Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 06:47 AM EDT

PDB ID	:	3I1F
Title	:	Gamma-subunit of the translation initiation factor 2 from S. solfataricus in complex with Gpp(CH2)p
Authors	:	Stolboushkina, E.A.; Nikonov, S.V.; Nikulin, A.D.; Blaesi, U.; Garber, M.B.; Nikonov, O.S.
Deposited on	:	2009-06-26
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

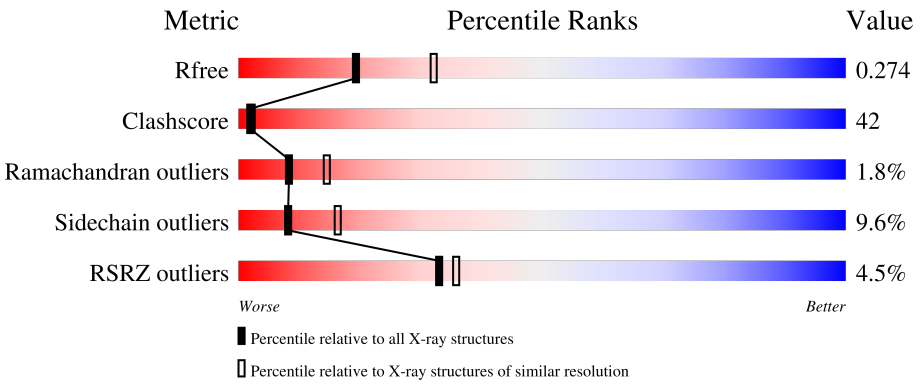
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	415	6% 44% 49% 6%
1	B	415	3% 31% 62% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GCP	A	416	-	-	X	-

2 Entry composition (i)

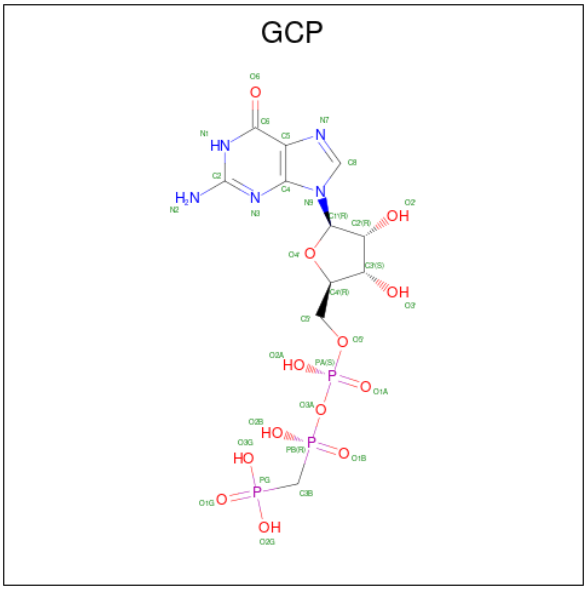
There are 4 unique types of molecules in this entry. The entry contains 6867 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Translation initiation factor 2 subunit gamma.

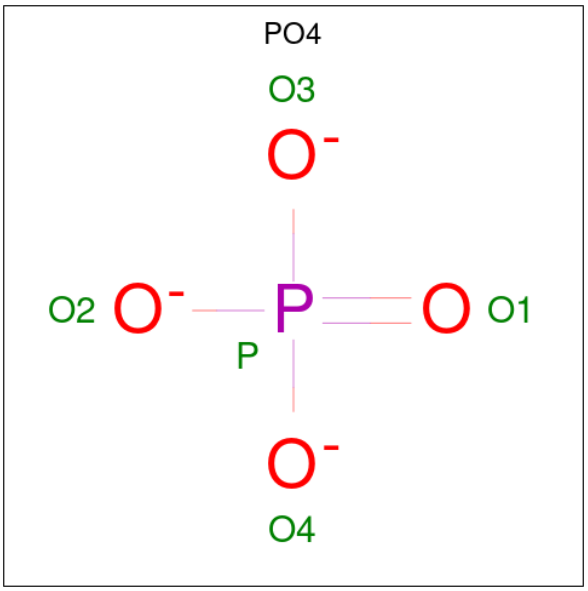
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	414	3213	2058	548	595	12	0	0	0
1	B	414	3213	2058	548	595	12	0	0	0

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	32	11	5	13	3	0	0
2	B	1	32	11	5	13	3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

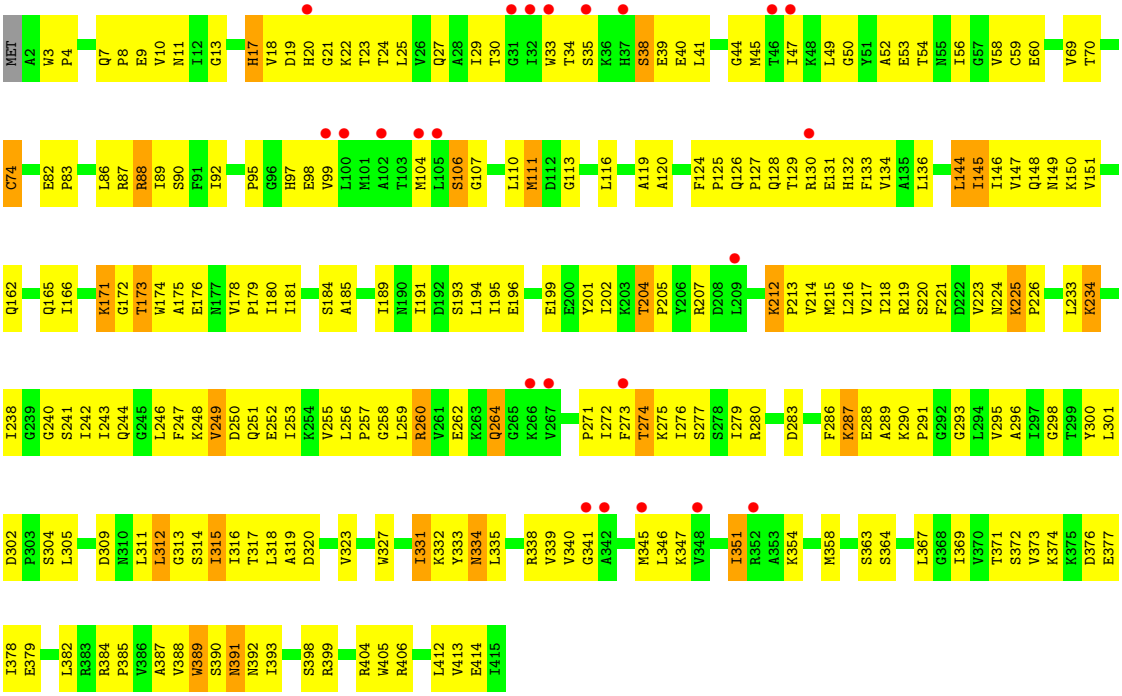
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	157	Total O 157 157	0	0
4	B	200	Total O 200 200	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

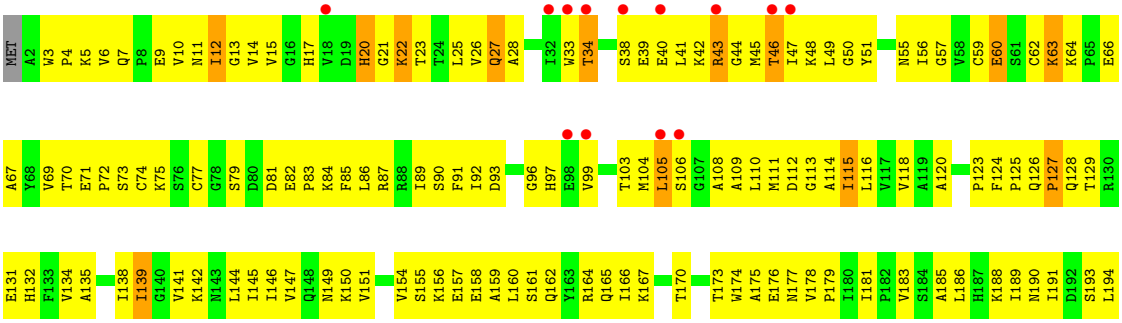
• Molecule 1: Translation initiation factor 2 subunit gamma

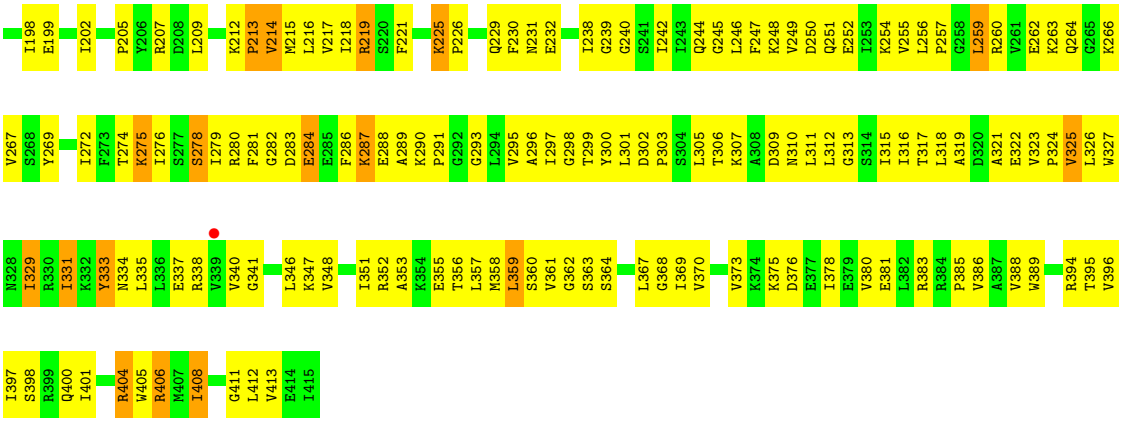
Chain A:



