.39	0.47
1:B:584:TYR:O	1:B:585:VAL:C	2.56	0.47
1:B:590:LYS:HG3	1:B:591:ARG:H	1.79	0.47
1:A:313:HIS:ND1	1:A:457:ARG:HA	2.29	0.47
1:B:373:TYR:N	1:B:468:LYS:O	2.42	0.47
1:A:5:ARG:NH1	1:A:272:MET:O	2.48	0.47
1:A:329:LEU:HB2	1:A:379:TYR:HB3	1.97	0.47
1:B:372:GLU:HG2	1:B:468:LYS:CB	2.45	0.47
1:B:469:VAL:O	1:B:582:LYS:HA	2.13	0.47
1:A:100:ILE:O	1:A:103:ILE:HG22	2.14	0.47
1:A:351:PHE:CZ	1:A:411:TRP:HB2	2.48	0.47
1:A:318:SER:O	1:A:448:GLY:HA3	2.15	0.47
1:A:323:PRO:C	1:A:325:PHE:H	2.23	0.47
1:A:334:LYS:HD2	1:A:347:ARG:CG	2.45	0.47
1:B:317:ILE:O	1:B:317:ILE:HD12	2.14	0.47
1:A:93:CYS:CB	1:A:94:PRO:HD2	2.45	0.47
1:A:259:PRO:HD2	3:A:1109:HOH:O	2.15	0.47
1:A:9:ASN:HD21	1:A:244:THR:HG21	1.80	0.47
1:B:528:PHE:O	1:B:529:LYS:CB	2.60	0.47
1:B:245:ILE:HB	1:B:281:MET:O	2.15	0.47
1:A:99:LEU:O	1:A:103:ILE:HG22	2.14	0.46
1:A:113:MET:HE3	1:A:113:MET:HB3	1.85	0.46
1:A:115:LEU:HD12	1:A:115:LEU:HA	1.60	0.46
1:A:224:PHE:CG	1:A:250:ILE:HD11	2.49	0.46
1:A:225:LEU:HD11	1:A:302:LEU:CD2	2.41	0.46
1:B:132:VAL:O	1:B:136:ILE:HG13	2.16	0.46
1:B:347:ARG:HG2	3:B:1106:HOH:O	2.15	0.46
1:B:364:LEU:C	1:B:451:LEU:HD21	2.40	0.46
1:B:202:ILE:CB	1:B:203:PRO:HD3	2.45	0.46
1:B:338:THR:HA	1:B:343:THR:HA	1.96	0.46
1:B:580:THR:HG23	1:B:590:LYS:HD2	1.88	0.46
1:A:466:ARG:NH1	1:B:589:HIS:ND1	2.64	0.46
1:B:346:GLY:O	1:B:347:ARG:HD3	2.16	0.46
1:A:477:GLY:HA3	1:A:492:SER:OG	2.15	0.46
1:A:258:ILE:CB	1:A:261:LEU:HG	2.44	0.46
1:B:8:VAL:CG2	1:B:88:VAL:HG22	2.45	0.46
1:B:348:LEU:HG	1:B:349:MET:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG11	1:A:167:MET:HE2	1.98	0.46
1:A:147:LYS:C	1:A:149:ASP:H	2.24	0.46
1:B:8:VAL:HG23	1:B:88:VAL:HG13	1.96	0.46
1:B:316:LEU:HD12	1:B:412:ALA:O	2.16	0.46
