Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 06:28 PM EDT

PDB ID	:	3TCM
Title	:	Crystal Structure of Alanine Aminotransferase from Hordeum vulgare
Authors	:	Rydel, T.J.; Sturman, E.J.; Halls, C.; Chen, S.; Zeng, J.; Evdokimov, A.; Duff, S.M.G.
Deposited on	:	2011-08-09
Resolution	:	2.71 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:

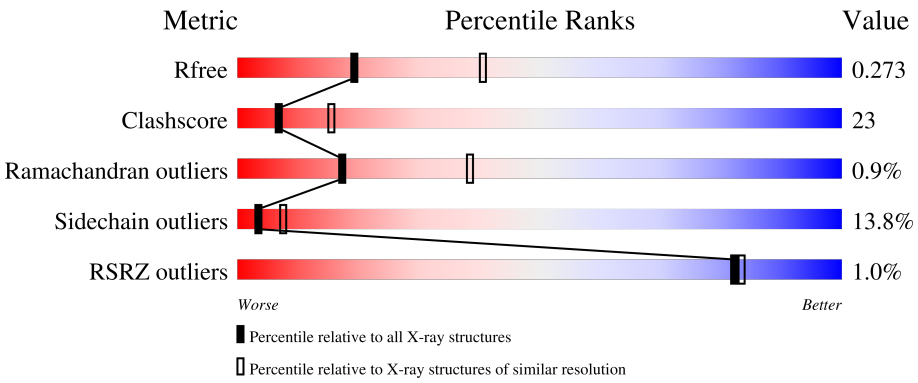
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

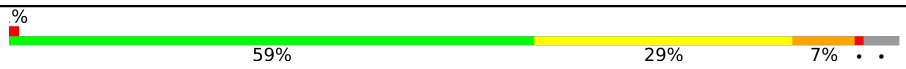
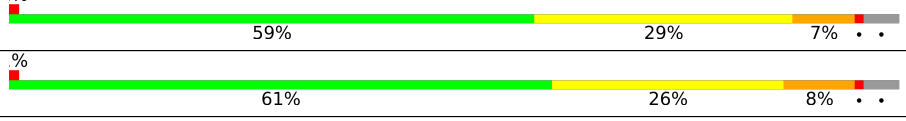
The reported resolution of this entry is 2.71 Å.

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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	500	
1	B	500	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7514 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 Alanine aminotransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	479	3706	2360	633	697	16	0	1	0
1	B	479	3703	2358	633	697	15	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

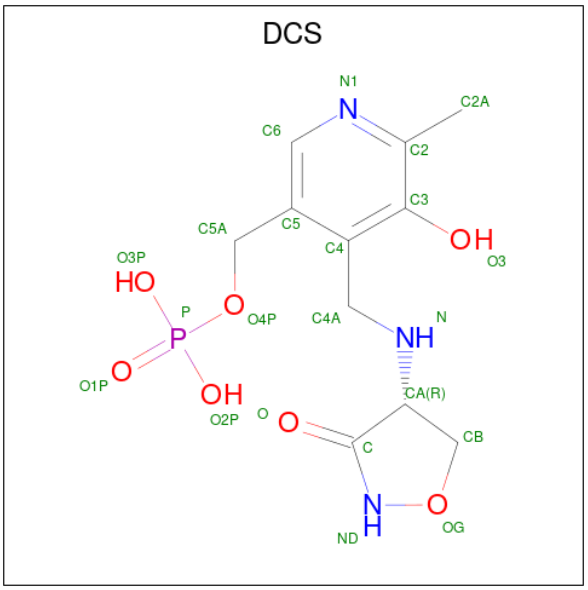
Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP P52894
A	-16	HIS	-	expression tag	UNP P52894
A	-15	HIS	-	expression tag	UNP P52894
A	-14	HIS	-	expression tag	UNP P52894
A	-13	HIS	-	expression tag	UNP P52894
A	-12	HIS	-	expression tag	UNP P52894
A	-11	HIS	-	expression tag	UNP P52894
A	-10	HIS	-	expression tag	UNP P52894
A	-9	HIS	-	expression tag	UNP P52894
A	-8	HIS	-	expression tag	UNP P52894
A	-7	HIS	-	expression tag	UNP P52894
A	-6	GLY	-	expression tag	UNP P52894
A	-5	THR	-	expression tag	UNP P52894
A	-4	ASP	-	expression tag	UNP P52894
A	-3	ASP	-	expression tag	UNP P52894
A	-2	ASP	-	expression tag	UNP P52894
A	-1	ASP	-	expression tag	UNP P52894
A	0	LYS	-	expression tag	UNP P52894
A	119	HIS	LYS	engineered mutation	UNP P52894
B	-17	MET	-	initiating methionine	UNP P52894
B	-16	HIS	-	expression tag	UNP P52894
B	-15	HIS	-	expression tag	UNP P52894
B	-14	HIS	-	expression tag	UNP P52894
B	-13	HIS	-	expression tag	UNP P52894
B	-12	HIS	-	expression tag	UNP P52894