• Molecule 1: Translation initiation factor 2 subunit gamma

Chain B:




I397 S398 R399 Q400 I401 R404 W405 R406 M407 I408 G411 L412 V413 E414 I415
N328 I329 R330 I331 K332 Y333 N334 L335 L336 E337 R338 V339 V340 G341 L346 K347 V348 I351 R352 A353 K354 E355 T356 L357 M358 L359 S360 V361 G362 S363 S364 L367 G368 I369 V370 V373 K374 K375 D376 E377 I378 E379 V380 E381 L382 R383 R384 P385 V386 A387 V388 W389 R394 T395 V396
V267 S268 Y269 I272 F273 T274 K275 I276 S277 S278 I279 R280 F281 G282 D283 E284 E285 F286 K287 E288 A289 K290 P291 G292 G293 L294 V295 A296 I297 G298 T299 Y300 L301 D302 P303 S304 L305 T306 K307 A308 D309 N310 L311 L312 G313 S314 I315 I316 T317 L318 A319 D320 A321 E322 V323 P324 V325 L326 W327
I198 E199 I202 P205 Y206 R207 D208 L209 K212 P213 V214 M215 L216 V217 I218 R219 S220 F221 K225 P226 Q229 F230 N231 E232 I238 G239 G240 S241 I242 I243 Q244 G245 L246 F247 K248 V249 D250 Q251 E252 I253 K254 V255 L256 P257 G258 L259 R260 V261 E262 K263 Q264 G265 K266

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	95.77Å 95.77Å 165.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.40 – 2.50 19.40 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.40-2.50) 98.7 (19.40-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.49Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.226 , 0.266 0.239 , 0.274	Depositor DCC
R_{free} test set	2887 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 92.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.064 for -h,-k,l 0.467 for h,-h-k,-l 0.063 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å^2)	123.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GCP, PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.25	0/3272	0.45	0/4430
1	B	0.25	0/3272	0.44	0/4430
All	All	0.25	0/6544	0.45	0/8860

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3213	0	3332	223	0
1	B	3213	0	3334	329	0
2	A	32	0	14	11	0
2	B	32	0	14	2	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
4	A	157	0	0	5	0
4	B	200	0	0	12	0
All	All	6867	0	6694	548	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 42.