1:B:477:GLY:HA3	1:B:492:SER:CB	2.30	0.46
1:A:485:ASP:O	1:A:536:LEU:N	2.49	0.46
1:B:347:ARG:O	1:B:348:LEU:HB2	2.16	0.46
1:A:13:LEU:HD11	1:A:113:MET:HB3	1.98	0.46
1:A:115:LEU:HB2	1:A:141:LEU:HD21	1.98	0.46
1:A:267:VAL:HG12	1:A:267:VAL:O	2.15	0.46
1:A:114:MET:CE	1:A:209:LEU:HD21	2.40	0.46
1:A:132:VAL:HG13	1:A:133:ILE:H	1.81	0.46
1:A:313:HIS:HE2	1:A:419:PRO:HB3	1.78	0.46
1:A:352:SER:CB	1:A:410:GLN:HE21	2.27	0.46
1:A:480:GLU:HG3	1:A:481:ARG:N	2.27	0.46
1:A:413:LEU:HD23	1:A:415:GLU:HG3	1.97	0.46
1:B:473:LYS:H	1:B:579:LEU:CD1	2.29	0.46
1:A:23:LEU:HD23	1:A:23:LEU:C	2.40	0.45
1:A:353:PRO:HG2	1:A:358:PHE:HD1	1.80	0.45
1:B:582:LYS:HB2	1:B:585:VAL:HG12	1.98	0.45
1:A:251:SER:N	1:A:254:ASP:OD2	2.49	0.45
1:A:590:LYS:HG3	1:A:591:ARG:H	1.79	0.45
1:B:187:LYS:O	2:B:1001:GDP:C5	2.66	0.45
1:B:417:GLU:HG3	3:B:1106:HOH:O	2.16	0.45
1:A:339:VAL:O	1:A:427:LEU:O	2.35	0.45
1:B:136:ILE:CD1	1:B:447:HIS:HB3	2.41	0.45
1:B:275:MET:N	1:B:276:PRO:CD	2.77	0.45
1:A:258:ILE:HB	1:A:261:LEU:CG	2.46	0.45
1:A:180:PRO:HG2	1:A:208:LEU:HD21	1.99	0.45
1:B:208:LEU:O	1:B:211:SER:CB	2.65	0.45
1:B:494:PHE:O	1:B:495:LYS:CB	2.64	0.45
1:A:113:MET:HB2	1:A:141:LEU:CD1	2.46	0.45
1:B:357:ASN:C	1:B:359:ASP:N	2.75	0.45
1:B:20:LYS:CA	2:B:1001:GDP:O1A	2.61	0.44
1:B:322:ILE:HG13	1:B:446:PHE:CA	2.45	0.44
1:A:140:LYS:CD	1:A:141:LEU:H	2.31	0.44
1:A:431:SER:CB	1:A:445:ALA:HB3	2.46	0.44
1:A:202:ILE:HB	1:A:203:PRO:HD3	2.00	0.44
1:B:411:TRP:O	1:B:412:ALA:HB2	2.17	0.44
1:A:220:PRO:HG3	1:A:281:MET:CE	2.47	0.44
1:A:349:MET:HE3	1:A:375:PHE:HE2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:SER:HA	1:B:411:TRP:CD1	2.53	0.44
1:A:21:THR:O	1:A:21:THR:HG22	2.16	0.44
1:A:424:ARG:HD2	1:B:486:TYR:CE2	2.53	0.44