All (548) 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:A:304:SER:HB3	1:B:307:LYS:HD2	1.27	1.07
1:B:216:LEU:HD21	1:B:363:SER:HB2	1.39	1.00
1:A:218:ILE:HG12	1:A:240:GLY:H	1.28	0.99
1:B:47:ILE:HB	1:B:219:ARG:HH22	1.34	0.93
1:B:131:GLU:HG2	1:B:340:VAL:HG21	1.52	0.91
1:B:12:ILE:HD11	1:B:89:ILE:HB	1.53	0.90
1:A:17:HIS:ND1	1:A:128:GLN:HB3	1.86	0.90
1:B:149:ASN:HD21	1:B:185:ALA:H	1.14	0.90
1:A:58:VAL:CG1	1:A:86:LEU:HD11	2.02	0.88
1:A:279:ILE:HD13	1:A:289:ALA:H	1.39	0.87
1:B:352:ARG:HH21	1:B:355:GLU:HA	1.39	0.87
1:B:115:ILE:HG22	1:B:145:ILE:HG13	1.56	0.87
1:B:329:ILE:HG13	1:B:413:VAL:HG13	1.55	0.87
1:A:20:HIS:HB2	1:A:150:LYS:HE3	1.55	0.86
1:A:258:GLY:HA3	1:A:271:PRO:HA	1.59	0.84
1:A:49:LEU:HD22	1:A:92:ILE:HD11	1.58	0.83
1:A:259:LEU:HD12	1:A:260:ARG:HH21	1.43	0.83
1:B:287:LYS:HE3	1:B:288:GLU:HG2	1.59	0.83
1:B:215:MET:HB2	1:B:247:PHE:CE1	2.14	0.82
1:A:58:VAL:HG12	1:A:86:LEU:HD11	1.58	0.82
1:B:69:VAL:HG12	1:B:71:GLU:H	1.47	0.80
1:B:23:THR:HG23	1:B:33:TRP:CD1	2.17	0.79
1:A:338:ARG:HD2	1:A:345:MET:HG3	1.63	0.78
1:A:59:CYS:CB	1:A:74:CYS:SG	2.72	0.77
1:A:280:ARG:HB3	2:A:416:GCP:HN21	1.47	0.77
1:B:11:ASN:HD21	1:B:293:GLY:H	1.33	0.77
1:B:205:PRO:HD2	1:B:207:ARG:HH12	1.49	0.77
1:B:28:ALA:HB1	1:B:191:ILE:HD13	1.67	0.77
1:B:216:LEU:CD2	1:B:363:SER:HB2	2.15	0.77
1:A:327:TRP:CE2	1:A:385:PRO:HG3	2.20	0.76
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.66	0.76
1:B:62:CYS:SG	1:B:77:CYS:HB3	2.25	0.76
1:B:97:HIS:HD2	1:B:99:VAL:H	1.33	0.76
1:B:173:THR:HG23	1:B:175:ALA:H	1.50	0.76
1:B:361:VAL:HG21	1:B:386:VAL:HG23	1.68	0.75
1:B:341:GLY:HA3	1:B:346:LEU:HD23	1.67	0.75
1:B:370:VAL:HA	1:B:380:VAL:HG12	1.68	0.75
1:B:62:CYS:SG	1:B:77:CYS:CB	2.75	0.75
1:A:59:CYS:HB2	1:A:74:CYS:SG	2.27	0.74
1:A:218:ILE:HG12	1:A:240:GLY:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:VAL:HG12	1:A:345:MET:HB3	1.68	0.74
1:A:296:ALA:HB3	2:A:416:GCP:N2	2.03	0.74
1:B:162:GLN:HA	1:B:165:GLN:HG2	1.69	0.74
1:A:275:LYS:HG2	1:A:276:ILE:N	2.03	0.73
1:B:47:ILE:H	1:B:219:ARG:HH12	1.36	0.73
1:B:59:CYS:HB2	1:B:62:CYS:HB2	1.70	0.72
1:B:142:LYS:HG3	1:B:174:TRP:CD1	2.24	0.72
1:A:259:LEU:HB2	1:A:272:ILE:HD11	1.70	0.72
1:B:325:VAL:HG12	1:B:385:PRO:HB2	1.71	0.72
1:A:279:ILE:HD13	1:A:289:ALA:N	2.04	0.71
1:B:360:SER:HB2	1:B:396:VAL:H	1.54	0.71
1:A:44:GLY:O	2:A:416:GCP:H3B1	1.90	0.71
1:B:215:MET:HB2	1:B:247:PHE:HE1	1.55	0.71
1:B:276:ILE:HG21	1:B:279:ILE:HD11	1.73	0.71
1:A:296:ALA:HB3	2:A:416:GCP:HN22	1.55	0.70
1:A:56:ILE:O	1:A:86:LEU:HB2	1.90	0.70
1:B:327:TRP:CE2	1:B:385:PRO:HG3	2.25	0.70
1:A:331:ILE:HG22	1:A:413:VAL:HA	1.74	0.70
1:B:28:ALA:HB1	1:B:191:ILE:CD1	2.23	0.69
1:B:33:TRP:HH2	1:B:50:GLY:HA3	1.58	0.69
1:B:134:VAL:O	1:B:138:ILE:HG12	1.92	0.69
1:A:373:VAL:HA	1:A:378:ILE:HG22	1.75	0.68
1:B:14:VAL:HB	1:B:93:ASP:HB3	1.75	0.68
1:B:262:GLU:HA	1:B:267:VAL:H	1.58	0.68
1:B:352:ARG:HB3	1:B:355:GLU:HB2	1.75	0.68
1:B:225:LYS:HG3	1:B:226:PRO:HD2	1.76	0.68
1:B:118:VAL:HG21	1:B:124:PHE:HB2	1.76	0.67
1:A:33:TRP:CD2	1:A:52:ALA:HB2	2.30	0.67
1:A:351:ILE:HD13	1:A:351:ILE:H	1.59	0.67
2:A:416:GCP:H3B2	2:A:416:GCP:O2A	1.94	0.67
1:B:164:ARG:HD3	4:B:523:HOH:O	1.95	0.67
1:A:207:ARG:NH1	1:A:291:PRO:HB3	2.10	0.66
1:B:49:LEU:HD11	1:B:103:THR:HB	1.76	0.66
1:A:30:THR:HG23	1:A:54:THR:HB	1.78	0.66
1:B:47:ILE:HB	1:B:219:ARG:NH2	2.10	0.66
1:B:259:LEU:O	1:B:269:TYR:HA	1.96	0.66
1:A:58:VAL:HG12	1:A:86:LEU:CD1	2.26	0.65
1:A:215:MET:HB3	1:A:316:ILE:HB	1.79	0.65
1:B:217:VAL:HG13	1:B:238:ILE:HG23	1.78	0.65
1:A:33:TRP:CG	1:A:52:ALA:HB2	2.31	0.65
1:A:243:ILE:HG13	1:A:244:GLN:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ARG:HH12	1:B:198:ILE:HG22	1.61	0.65
1:A:17:HIS:CD2	1:A:18:VAL:HG22	2.32	0.65
1:A:171:LYS:HG3	1:A:172:GLY:H	1.61	0.64
1:A:274:THR:HG21	1:A:301:LEU:HG	1.79	0.64
1:B:59:CYS:CB	1:B:62:CYS:HB2	2.28	0.64
1:A:162:GLN:HA	1:A:165:GLN:HE21	1.62	0.64
1:B:15:VAL:HG13	1:B:116:LEU:HA	1.77	0.64
1:A:217:VAL:HG13	1:A:238:ILE:HG23	1.79	0.64
1:B:400:GLN:HA	1:B:405:TRP:HA	1.80	0.64
1:B:11:ASN:HD21	1:B:293:GLY:N	1.95	0.63
1:B:155:SER:H	1:B:158:GLU:HG2	1.62	0.63
1:B:361:VAL:HG12	1:B:362:GLY:H	1.61	0.63
1:A:56:ILE:HG13	1:A:89:ILE:HD12	1.80	0.63
1:A:218:ILE:O	1:A:312:LEU:HD13	1.99	0.63
1:A:280:ARG:HB3	2:A:416:GCP:N2	2.12	0.63
1:B:10:VAL:HG12	1:B:11:ASN:N	2.13	0.62
1:B:33:TRP:CH2	1:B:50:GLY:HA3	2.34	0.62
1:B:116:LEU:HB3	1:B:146:ILE:HD12	1.81	0.62
1:B:331:ILE:HG13	1:B:378:ILE:HG13	1.79	0.62
1:A:20:HIS:C	1:A:149:ASN:HD22	2.01	0.62
1:B:97:HIS:CD2	1:B:99:VAL:H	2.18	0.62
1:A:17:HIS:C	1:A:19:ASP:H	2.03	0.62
1:B:274:THR:HG21	1:B:301:LEU:HG	1.81	0.62
1:B:238:ILE:HD11	1:B:311:LEU:HD12	1.80	0.62
1:A:95:PRO:HD2	1:A:97:HIS:CE1	2.35	0.61
1:B:214:VAL:HG22	1:B:244:GLN:HG2	1.82	0.61
1:A:382:LEU:HD13	1:A:384:ARG:O	2.00	0.61
1:B:45:MET:HB3	1:B:48:LYS:HG3	1.82	0.61
1:B:247:PHE:HZ	1:B:317:THR:HA	1.66	0.61
1:A:10:VAL:HG22	1:A:11:ASN:H	1.64	0.61
1:B:255:VAL:HG22	1:B:316:ILE:HD12	1.82	0.61
1:A:246:LEU:HD23	1:A:247:PHE:N	2.16	0.61
1:A:224:ASN:OD1	1:A:233:LEU:HB2	2.00	0.60
1:B:155:SER:N	1:B:158:GLU:HG2	2.15	0.60
1:B:209:LEU:HG	1:B:246:LEU:HD23	1.83	0.60
1:B:186:LEU:HB3	4:B:504:HOH:O	2.01	0.60
1:A:289:ALA:O	1:A:290:LYS:HG3	2.02	0.59
1:B:149:ASN:ND2	1:B:150:LYS:H	2.00	0.59
1:B:183:VAL:HG12	1:B:190:ASN:HD22	1.66	0.59
1:B:60:GLU:H	1:B:60:GLU:CD	2.05	0.59
1:B:142:LYS:HG3	1:B:174:TRP:HD1	1.63	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:HIS:O	1:B:20:HIS:HB2	2.03	0.59
1:B:207:ARG:HE	1:B:291:PRO:HB2	1.66	0.59
1:B:287:LYS:N	1:B:287:LYS:HE2	2.16	0.59
1:A:20:HIS:CB	1:A:150:LYS:HE3	2.29	0.59
1:A:127:PRO:O	1:A:130:ARG:HG2	2.02	0.59
1:A:351:ILE:HD13	1:A:351:ILE:N	2.17	0.59
1:B:42:LYS:HG2	1:B:282:GLY:HA3	1.85	0.59
1:B:73:SER:HA	1:B:83:PRO:HD3	1.85	0.59
1:B:331:ILE:HG21	1:B:395:THR:HG21	1.84	0.59
1:A:23:THR:O	1:A:27:GLN:HG3	2.03	0.59
1:A:107:GLY:HA2	1:A:110:LEU:HD22	1.85	0.59
1:B:217:VAL:HG22	1:B:238:ILE:HG21	1.83	0.59
1:A:8:PRO:HB2	1:A:293:GLY:HA3	1.85	0.59
1:A:338:ARG:HD2	1:A:345:MET:CG	2.31	0.59
1:A:173:THR:HG22	1:A:174:TRP:H	1.67	0.59
1:A:224:ASN:HA	4:A:548:HOH:O	2.03	0.59
1:B:219:ARG:HE	1:B:219:ARG:HA	1.67	0.59
1:B:275:LYS:HB2	1:B:300:TYR:CD2	2.38	0.59
1:B:46:THR:HG22	1:B:47:ILE:H	1.68	0.58
1:A:338:ARG:NH1	1:A:347:LYS:HE2	2.18	0.58
1:B:124:PHE:CD2	1:B:125:PRO:HD3	2.38	0.58
1:B:249:VAL:HG23	1:B:287:LYS:O	2.04	0.58
1:A:327:TRP:HA	1:A:382:LEU:HD11	1.85	0.58
1:B:42:LYS:CG	1:B:282:GLY:HA3	2.34	0.58
1:A:39:GLU:HA	1:A:41:LEU:H	1.68	0.58
1:B:329:ILE:HD11	1:B:331:ILE:HG23	1.85	0.57
1:B:33:TRP:CG	1:B:34:THR:N	2.72	0.57
1:B:150:LYS:HE2	1:B:186:LEU:H	1.69	0.57
1:B:213:PRO:HB3	1:B:246:LEU:O	2.04	0.57
1:B:299:THR:OG1	1:B:301:LEU:HB2	2.04	0.57
1:B:299:THR:C	1:B:301:LEU:H	2.08	0.57
1:A:387:ALA:HB1	4:A:424:HOH:O	2.05	0.57
1:B:45:MET:HB3	1:B:48:LYS:CG	2.35	0.57
1:B:51:TYR:CE2	1:B:90:SER:HB2	2.40	0.57
1:B:376:ASP:HB2	4:B:537:HOH:O	2.03	0.57
1:A:145:ILE:HA	1:A:179:PRO:HD2	1.86	0.57
4:A:572:HOH:O	1:B:275:LYS:HE2	2.05	0.57
1:B:128:GLN:HG3	1:B:132:HIS:CD2	2.40	0.57
1:B:22:LYS:HE3	1:B:23:THR:H	1.69	0.56
1:B:154:VAL:HG21	1:B:159:ALA:HB2	1.86	0.56
1:B:275:LYS:HB2	1:B:300:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:HIS:HB2	1:B:97:HIS:HA	1.87	0.56
1:B:274:THR:HG21	1:B:299:THR:HB	1.86	0.56
1:A:126:GLN:HB3	1:A:129:THR:HB	1.88	0.56
1:B:56:ILE:HG22	1:B:86:LEU:HB2	1.87	0.56
1:B:57:GLY:HA2	1:B:84:LYS:O	2.06	0.56
1:B:131:GLU:CG	1:B:340:VAL:HG21	2.31	0.56
1:A:13:GLY:HA2	1:A:92:ILE:O	2.04	0.56
1:A:391:ASN:HD21	1:A:414:GLU:HA	1.69	0.56
1:A:259:LEU:HD12	1:A:260:ARG:NH2	2.18	0.56
1:B:3:TRP:CD1	1:B:85:PHE:HB2	2.41	0.56
1:B:39:GLU:O	1:B:42:LYS:HB2	2.06	0.56
1:B:79:SER:HB3	1:B:81:ASP:OD1	2.06	0.56
1:B:21:GLY:O	1:B:25:LEU:HB2	2.05	0.55
1:B:47:ILE:N	1:B:219:ARG:HH12	2.03	0.55
1:B:333:TYR:CE1	1:B:335:LEU:HD13	2.41	0.55
1:A:216:LEU:HB3	1:A:363:SER:HB2	1.87	0.55
1:B:44:GLY:O	1:B:46:THR:HB	2.06	0.55
1:B:127:PRO:HA	4:B:466:HOH:O	2.06	0.55
1:B:326:LEU:O	1:B:385:PRO:HA	2.06	0.55
1:B:22:LYS:O	1:B:26:VAL:HG23	2.07	0.55