1:B:590:LYS:CG	1:B:591:ARG:N	2.81	0.44
1:A:5:ARG:CZ	1:A:272:MET:HE2	2.48	0.44
1:A:258:ILE:HG22	1:A:261:LEU:HG	2.00	0.44
1:A:7:ASN:HD21	1:A:89:THR:CG2	2.31	0.44
1:A:256:VAL:O	1:A:264:VAL:HA	2.18	0.44
1:A:338:THR:HA	1:A:343:THR:HA	1.99	0.44
1:A:423:PRO:HB2	1:A:426:CYS:HB3	1.99	0.44
1:A:450:LEU:HD23	1:A:450:LEU:C	2.43	0.44
1:A:224:PHE:CZ	1:A:226:MET:HB2	2.53	0.44
1:A:431:SER:CB	1:A:445:ALA:H	2.30	0.44
1:A:590:LYS:CG	1:A:591:ARG:N	2.81	0.44
1:B:148:ILE:HB	1:B:185:ALA:HB2	2.00	0.44
1:B:527:LYS:O	1:B:528:PHE:HB2	2.17	0.44
1:A:319:VAL:HG12	1:A:320:GLU:N	2.33	0.44
1:A:334:LYS:HB3	1:A:433:LEU:HD21	1.99	0.44
1:A:588:THR:HG23	1:A:589:HIS:N	2.13	0.44
1:B:425:LEU:N	1:B:425:LEU:HD23	2.32	0.44
1:A:142:VAL:HG22	1:A:180:PRO:HG2	1.99	0.43
1:A:144:VAL:HG11	1:A:205:LEU:HD13	2.00	0.43
1:B:579:LEU:HA	1:B:590:LYS:HB2	2.00	0.43
1:A:323:PRO:O	1:A:325:PHE:N	2.51	0.43
1:A:332:LYS:O	1:A:347:ARG:NH1	2.52	0.43
1:B:117:ILE:CG1	1:B:167:MET:HE1	2.46	0.43
1:A:118:ASP:C	1:A:120:THR:H	2.26	0.43
1:A:322:ILE:HG23	1:A:323:PRO:HD2	2.00	0.43
1:B:166:LYS:HG2	1:B:167:MET:N	2.33	0.43
1:B:224:PHE:HD2	1:B:304:CYS:CA	2.28	0.43
1:A:100:ILE:HA	1:A:103:ILE:HG22	2.01	0.43
1:B:245:ILE:HD12	1:B:280:ALA:CB	2.48	0.43
1:B:316:LEU:CD2	1:B:367:PHE:CE2	3.02	0.43
1:A:420:VAL:CG2	1:A:421:THR:H	2.30	0.43
1:A:477:GLY:HA2	1:A:492:SER:HB3	2.01	0.43
1:A:7:ASN:OD1	1:A:8:VAL:N	2.51	0.43
1:A:113:MET:HG2	1:A:138:CYS:CB	2.49	0.43
1:A:317:ILE:HA	1:A:449:ILE:O	2.18	0.43
1:A:317:ILE:HG23	1:A:414:VAL:CG2	2.48	0.43
1:A:339:VAL:HG12	1:A:426:CYS:SG	2.58	0.43
1:B:26:ALA:O	1:B:30:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:O	1:A:99:LEU:HD11	2.19	0.43
1:A:377:GLU:O	1:A:377:GLU:HG3	2.19	0.43
1:B:220:PRO:CB	1:B:249:SER:HB2	2.47	0.43
1:B:502:LEU:HD12	1:B:502:LEU:N	2.34	0.43
1:B:545:THR:CB	1:B:546:PRO:HD2	2.49	0.43
1:A:319:VAL:CG2	1:A:412:ALA:HB3	2.49	0.42
1:B:347:ARG:CZ	1:B:417:GLU:OE2	2.67	0.42
1:B:450:LEU:C	1:B:450:LEU:HD23	2.44	0.42
1:A:99:LEU:HD23	1:A:99:LEU:C	2.44	0.42
1:A:116:VAL:O	1:A:117:ILE:HD13	2.19	0.42
1:A:117:ILE:HG23	1:A:122:GLY:O	2.17	0.42
1:A:406:CYS:CB	1:A:407:PRO:CD	2.97	0.42
1:A:466:ARG:HD2	1:B:589:HIS:CE1	2.54	0.42
1:B:450:LEU:HD23	1:B:452:HIS:N	2.34	0.42
1:B:484:ASP:O	1:B:536:LEU:HD11	2.20	0.42
1:B:525:SER:C	1:B:527:LYS:H	2.27	0.42
1:B:568:ARG:O	1:B:569:SER:CB	2.66	0.42
1:A:132:VAL:O	1:A:133:ILE:C	2.62	0.42
1:A:360:GLN:HG2	1:A:361:GLU:N	2.34	0.42
1:B:362:PRO:HA	1:B:409:GLN:HE21	1.78	0.42
1:B:447:HIS:O	1:B:447:HIS:ND1	2.52	0.42
1:B:473:LYS:H	1:B:579:LEU:HD12	1.84	0.42
1:B:337:ILE:HA	1:B:430:GLY:CA	2.49	0.42
1:A:13:LEU:CD1	1:A:113:MET:HE3	2.45	0.42
1:A:420:VAL:CG2	1:A:421:THR:N	2.82	0.42
1:A:466:ARG:CD	1:B:589:HIS:HE1	2.32	0.42
1:A:466:ARG:HD3	1:A:466:ARG:HA	1.92	0.42
1:A:140:LYS:CG	1:A:141:LEU:H	2.33	0.42
1:A:250:ILE:HG23	1:A:250:ILE:HD12	1.76	0.42
1:B:95:GLY:O	1:B:96:HIS:C	2.63	0.42
1:A:427:LEU:HD23	1:A:427:LEU:C	2.45	0.42
1:B:322:ILE:HD12	1:B:445:ALA:N	2.34	0.42
1:A:144:VAL:HG12	1:A:182:ILE:CB	2.39	0.42
1:A:368:ASN:O	1:A:371:GLN:HG2	2.19	0.42
1:A:579:LEU:HA	1:A:590:LYS:CB	2.39	0.42
1:A:149:ASP:OD1	1:A:150:LEU:HD13	2.20	0.42
1:B:587:ASP:O	1:B:588:THR:HB	2.20	0.42
1:A:208:LEU:O	1:A:209:LEU:C	2.63	0.41
1:B:152:PRO:C	1:B:154:GLY:H	2.28	0.41
1:B:245:ILE:HD12	1:B:280:ALA:HB3	2.02	0.41
1:A:114:MET:HA	1:A:142:VAL:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:CYS:CB	1:A:423:PRO:CD	2.97	0.41