1:A:128:GLN:O	1:A:131:GLU:HG2	2.06	0.55
1:B:278:SER:HB2	1:B:298:GLY:HA3	1.87	0.55
1:A:280:ARG:HD2	2:A:416:GCP:C2	2.37	0.55
1:B:72:PRO:O	1:B:82:GLU:HG2	2.07	0.55
1:B:309:ASP:O	1:B:312:LEU:HD22	2.07	0.55
1:B:14:VAL:HG21	1:B:26:VAL:HG22	1.88	0.55
1:A:272:ILE:HD13	1:A:305:LEU:HD13	1.89	0.54
1:B:124:PHE:O	1:B:129:THR:HG21	2.06	0.54
1:B:275:LYS:H	1:B:275:LYS:HD2	1.72	0.54
1:A:253:ILE:HD12	1:A:316:ILE:HD12	1.90	0.54
1:A:8:PRO:HA	1:A:88:ARG:HB3	1.88	0.54
1:A:20:HIS:HB2	1:A:150:LYS:CE	2.34	0.54
1:B:126:GLN:HB3	1:B:127:PRO:HD2	1.88	0.54
1:B:138:ILE:C	1:B:394:ARG:HH21	2.11	0.54
1:B:255:VAL:HB	1:B:272:ILE:HB	1.89	0.54
1:B:263:LYS:O	1:B:264:GLN:HB3	2.07	0.54
1:A:34:THR:HB	1:A:35:SER:HA	1.89	0.54
1:A:213:PRO:HG2	1:A:318:LEU:HD13	1.89	0.54
1:A:106:SER:O	1:A:110:LEU:HD13	2.08	0.54
1:A:304:SER:HB3	1:B:307:LYS:CD	2.20	0.54
1:B:22:LYS:NZ	1:B:96:GLY:H	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:LYS:HD2	4:B:504:HOH:O	2.08	0.54
1:A:191:ILE:O	1:A:195:ILE:HG12	2.08	0.53
1:B:12:ILE:HD13	1:B:12:ILE:N	2.23	0.53
1:B:194:LEU:O	1:B:198:ILE:HG13	2.08	0.53
1:A:10:VAL:HG22	1:A:11:ASN:N	2.22	0.53
1:A:87:ARG:HG3	1:A:199:GLU:OE1	2.08	0.53
1:B:9:GLU:HG2	4:B:422:HOH:O	2.07	0.53
1:B:74:CYS:SG	1:B:83:PRO:HG3	2.49	0.53
1:A:17:HIS:NE2	1:A:18:VAL:HG22	2.24	0.53
1:A:17:HIS:CG	1:A:18:VAL:H	2.26	0.53
1:A:257:PRO:HD2	4:A:537:HOH:O	2.08	0.53
1:B:22:LYS:HZ1	1:B:96:GLY:H	1.56	0.53
1:A:175:ALA:HB1	1:A:178:VAL:HB	1.91	0.53
1:A:286:PHE:HD2	1:A:287:LYS:HD2	1.73	0.53
1:B:138:ILE:HG22	1:B:396:VAL:HG22	1.91	0.53
1:B:212:LYS:O	1:B:244:GLN:HG3	2.09	0.53
1:B:302:ASP:HB3	1:B:305:LEU:HD23	1.91	0.53
1:B:359:LEU:HB3	1:B:395:THR:OG1	2.09	0.53
1:B:369:ILE:HG13	1:B:383:ARG:NH2	2.25	0.53
1:A:374:LYS:HD2	1:A:377:GLU:O	2.09	0.52
1:A:17:HIS:CG	1:A:18:VAL:N	2.77	0.52
1:A:25:LEU:O	1:A:29:ILE:HG13	2.09	0.52
1:B:134:VAL:HG23	1:B:135:ALA:H	1.74	0.52
1:A:351:ILE:HA	1:A:399:ARG:HH22	1.74	0.52
1:B:51:TYR:CZ	1:B:90:SER:HB2	2.45	0.52
1:B:264:GLN:HG3	1:B:264:GLN:O	2.08	0.52
1:A:311:LEU:O	1:A:314:SER:HB2	2.09	0.52
1:B:5:LYS:O	1:B:286:PHE:HE2	1.93	0.52
1:B:305:LEU:O	1:B:310:ASN:HB3	2.09	0.52
1:A:124:PHE:CG	1:A:125:PRO:HA	2.44	0.52
1:B:63:LYS:O	1:B:66:GLU:HB2	2.10	0.52
1:B:334:ASN:HB2	4:B:470:HOH:O	2.08	0.52
1:B:280:ARG:HB2	1:B:284:GLU:O	2.10	0.52
1:B:22:LYS:HE2	1:B:22:LYS:H	1.74	0.51
1:B:212:LYS:O	1:B:214:VAL:HG13	2.09	0.51
1:B:256:LEU:HA	1:B:257:PRO:C	2.31	0.51
1:A:130:ARG:O	1:A:134:VAL:HG23	2.10	0.51
1:B:110:LEU:HD21	1:B:216:LEU:HD13	1.92	0.51
1:B:287:LYS:HE2	1:B:287:LYS:H	1.74	0.51
1:B:97:HIS:CD2	1:B:99:VAL:HG22	2.45	0.51
1:A:17:HIS:C	1:A:19:ASP:N	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:LEU:HD13	1:B:218:ILE:HD11	1.92	0.51
1:B:173:THR:HG23	1:B:175:ALA:N	2.24	0.51
1:B:51:TYR:HA	1:B:91:PHE:O	2.11	0.51
1:B:406:ARG:O	1:B:408:ILE:HD13	2.10	0.51
1:B:353:ALA:C	1:B:355:GLU:H	2.13	0.51
1:A:69:VAL:HG12	1:A:70:THR:H	1.77	0.50
1:B:22:LYS:H	1:B:22:LYS:CE	2.24	0.50
1:B:302:ASP:OD1	1:B:303:PRO:HD2	2.11	0.50
1:A:392:ASN:HA	1:A:412:LEU:HD23	1.93	0.50
1:B:59:CYS:H	1:B:67:ALA:HB1	1.77	0.50
1:B:149:ASN:ND2	1:B:185:ALA:H	1.96	0.50
1:A:147:VAL:HG12	1:A:181:ILE:HB	1.94	0.50
1:B:154:VAL:HA	1:B:158:GLU:OE1	2.11	0.50
1:B:356:THR:O	1:B:357:LEU:HD12	2.12	0.50
1:A:252:GLU:HB3	1:A:319:ALA:HB2	1.94	0.50
1:B:23:THR:HB	2:B:416:GCP:O2G	2.11	0.49
1:A:212:LYS:HE2	1:A:213:PRO:HD2	1.92	0.49
1:A:391:ASN:ND2	1:A:414:GLU:HA	2.26	0.49
1:B:400:GLN:HG2	1:B:405:TRP:HA	1.93	0.49
1:A:132:HIS:O	1:A:136:LEU:HD13	2.13	0.49
1:B:63:LYS:O	1:B:63:LYS:HG3	2.12	0.49
1:B:104:MET:O	1:B:108:ALA:HB3	2.12	0.49
1:B:306:THR:HG22	1:B:311:LEU:HD12	1.94	0.49
1:A:92:ILE:CG2	1:A:111:MET:HE1	2.42	0.49
1:B:279:ILE:HA	1:B:297:ILE:HD13	1.94	0.49
1:B:279:ILE:HG12	1:B:297:ILE:HD12	1.93	0.49
1:B:394:ARG:HA	1:B:412:LEU:HD23	1.93	0.49
1:A:317:THR:HG21	1:A:323:VAL:HG11	1.95	0.49
1:B:55:ASN:HB3	1:B:85:PHE:CE2	2.48	0.49
1:B:70:THR:HG23	4:B:430:HOH:O	2.12	0.49
1:B:290:LYS:HB3	1:B:291:PRO:HD2	1.95	0.49
1:A:148:GLN:O	1:A:151:VAL:HG23	2.13	0.49
1:A:295:VAL:HG22	1:A:296:ALA:N	2.28	0.49
1:A:332:LYS:HA	1:A:376:ASP:O	2.12	0.49
1:B:156:LYS:O	1:B:160:LEU:HD13	2.13	0.49
1:B:248:LYS:H	1:B:251:GLN:NE2	2.11	0.49
1:A:193:SER:O	1:A:196:GLU:HB3	2.13	0.49
1:A:339:VAL:HG13	1:A:346:LEU:HB3	1.94	0.49
1:B:59:CYS:HB2	1:B:67:ALA:HA	1.95	0.49
1:A:136:LEU:HD23	1:A:144:LEU:CD1	2.42	0.48
1:B:284:GLU:HB2	1:B:286:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HD23	1:A:271:PRO:HB3	1.95	0.48
1:A:338:ARG:HG3	1:A:345:MET:HB2	1.95	0.48
1:B:359:LEU:HD12	1:B:397:ILE:HA	1.96	0.48
1:A:19:ASP:HB3	1:A:119:ALA:H	1.78	0.48
1:A:388:VAL:HG12	1:A:389:TRP:N	2.29	0.48
1:B:25:LEU:HD21	1:B:194:LEU:HD23	1.95	0.48
1:A:40:GLU:C	1:A:41:LEU:HD12	2.34	0.48
1:A:98:GLU:HG3	1:A:99:VAL:HG13	1.94	0.48
1:A:223:VAL:HG11	2:A:416:GCP:H8	1.94	0.48
1:A:255:VAL:CG1	1:A:272:ILE:HB	2.44	0.48
1:A:346:LEU:HG	1:A:347:LYS:N	2.28	0.48
1:B:56:ILE:HB	1:B:87:ARG:O	2.13	0.48
1:A:191:ILE:O	1:A:194:LEU:HB3	2.14	0.48
1:A:246:LEU:CD2	1:A:248:LYS:HG3	2.43	0.48
1:A:212:LYS:HE2	1:A:212:LYS:CA	2.40	0.48
1:A:351:ILE:H	1:A:351:ILE:CD1	2.26	0.48
1:B:149:ASN:HD21	1:B:185:ALA:N	1.97	0.48
1:B:400:GLN:HG2	1:B:405:TRP:CG	2.49	0.48
1:A:44:GLY:C	2:A:416:GCP:H3B1	2.34	0.48
1:A:260:ARG:H	1:A:260:ARG:CZ	2.26	0.48
1:A:393:ILE:HB	1:A:413:VAL:HG12	1.94	0.48
1:B:213:PRO:HA	1:B:245:GLY:HA3	1.96	0.48
1:A:24:THR:HA	1:A:27:GLN:OE1	2.14	0.47
1:A:226:PRO:HG3	1:B:259:LEU:CD1	2.44	0.47
1:B:10:VAL:CG1	1:B:11:ASN:N	2.77	0.47
1:A:144:LEU:HG	1:A:145:ILE:N	2.30	0.47
1:A:53:GLU:HA	1:A:90:SER:HA	1.97	0.47
1:A:146:ILE:O	1:A:180:ILE:HA	2.13	0.47
1:B:12:ILE:HG12	1:B:90:SER:O	2.14	0.47
1:B:212:LYS:HZ2	1:B:323:VAL:HG22	1.79	0.47
1:A:212:LYS:O	1:A:214:VAL:HG23	2.14	0.47
1:A:288:GLU:O	1:A:288:GLU:HG3	2.14	0.47
1:B:361:VAL:CG2	1:B:386:VAL:HG23	2.41	0.47
1:A:216:LEU:HD22	1:A:243:ILE:HG21	1.96	0.47
1:A:242:ILE:HD12	1:A:242:ILE:N	2.29	0.47
1:B:45:MET:HA	1:B:46:THR:HB	1.97	0.47
1:B:123:PRO:O	1:B:126:GLN:HG2	2.14	0.47
1:B:352:ARG:HE	1:B:355:GLU:HB2	1.79	0.47
1:B:355:GLU:HG2	1:B:356:THR:N	2.29	0.47
1:B:357:LEU:HD23	1:B:397:ILE:CG2	2.44	0.47
1:B:411:GLY:O	1:B:412:LEU:HD23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HB3	1:A:146:ILE:HD12	1.96	0.47
1:B:215:MET:HA	1:B:242:ILE:HA	1.95	0.47
1:B:272:ILE:HD13	1:B:305:LEU:HD12	1.96	0.47
1:A:226:PRO:HG3	1:B:259:LEU:HD13	1.97	0.47
1:A:277:SER:HB3	1:A:298:GLY:C	2.35	0.47
1:B:75:LYS:HA	1:B:79:SER:H	1.80	0.47
1:B:260:ARG:HB2	1:B:269:TYR:CE2	2.49	0.47
1:A:34:THR:OG1	1:A:50:GLY:HA2	2.13	0.47
1:A:136:LEU:HD23	1:A:144:LEU:HD13	1.97	0.47
1:B:351:ILE:HD12	1:B:357:LEU:HD21	1.96	0.47
1:B:11:ASN:ND2	1:B:293:GLY:H	2.07	0.47
1:B:17:HIS:CA	1:B:97:HIS:HA	2.45	0.47
1:B:55:ASN:HB3	1:B:85:PHE:HE2	1.80	0.47
1:B:69:VAL:HG12	1:B:71:GLU:N	2.22	0.47
1:B:128:GLN:HA	1:B:131:GLU:HB2	1.96	0.47
1:B:134:VAL:HG23	1:B:135:ALA:N	2.29	0.47
1:A:56:ILE:HG13	1:A:89:ILE:CD1	2.45	0.47
1:A:146:ILE:HG12	1:A:178:VAL:CG2	2.45	0.47
1:A:256:LEU:CD1	1:A:323:VAL:HB	2.45	0.47
1:B:71:GLU:HA	1:B:72:PRO:HD3	1.79	0.47
1:B:275:LYS:HD2	1:B:275:LYS:N	2.29	0.47
1:B:327:TRP:CZ2	1:B:385:PRO:HG3	2.50	0.46
1:A:372:SER:OG	1:A:379:GLU:HG2	2.15	0.46
1:B:247:PHE:CZ	1:B:317:THR:HA	2.47	0.46
1:A:119:ALA:HB1	1:A:150:LYS:HG3	1.98	0.46
1:B:162:GLN:CA	1:B:165:GLN:HG2	2.44	0.46
1:B:322:GLU:H	1:B:322:GLU:CD	2.19	0.46
1:A:234:LYS:HB2	1:A:234:LYS:NZ	2.30	0.46
1:A:302:ASP:OD2	1:A:304:SER:HB2	2.15	0.46
1:A:327:TRP:NE1	1:A:385:PRO:HG3	2.30	0.46
1:B:105:LEU:O	1:B:109:ALA:HB2	2.14	0.46
1:B:155:SER:HB3	1:B:158:GLU:H	1.80	0.46
1:B:254:LYS:NZ	1:B:256:LEU:HD11	2.30	0.46
1:A:392:ASN:HB2	4:A:436:HOH:O	2.15	0.46
1:B:64:LYS:HE2	1:B:64:LYS:HB3	1.72	0.46
1:B:246:LEU:HB2	1:B:289:ALA:O	2.16	0.46
1:A:215:MET:HG2	1:A:241:SER:C	2.35	0.46
1:A:315:ILE:HG21	1:A:387:ALA:HB3	1.97	0.46
1:A:371:THR:O	1:A:372:SER:HB3	2.16	0.46
1:B:315:ILE:HD13	1:B:389:TRP:CE3	2.50	0.46
1:B:49:LEU:H	1:B:49:LEU:HD12	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:PRO:HG2	1:B:318:LEU:HD11	1.97	0.46