1:B:471:LYS:HB2	1:B:581:PHE:HB3	2.02	0.41
1:A:140:LYS:HD2	1:A:141:LEU:N	2.36	0.41
1:A:185:ALA:HB3	1:A:200:GLN:OE1	2.20	0.41
1:A:466:ARG:HH11	1:B:589:HIS:CE1	2.38	0.41
1:B:224:PHE:CE2	1:B:304:CYS:HA	2.55	0.41
1:B:486:TYR:HB3	1:B:532:ILE:O	2.20	0.41
1:A:469:VAL:O	1:A:582:LYS:HA	2.20	0.41
1:A:490:GLY:CA	1:A:528:PHE:HD2	2.33	0.41
1:A:579:LEU:HD12	1:A:579:LEU:C	2.46	0.41
1:B:313:HIS:CD2	1:B:419:PRO:HB3	2.55	0.41
1:B:346:GLY:O	1:B:347:ARG:NH1	2.49	0.41
1:B:475:LYS:HB3	1:B:493:LEU:CB	2.50	0.41
1:A:106:GLY:O	1:A:107:ALA:C	2.63	0.41
1:A:148:ILE:HG22	1:A:184:VAL:C	2.45	0.41
1:A:19:GLY:HA3	1:A:146:ASN:ND2	2.36	0.41
1:A:590:LYS:CG	1:A:591:ARG:H	2.34	0.41
1:B:590:LYS:O	1:B:591:ARG:CB	2.69	0.41
1:A:149:ASP:OD1	1:A:150:LEU:CD1	2.69	0.41
1:A:312:VAL:HG13	1:A:314:ALA:O	2.21	0.41
1:B:335:PHE:CE2	1:B:446:PHE:HE2	2.39	0.41
1:B:529:LYS:O	1:B:530:ILE:HD12	2.21	0.41
1:A:344:VAL:HG11	1:A:420:VAL:HB	2.03	0.41
1:A:451:LEU:O	1:A:452:HIS:HB2	2.20	0.41
1:B:372:GLU:CG	1:B:582:LYS:HZ2	2.33	0.41
1:B:528:PHE:HD1	1:B:529:LYS:H	1.67	0.41
1:A:240:VAL:HG12	1:A:241:MET:N	2.36	0.40
1:A:590:LYS:O	1:A:591:ARG:CB	2.69	0.40
1:A:272:MET:O	1:A:272:MET:HG3	2.21	0.40
1:A:357:ASN:ND2	1:A:360:GLN:OE1	2.54	0.40
1:A:418:LYS:O	1:A:420:VAL:N	2.54	0.40
1:B:318:SER:HA	1:B:411:TRP:HD1	1.86	0.40
1:A:528:PHE:HD1	1:A:528:PHE:HA	1.66	0.40
1:A:86:LEU:HD12	1:A:87:GLN:N	2.36	0.40
1:A:126:GLN:C	1:A:128:ALA:H	2.30	0.40
1:A:511:SER:CB	1:A:574:HIS:CB	2.99	0.40
1:B:533:PRO:C	1:B:535:GLY:H	2.30	0.40
1:A:178:GLY:O	1:A:179:ALA:C	2.65	0.40
1:A:492:SER:O	1:A:493:LEU:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/616 (74%)	340 (74%)	99 (22%)	20 (4%)	2	12
1	B	428/616 (70%)	330 (77%)	82 (19%)	16 (4%)	2	15