1:B:124:PHE:CE2	1:B:165:GLN:HG3	2.51	0.46
1:B:264:GLN:HB3	1:B:266:LYS:HG2	1.98	0.46
1:B:358:MET:C	1:B:359:LEU:HD13	2.36	0.46
1:A:331:ILE:HD13	1:A:331:ILE:H	1.81	0.45
1:B:7:GLN:HB2	1:B:281:PHE:CE1	2.51	0.45
1:A:252:GLU:CD	1:A:273:PHE:CE1	2.89	0.45
1:A:390:SER:H	1:A:393:ILE:HD11	1.80	0.45
1:B:175:ALA:HA	1:B:178:VAL:HG23	1.97	0.45
1:B:254:LYS:HA	1:B:272:ILE:O	2.17	0.45
1:A:314:SER:HB3	1:A:315:ILE:H	1.60	0.45
1:A:3:TRP:HZ2	1:A:83:PRO:HB2	1.80	0.45
1:B:322:GLU:O	1:B:322:GLU:HG2	2.15	0.45
1:B:279:ILE:HG12	1:B:297:ILE:CD1	2.46	0.45
1:B:10:VAL:HG12	1:B:11:ASN:H	1.80	0.45
1:B:41:LEU:H	1:B:43:ARG:HE	1.62	0.45
1:B:335:LEU:HG	1:B:348:VAL:HG11	1.99	0.45
1:B:159:ALA:C	1:B:161:SER:H	2.20	0.45
1:A:333:TYR:CE2	1:A:378:ILE:HG23	2.52	0.45
1:A:371:THR:OG1	1:A:379:GLU:HG3	2.17	0.45
1:B:40:GLU:OE2	1:B:40:GLU:HA	2.17	0.45
1:B:97:HIS:NE2	1:B:99:VAL:HG22	2.32	0.45
1:B:144:LEU:HD11	1:B:146:ILE:HD13	1.98	0.45
1:A:216:LEU:HD11	1:A:243:ILE:HD13	1.99	0.45
1:B:114:ALA:O	1:B:144:LEU:HA	2.17	0.44
1:B:124:PHE:CZ	1:B:166:ILE:HA	2.52	0.44
1:B:358:MET:CG	1:B:398:SER:HB2	2.47	0.44
1:A:113:GLY:HA3	1:A:202:ILE:HG23	1.99	0.44
1:A:184:SER:OG	1:A:189:ILE:HB	2.17	0.44
1:A:238:ILE:O	1:A:296:ALA:HA	2.18	0.44
1:A:354:LYS:O	1:A:354:LYS:HG2	2.16	0.44
1:B:217:VAL:HG22	1:B:238:ILE:CG2	2.48	0.44
1:B:368:GLY:HA2	1:B:383:ARG:HD3	1.99	0.44
1:B:55:ASN:C	1:B:56:ILE:HD12	2.38	0.44
1:B:252:GLU:OE1	1:B:252:GLU:HA	2.16	0.44
1:A:34:THR:CB	1:A:35:SER:HA	2.46	0.44
1:B:262:GLU:HA	1:B:267:VAL:N	2.30	0.44
1:A:382:LEU:HD12	1:A:382:LEU:O	2.18	0.44
1:B:13:GLY:HA3	1:B:111:MET:SD	2.56	0.44
1:B:245:GLY:O	1:B:291:PRO:HD3	2.17	0.44
1:B:375:LYS:HB3	1:B:376:ASP:H	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:TRP:HE3	1:A:34:THR:HG1	1.66	0.44
1:A:82:GLU:HG2	1:A:83:PRO:HD2	2.00	0.44
1:A:223:VAL:HG11	2:A:416:GCP:C8	2.47	0.44
1:A:251:GLN:O	1:A:275:LYS:HG3	2.18	0.44
1:B:4:PRO:HB2	1:B:6:VAL:HG13	1.99	0.44
1:B:367:LEU:N	1:B:367:LEU:HD23	2.33	0.44
1:B:401:ILE:HG22	1:B:406:ARG:HB3	1.99	0.44
1:A:275:LYS:CG	1:A:276:ILE:N	2.79	0.44
2:B:416:GCP:N3	2:B:416:GCP:H2'	2.32	0.44
1:A:20:HIS:C	1:A:149:ASN:ND2	2.71	0.44
1:B:216:LEU:C	1:B:216:LEU:HD23	2.37	0.44
1:B:405:TRP:O	1:B:406:ARG:HB2	2.18	0.44
1:A:58:VAL:HG11	1:A:86:LEU:HD11	1.95	0.43
1:A:225:LYS:HD2	1:A:225:LYS:HA	1.56	0.43
1:B:358:MET:HG3	1:B:398:SER:HB2	2.00	0.43
1:B:40:GLU:O	1:B:41:LEU:HB2	2.18	0.43
1:B:360:SER:OG	1:B:396:VAL:HB	2.18	0.43
1:A:295:VAL:HG22	1:A:296:ALA:H	1.83	0.43
1:B:138:ILE:HG22	1:B:138:ILE:O	2.18	0.43
1:B:238:ILE:HD11	1:B:311:LEU:CD1	2.47	0.43
1:B:316:ILE:HG22	1:B:317:THR:N	2.33	0.43
1:A:39:GLU:HA	1:A:41:LEU:N	2.31	0.43
1:A:388:VAL:HG12	1:A:389:TRP:H	1.82	0.43
1:B:113:GLY:HA3	1:B:202:ILE:HG23	2.01	0.43
1:B:225:LYS:HE2	1:B:225:LYS:HA	2.00	0.43
1:B:400:GLN:OE1	1:B:404:ARG:HA	2.19	0.43
1:B:404:ARG:HD2	1:B:405:TRP:CE3	2.53	0.43
1:B:170:THR:HB	1:B:173:THR:HG22	2.00	0.43
1:A:242:ILE:HD12	1:A:242:ILE:H	1.82	0.43
1:B:134:VAL:HG21	1:B:406:ARG:HH22	1.84	0.43
1:B:338:ARG:HB3	1:B:347:LYS:HG3	2.00	0.43
1:A:248:LYS:O	1:A:251:GLN:HB3	2.19	0.43
1:B:87:ARG:NH2	1:B:199:GLU:HA	2.34	0.43
1:B:183:VAL:HB	1:B:189:ILE:O	2.19	0.43
1:B:215:MET:N	1:B:247:PHE:HE1	2.17	0.43
1:A:74:CYS:SG	1:A:83:PRO:HG3	2.59	0.43
1:A:341:GLY:HA3	1:A:406:ARG:NH2	2.34	0.43
1:B:34:THR:HB	1:B:38:SER:HA	2.01	0.43
1:B:97:HIS:CD2	1:B:99:VAL:HG13	2.53	0.43
1:B:144:LEU:O	1:B:178:VAL:HG22	2.19	0.43
1:A:22:LYS:HG2	1:A:23:THR:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ILE:N	1:A:369:ILE:HD12	2.34	0.43
1:A:133:PHE:CE1	1:A:173:THR:HG21	2.53	0.42
1:A:234:LYS:HA	1:B:230:PHE:CZ	2.53	0.42
1:B:50:GLY:O	1:B:92:ILE:HA	2.19	0.42
1:B:239:GLY:HA2	1:B:296:ALA:HA	2.00	0.42
1:A:179:PRO:HG3	1:A:201:TYR:CD1	2.54	0.42
1:B:75:LYS:HG2	4:B:455:HOH:O	2.18	0.42
1:B:315:ILE:O	1:B:315:ILE:HG13	2.18	0.42
1:A:264:GLN:HE21	1:A:264:GLN:HB2	1.64	0.42
1:A:312:LEU:HD12	1:A:313:GLY:N	2.34	0.42
1:A:124:PHE:CD1	1:A:125:PRO:HA	2.54	0.42
1:B:49:LEU:HD12	1:B:49:LEU:N	2.33	0.42
1:B:115:ILE:HA	1:B:145:ILE:O	2.19	0.42
1:B:145:ILE:HG22	1:B:179:PRO:HD2	1.99	0.42
1:B:242:ILE:O	1:B:291:PRO:HA	2.18	0.42
1:A:279:ILE:CD1	1:A:289:ALA:H	2.19	0.42
1:B:120:ALA:CB	1:B:154:VAL:HG11	2.49	0.42
1:B:188:LYS:HA	1:B:191:ILE:HD12	2.02	0.42
1:A:20:HIS:CB	1:A:21:GLY:HA2	2.49	0.42
1:A:393:ILE:HB	1:A:413:VAL:CG1	2.49	0.42
1:B:42:LYS:HE3	1:B:51:TYR:HE1	1.83	0.42
1:B:176:GLU:HG3	1:B:177:ASN:OD1	2.19	0.42
1:B:299:THR:C	1:B:301:LEU:N	2.72	0.42
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.84	0.42
1:A:300:TYR:HB3	1:B:230:PHE:HB2	2.01	0.42
1:B:46:THR:HG22	1:B:47:ILE:N	2.32	0.42
1:B:64:LYS:H	1:B:64:LYS:HG2	1.52	0.42
1:A:204:THR:HA	1:A:205:PRO:HD3	1.78	0.42
1:A:251:GLN:C	1:A:275:LYS:HG3	2.40	0.42
1:A:313:GLY:O	1:A:364:SER:HB3	2.20	0.42
1:B:319:ALA:C	1:B:321:ALA:H	2.22	0.42
1:B:333:TYR:CD1	1:B:335:LEU:HD13	2.55	0.42
1:A:220:SER:O	1:A:309:ASP:N	2.49	0.42
1:A:275:LYS:HG2	1:A:276:ILE:H	1.80	0.41
1:A:388:VAL:HG13	1:A:413:VAL:HG11	2.02	0.41
1:B:69:VAL:C	1:B:71:GLU:H	2.24	0.41
1:B:146:ILE:HG12	1:B:178:VAL:CG1	2.49	0.41
1:A:3:TRP:HA	1:A:4:PRO:HD3	1.79	0.41
1:A:313:GLY:HA2	1:A:363:SER:O	2.20	0.41
1:B:17:HIS:CB	1:B:97:HIS:HA	2.49	0.41
1:B:87:ARG:HD2	1:B:89:ILE:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:VAL:HB	1:B:158:GLU:CG	2.50	0.41
1:A:331:ILE:HD13	1:A:331:ILE:N	2.36	0.41
1:A:331:ILE:O	1:A:331:ILE:HG12	2.20	0.41
1:A:393:ILE:O	1:A:412:LEU:HA	2.20	0.41
1:B:190:ASN:ND2	1:B:193:SER:HB2	2.36	0.41
1:A:7:GLN:OE1	1:A:290:LYS:HB2	2.19	0.41
1:B:139:ILE:HA	1:B:394:ARG:HE	1.84	0.41
1:B:219:ARG:O	1:B:239:GLY:N	2.54	0.41
1:A:262:GLU:HG3	1:A:262:GLU:O	2.20	0.41
1:A:280:ARG:HB3	2:A:416:GCP:HN1	1.84	0.41
1:B:47:ILE:H	1:B:219:ARG:NH1	2.12	0.41
1:A:162:GLN:O	1:A:166:ILE:HG13	2.20	0.41
1:A:246:LEU:HD23	1:A:246:LEU:C	2.40	0.41
1:B:27:GLN:HG2	1:B:33:TRP:CB	2.51	0.41
1:B:134:VAL:HA	4:B:514:HOH:O	2.21	0.41
1:A:249:VAL:O	1:A:250:ASP:HB2	2.21	0.41
1:A:388:VAL:HG13	1:A:393:ILE:HD12	2.01	0.41
1:B:14:VAL:HG22	1:B:115:ILE:HD11	2.03	0.41
1:B:42:LYS:HG3	1:B:282:GLY:HA3	2.03	0.41
1:B:87:ARG:HH22	1:B:199:GLU:HA	1.84	0.41
1:B:103:THR:HA	1:B:106:SER:OG	2.21	0.41
1:B:151:VAL:HG22	1:B:151:VAL:O	2.21	0.41
1:B:246:LEU:C	1:B:246:LEU:HD12	2.41	0.41
1:B:337:GLU:H	1:B:337:GLU:CD	2.24	0.41
1:A:111:MET:HG3	1:A:113:GLY:O	2.21	0.41
1:A:120:ALA:N	1:A:149:ASN:O	2.51	0.41
1:A:220:SER:H	1:A:309:ASP:HA	1.86	0.41
1:B:12:ILE:HG13	1:B:91:PHE:CE2	2.55	0.41
1:B:167:LYS:HD3	4:B:443:HOH:O	2.19	0.41
1:B:205:PRO:CD	1:B:207:ARG:HH12	2.26	0.41
1:B:219:ARG:HG2	1:B:221:PHE:HE2	1.86	0.41
1:B:249:VAL:HG12	1:B:250:ASP:OD2	2.21	0.41
1:B:313:GLY:HA2	1:B:363:SER:OG	2.20	0.41
1:B:346:LEU:HD12	1:B:401:ILE:HD11	2.02	0.41
1:B:333:TYR:HE1	1:B:335:LEU:HD13	1.83	0.41
1:A:133:PHE:O	1:A:174:TRP:CZ2	2.74	0.40
1:A:179:PRO:HG3	1:A:201:TYR:CG	2.56	0.40
1:A:358:MET:HB2	1:A:405:TRP:CE3	2.56	0.40
1:A:358:MET:HB3	1:A:398:SER:HB2	2.04	0.40
1:B:17:HIS:O	1:B:22:LYS:HD3	2.21	0.40
1:B:116:LEU:O	1:B:146:ILE:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLN:HG3	1:B:132:HIS:NE2	2.36	0.40
1:B:218:ILE:HB	1:B:240:GLY:HA2	2.03	0.40
1:B:231:ASN:CG	1:B:232:GLU:H	2.24	0.40
1:B:134:VAL:O	1:B:138:ILE:N	2.52	0.40
1:A:338:ARG:HH12	1:A:347:LYS:HE2	1.84	0.40
1:A:351:ILE:HA	1:A:399:ARG:NH2	2.36	0.40
1:A:390:SER:O	1:A:393:ILE:HG13	2.21	0.40
1:B:128:GLN:HE21	1:B:132:HIS:CE1	2.40	0.40
1:B:255:VAL:HG22	1:B:316:ILE:CD1	2.48	0.40
1:B:34:THR:HG21	1:B:45:MET:CE	2.52	0.40
1:B:275:LYS:HD3	1:B:300:TYR:CG	2.57	0.40
1:A:259:LEU:N	1:A:272:ILE:HG13	2.37	0.40
1:B:45:MET:HA	1:B:46:THR:C	2.42	0.40
1:B:188:LYS:HA	1:B:191:ILE:CD1	2.51	0.40
1:B:287:LYS:HD3	4:B:524:HOH:O	2.21	0.40
1:B:324:PRO:HD2	1:B:388:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	412/415 (99%)	339 (82%)	65 (16%)	8 (2%)	8 13
1	B	412/415 (99%)	332 (81%)	73 (18%)	7 (2%)	9 16
All	All	824/830 (99%)	671 (81%)	138 (17%)	15 (2%)	8 14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ALA
1	B	43	ARG

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Mol	Chain	Res	Type
1	B	406	ARG
1	A	171	LYS
1	B	127	PRO
1	A	17	HIS
1	A	38	SER
1	A	47	ILE
1	A	106	SER
1	A	334	ASN
1	A	389	TRP
1	B	141	VAL
1	B	404	ARG
1	B	373	VAL
1	B	213	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	356/357 (100%)	322 (90%)	34 (10%)	8 16
1	B	356/357 (100%)	322 (90%)	34 (10%)	8 16
All	All	712/714 (100%)	644 (90%)	68 (10%)	8 16

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	38	SER
1	A	45	MET
1	A	60	GLU
1	A	74	CYS
1	A	88	ARG
1	A	104	MET
1	A	111	MET
1	A	144	LEU
1	A	145	ILE

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Mol	Chain	Res	Type
1	A	173	THR
1	A	176	GLU
1	A	204	THR
1	A	212	LYS
1	A	219	ARG
1	A	221	PHE
1	A	225	LYS
1	A	234	LYS
1	A	249	VAL
1	A	260	ARG
1	A	264	GLN
1	A	274	THR
1	A	283	ASP
1	A	287	LYS
1	A	312	LEU
1	A	315	ILE
1	A	320	ASP
1	A	331	ILE
1	A	334	ASN
1	A	335	LEU
1	A	351	ILE
1	A	367	LEU
1	A	391	ASN
1	A	404	ARG
1	B	12	ILE
1	B	20	HIS
1	B	22	LYS
1	B	27	GLN
1	B	34	THR
1	B	46	THR
1	B	60	GLU
1	B	63	LYS
1	B	105	LEU
1	B	112	ASP
1	B	115	ILE
1	B	139	ILE
1	B	147	VAL
1	B	157	GLU
1	B	181	ILE
1	B	214	VAL
1	B	219	ARG
1	B	225	LYS