All	All	887/1232 (72%)	670 (76%)	181 (20%)	36 (4%)	2	13

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	500	ILE
1	A	275	MET
1	A	277	ILE
1	A	324	TYR
1	A	369	PHE
1	B	166	LYS
1	A	31	ALA
1	A	119	VAL
1	A	291	THR
1	B	23	LEU
1	B	545	THR
1	A	148	ILE
1	A	216	PRO
1	A	493	LEU
1	A	533	PRO
1	B	100	ILE
1	B	527	LYS
1	B	533	PRO
1	B	572	SER
1	A	24	ALA
1	B	202	ILE
1	B	277	ILE
1	B	472	LEU
1	B	491	ARG
1	A	191	PRO

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Mol	Chain	Res	Type
1	A	571	PRO
1	B	571	PRO
1	A	61	PRO
1	A	104	ILE
1	B	148	ILE
1	B	213	ILE
1	A	263	VAL
1	A	518	ILE
1	A	419	PRO
1	B	488	VAL
1	B	543	ILE

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	A	261/524 (50%)	243 (93%)	18 (7%)	14	41
1	B	160/524 (30%)	154 (96%)	6 (4%)	29	55
All	All	421/1048 (40%)	397 (94%)	24 (6%)	18	46

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	88	VAL
1	A	119	VAL
1	A	132	VAL
1	A	174	THR
1	A	184	VAL
1	A	228	VAL
1	A	274	HIS
1	A	311	THR
1	A	348	LEU
1	A	358	PHE
1	A	414	VAL

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Mol	Chain	Res	Type
1	A	421	THR
1	A	473	LYS
1	A	528	PHE
1	A	529	LYS
1	A	586	PHE
1	A	589	HIS
1	B	135	GLN
1	B	324	TYR
1	B	377	GLU
1	B	471	LYS
1	B	532	ILE
1	B	589	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	310	HIS
1	A	341	HIS
1	A	410	GLN
1	A	509	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GDP	B	1001	-	29,30,30	1.24	4 (13%)	45,47,47	1.74	11 (24%)
2	GDP	A	1001	-	29,30,30	1.24	3 (10%)	45,47,47	1.72	10 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GDP	B	1001	-	-	3/16/32/32	0/3/3/3
2	GDP	A	1001	-	-	3/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GDP	C5-C6	-2.98	1.33	1.44
2	B	1001	GDP	C5-C6	-2.98	1.33	1.44
2	A	1001	GDP	C5-N7	-2.82	1.33	1.39
2	B	1001	GDP	C5-N7	-2.79	1.33	1.39
2	B	1001	GDP	PB-O2B	-2.01	1.47	1.54
2	A	1001	GDP	PB-O2B	-2.00	1.47	1.54
2	B	1001	GDP	PB-O3B	-2.00	1.47	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	GDP	C2-N3-C4	4.90	120.74	112.30
2	A	1001	GDP	C2-N3-C4	4.86	120.67	112.30
2	A	1001	GDP	C5-C4-N3	-4.54	121.17	128.39
2	B	1001	GDP	C5-C4-N3	-4.53	121.18	128.39
2	A	1001	GDP	C2-N1-C6	-3.79	118.23	125.11
2	B	1001	GDP	C2-N1-C6	-3.77	118.28	125.11
2	A	1001	GDP	N9-C8-N7	-3.02	107.80	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	GDP	N9-C8-N7	-3.00	107.84	113.40
2	A	1001	GDP	N9-C4-N3	2.59	131.14	125.95
2	B	1001	GDP	N9-C4-N3	2.59	131.13	125.95
2	B	1001	GDP	C5-C6-N1	2.52	119.68	113.25
2	A	1001	GDP	C5-C6-N1	2.52	119.66	113.25
2	A	1001	GDP	C4'-O4'-C1'	-2.49	103.97	109.47
2	B	1001	GDP	C4'-O4'-C1'	-2.48	104.00	109.47
2	B	1001	GDP	O3B-PB-O2B	2.25	116.25	107.80
2	A	1001	GDP	C8-N7-C5	2.22	108.22	104.26
2	B	1001	GDP	O6-C6-C5	-2.21	120.69	126.53
2	B	1001	GDP	N1-C2-N3	-2.21	119.28	123.32
2	B	1001	GDP	C8-N7-C5	2.20	108.19	104.26
2	A	1001	GDP	O6-C6-C5	-2.20	120.73	126.53
2	A	1001	GDP	N1-C2-N3	-2.15	119.38	123.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	GDP	C5'-O5'-PA-O3A
2	A	1001	GDP	C5'-O5'-PA-O1A
2	B	1001	GDP	C5'-O5'-PA-O3A
2	B	1001	GDP	C5'-O5'-PA-O1A
2	B	1001	GDP	C5'-O5'-PA-O2A
2	A	1001	GDP	C5'-O5'-PA-O2A

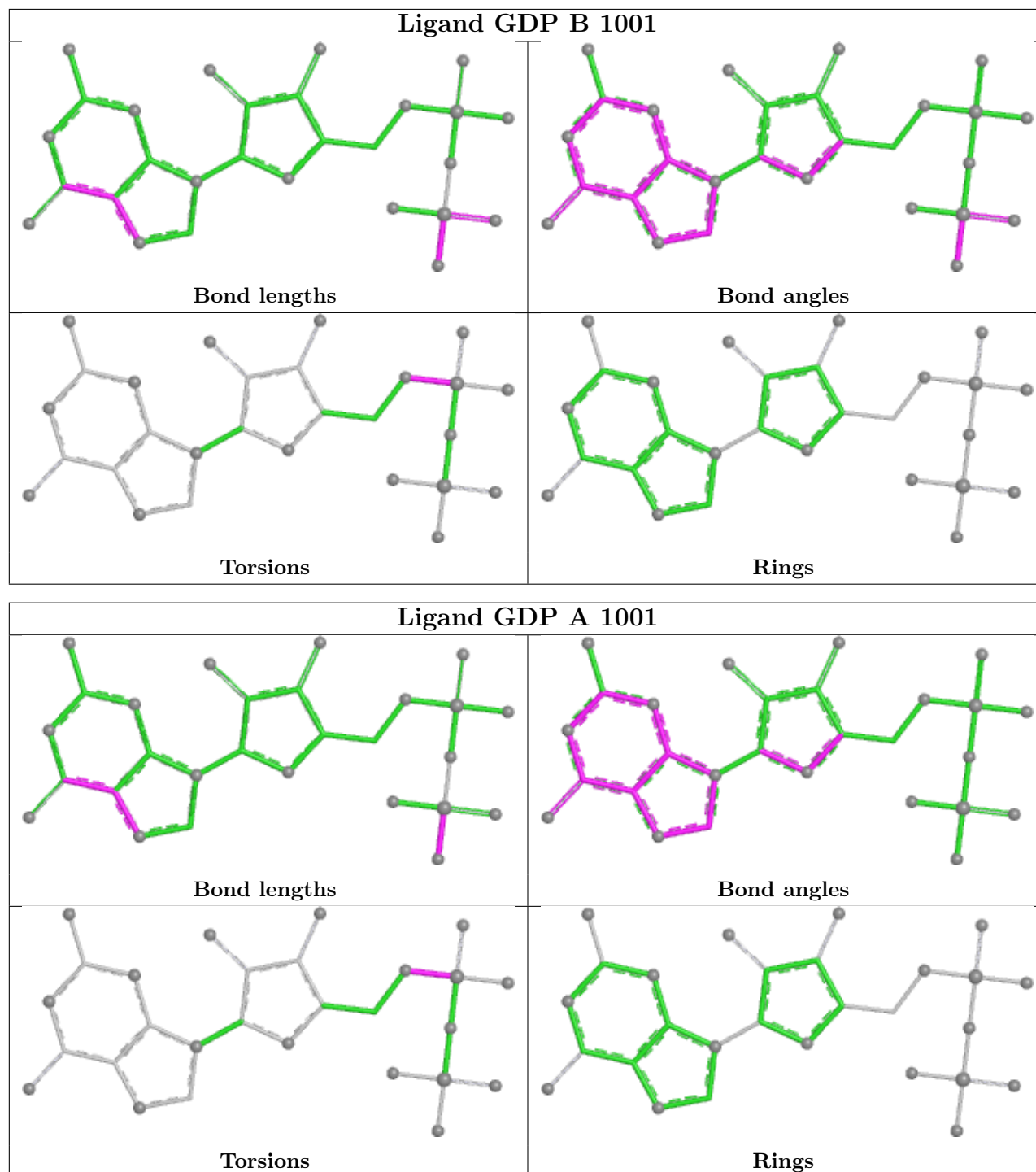
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	GDP	7	0
2	A	1001	GDP	4	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	A	480/616 (77%)	0.33	12 (2%) 58 39	27, 69, 101, 114	1 (0%)
1	B	451/616 (73%)	0.75	43 (9%) 14 11	44, 95, 149, 168	1 (0%)