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	259	LEU
1	B	275	LYS
1	B	278	SER
1	B	283	ASP
1	B	284	GLU
1	B	287	LYS
1	B	295	VAL
1	B	325	VAL
1	B	329	ILE
1	B	331	ILE
1	B	333	TYR
1	B	359	LEU
1	B	364	SER
1	B	381	GLU
1	B	408	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	126	GLN
1	A	165	GLN
1	A	190	ASN
1	A	229	GLN
1	A	244	GLN
1	A	264	GLN
1	A	334	ASN
1	A	391	ASN
1	A	392	ASN
1	B	11	ASN
1	B	20	HIS
1	B	97	HIS
1	B	128	GLN
1	B	149	ASN
1	B	190	ASN
1	B	231	ASN
1	B	251	GLN
1	B	392	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GCP	A	416	-	27,34,34	1.19	3 (11%)	34,54,54	1.74	6 (17%)
2	GCP	B	416	-	27,34,34	1.21	3 (11%)	34,54,54	1.77	6 (17%)
3	PO4	A	418	-	4,4,4	0.93	0	6,6,6	0.43	0
3	PO4	A	417	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	B	417	-	4,4,4	0.93	0	6,6,6	0.44	0
3	PO4	B	418	-	4,4,4	0.92	0	6,6,6	0.41	0

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	GCP	B	416	-	-	7/15/38/38	0/3/3/3
2	GCP	A	416	-	-	8/15/38/38	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	416	GCP	C6-N1	3.00	1.38	1.33
2	A	416	GCP	C6-N1	2.97	1.38	1.33
2	B	416	GCP	PB-O3A	2.97	1.61	1.58
2	A	416	GCP	PB-O3A	2.90	1.61	1.58
2	B	416	GCP	PB-O2B	-2.09	1.51	1.56
2	A	416	GCP	PB-O2B	-2.04	1.51	1.56

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	416	GCP	N3-C2-N1	-5.22	120.26	127.22
2	B	416	GCP	N3-C2-N1	-5.22	120.26	127.22
2	B	416	GCP	C2-N3-C4	4.53	120.54	115.36
2	A	416	GCP	C2-N3-C4	4.35	120.32	115.36
2	B	416	GCP	PB-O3A-PA	-3.78	120.58	132.56
2	A	416	GCP	PB-O3A-PA	-3.56	121.27	132.56
2	B	416	GCP	C3'-C2'-C1'	3.21	105.81	100.98
2	A	416	GCP	C5-C6-N1	-2.95	119.39	123.43
2	A	416	GCP	C3'-C2'-C1'	2.88	105.32	100.98
2	B	416	GCP	C5-C6-N1	-2.87	119.50	123.43
2	A	416	GCP	C2-N1-C6	2.51	119.91	115.93
2	B	416	GCP	C2-N1-C6	2.43	119.79	115.93

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	416	GCP	C5'-O5'-PA-O1A
2	B	416	GCP	C5'-O5'-PA-O1A
2	B	416	GCP	O4'-C4'-C5'-O5'
2	A	416	GCP	O4'-C4'-C5'-O5'
2	A	416	GCP	C3'-C4'-C5'-O5'
2	B	416	GCP	C4'-C5'-O5'-PA
2	B	416	GCP	C3'-C4'-C5'-O5'
2	A	416	GCP	C5'-O5'-PA-O3A
2	B	416	GCP	C5'-O5'-PA-O3A
2	A	416	GCP	C5'-O5'-PA-O2A
2	B	416	GCP	C5'-O5'-PA-O2A
2	A	416	GCP	PG-C3B-PB-O2B
2	B	416	GCP	PB-O3A-PA-O1A
2	A	416	GCP	PG-C3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	A	416	GCP	C4'-C5'-O5'-PA

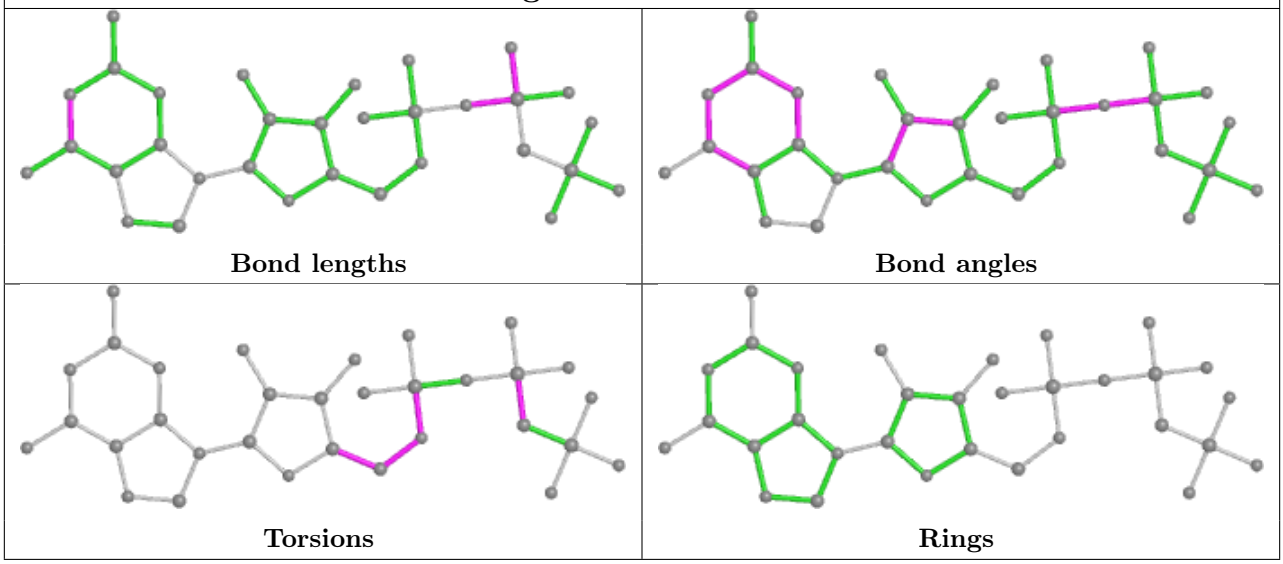
There are no ring outliers.

2 monomers are involved in 13 short contacts:

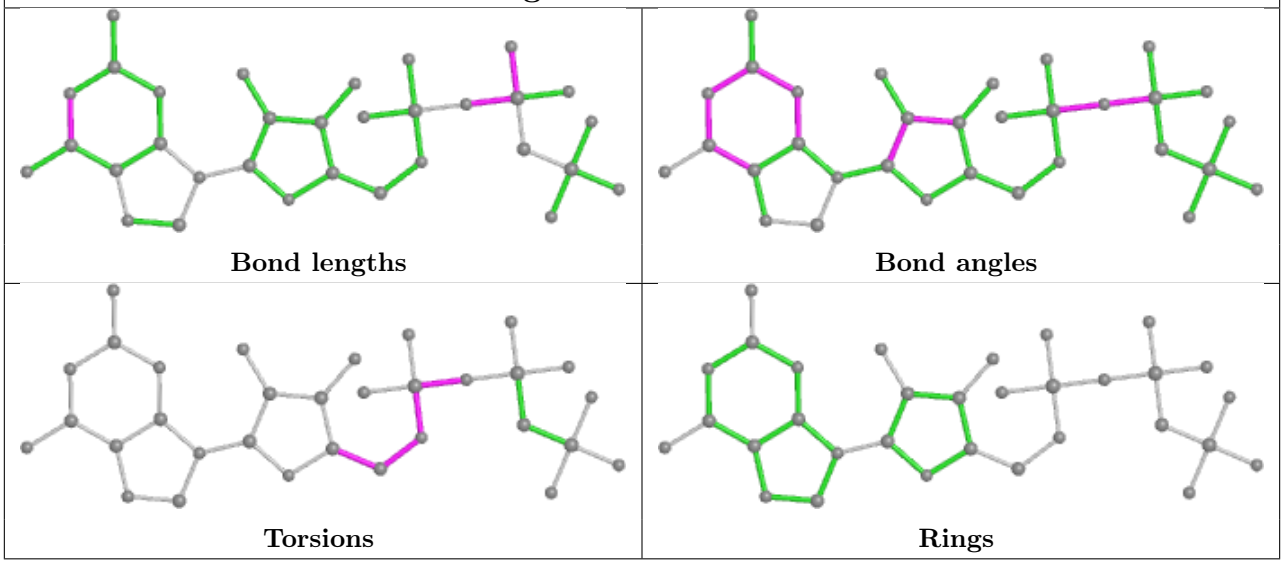
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	416	GCP	11	0
2	B	416	GCP	2	0