All	All	931/1232 (75%)	0.53	55 (5%) 28 19	27, 81, 129, 168	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ILE	5.3
1	B	267	VAL	5.2
1	B	298	LEU	4.6
1	B	287	GLY	4.2
1	B	534	GLY	3.9
1	A	442	CYS	3.9
1	A	155	LYS	3.7
1	A	372	GLU	3.7
1	B	299	GLU	3.7
1	B	268	LYS	3.5
1	B	285	ARG	3.5
1	B	251	SER	3.4
1	B	255	SER	3.4
1	B	584	TYR	3.3
1	B	247	SER	3.2
1	B	533	PRO	3.0
1	B	19	GLY	3.0
1	B	10	VAL	3.0
1	B	294	ASP	2.9
1	B	13	LEU	2.9
1	B	286	LEU	2.9
1	B	571	PRO	2.9
1	B	424	ARG	2.8
1	B	117	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	535	GLY	2.7
1	B	23	LEU	2.7
1	B	483	MET	2.6
1	B	88	VAL	2.6
1	B	491	ARG	2.6
1	B	590	LYS	2.6
1	B	422	CYS	2.5
1	A	534	GLY	2.5
1	B	359	ASP	2.5
1	B	265	LYS	2.5
1	B	129	GLU	2.4
1	B	333	ALA	2.4
1	A	371	GLN	2.3
1	B	244	THR	2.3
1	B	569	SER	2.3
1	B	572	SER	2.2
1	B	308	SER	2.2
1	A	467	LEU	2.2
1	B	316	LEU	2.2
1	A	240	VAL	2.2
1	A	349	MET	2.2
1	B	423	PRO	2.2
1	A	130	CYS	2.2
1	B	341	HIS	2.2
1	A	129	GLU	2.1
1	B	243	GLY	2.1
1	A	577	LEU	2.1
1	A	275	MET	2.1
1	B	55	CYS	2.1
1	B	442	CYS	2.1
1	B	219	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

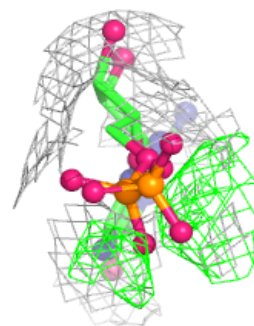
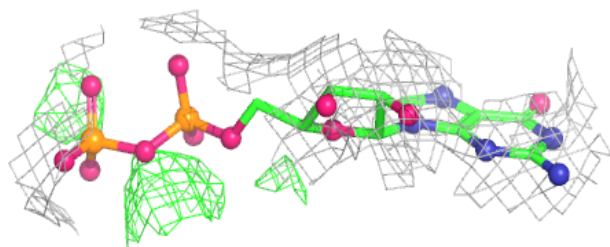
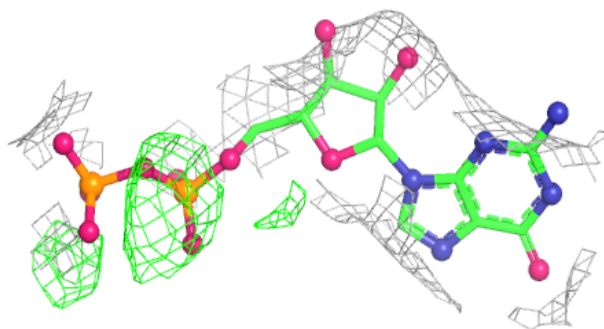
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GDP	B	1001	28/28	0.74	0.13	122,135,153,158	0
2	GDP	A	1001	28/28	0.81	0.14	72,93,113,129	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.

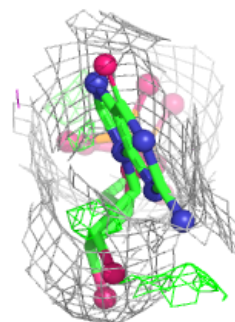
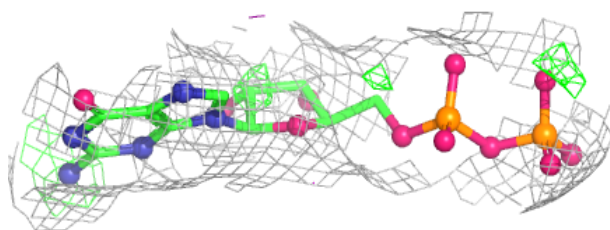
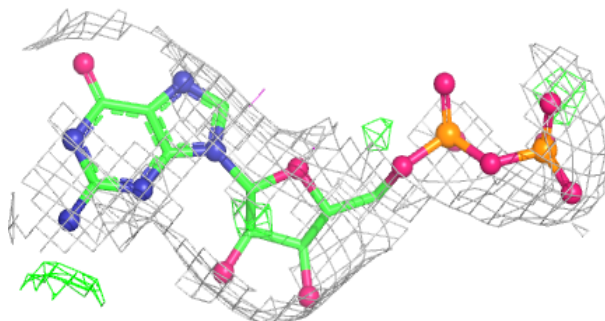
Electron density around GDP B 1001:

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 GDP A 1001:

$2mF_o-DF_c$ (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.