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

Ligand GCP A 416



Ligand GCP B 416



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	414/415 (99%)	0.25	23 (5%)	24	25	75, 121, 203, 288	0
1	B	414/415 (99%)	0.07	14 (3%)	45	48	73, 109, 202, 297	0
All	All	828/830 (99%)	0.16	37 (4%)	33	36	73, 114, 203, 297	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	SER	7.5
1	A	47	ILE	5.9
1	A	104	MET	5.4
1	B	38	SER	5.1
1	A	32	ILE	4.9
1	B	99	VAL	4.9
1	A	20	HIS	4.9
1	B	40	GLU	4.8
1	A	102	ALA	4.7
1	B	46	THR	4.6
1	A	105	LEU	3.8
1	B	47	ILE	3.6
1	A	46	THR	3.4
1	A	267	VAL	3.3
1	A	33	TRP	3.3
1	A	342	ALA	3.2
1	B	34	THR	3.2
1	B	106	SER	3.1
1	A	348	VAL	3.0
1	A	37	HIS	2.9
1	A	209	LEU	2.9
1	A	99	VAL	2.8
1	B	43	ARG	2.7
1	A	31	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	100	LEU	2.7
1	A	266	LYS	2.5
1	B	105	LEU	2.5
1	B	339	VAL	2.5
1	B	33	TRP	2.4
1	A	341	GLY	2.4
1	A	352	ARG	2.4
1	A	273	PHE	2.4
1	B	98	GLU	2.3
1	B	18	VAL	2.2
1	A	345	MET	2.2
1	A	130	ARG	2.2
1	B	32	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

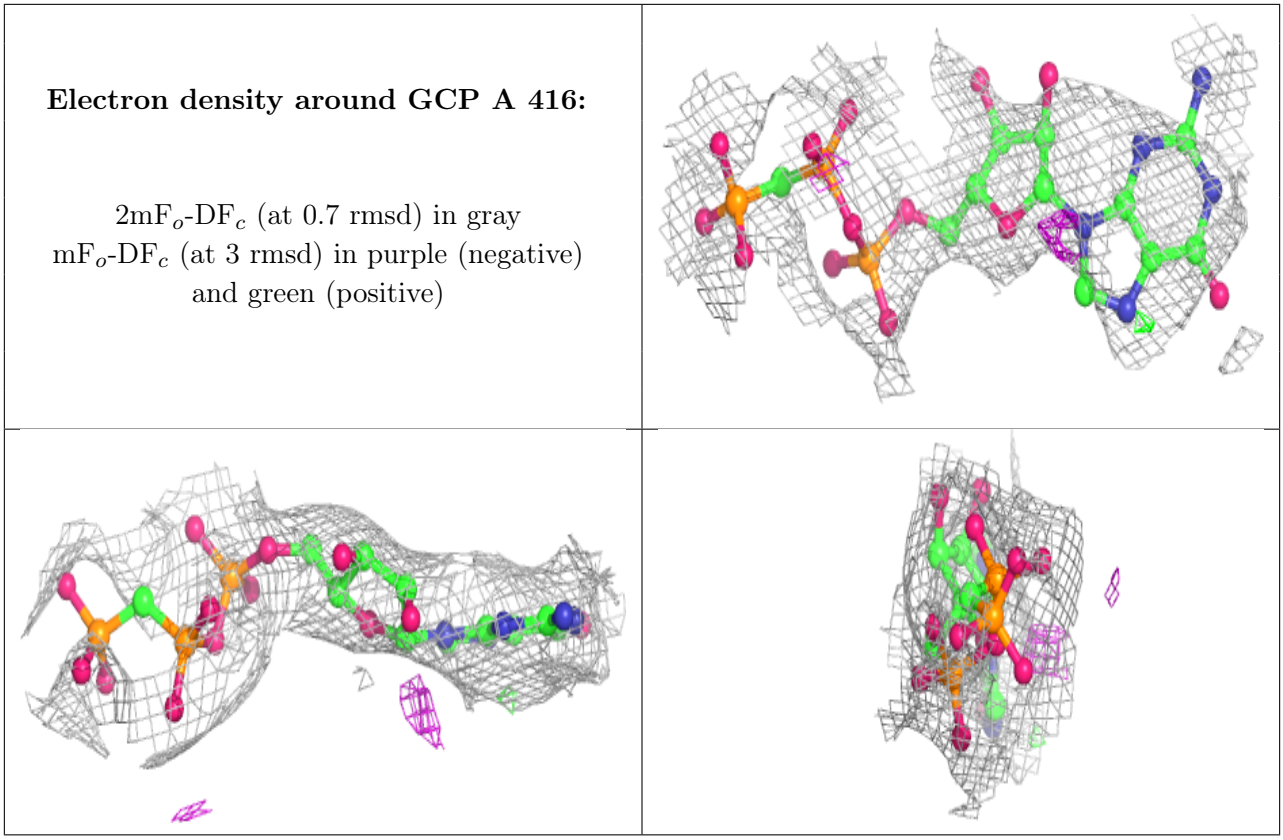
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	418	5/5	0.70	0.35	267,271,280,283	0
2	GCP	A	416	32/32	0.81	0.20	209,228,247,252	0
2	GCP	B	416	32/32	0.86	0.14	193,214,233,238	0
3	PO4	B	418	5/5	0.91	0.19	190,194,199,203	0
3	PO4	B	417	5/5	0.97	0.13	131,145,151,155	0
3	PO4	A	417	5/5	0.98	0.14	133,136,143,147	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.

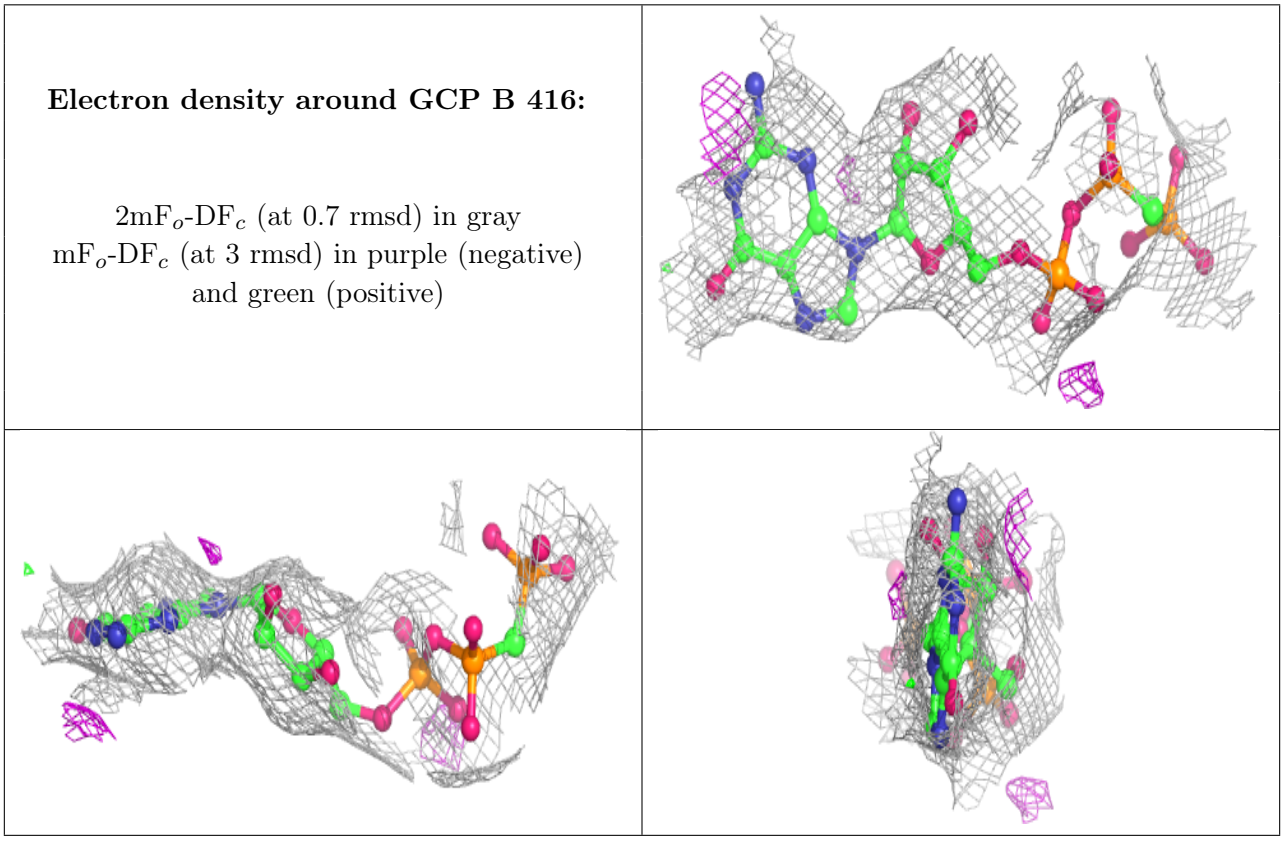
Electron density around GCP A 416:

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



Electron density around GCP B 416:

$2mF_o$-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.