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P52894
B	-10	HIS	-	expression tag	UNP P52894
B	-9	HIS	-	expression tag	UNP P52894
B	-8	HIS	-	expression tag	UNP P52894
B	-7	HIS	-	expression tag	UNP P52894
B	-6	GLY	-	expression tag	UNP P52894
B	-5	THR	-	expression tag	UNP P52894
B	-4	ASP	-	expression tag	UNP P52894
B	-3	ASP	-	expression tag	UNP P52894
B	-2	ASP	-	expression tag	UNP P52894
B	-1	ASP	-	expression tag	UNP P52894
B	0	LYS	-	expression tag	UNP P52894
B	119	HIS	LYS	engineered mutation	UNP P52894

- Molecule 2 is D-[3-HYDROXY-2-METHYL-5-PHOSPHONOOXYMETHYL-PYRIDIN-4-YLMETHYL]-N,O-CYCLOSERYLAMIDE (three-letter code: DCS) (formula: $C_{11}H_{16}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			22	11	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			22	11	3	7	1		

- Molecule 3 is water.

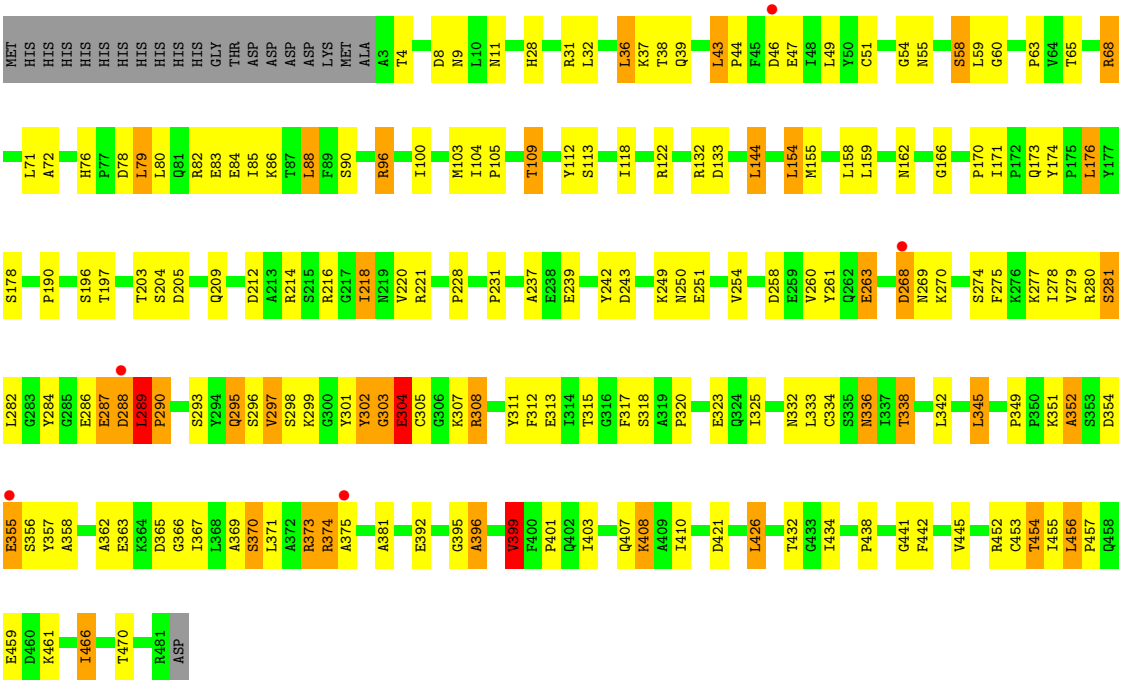
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	29	29	29	0	0
			Total	O		
3	B	32	32	32	0	0

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.

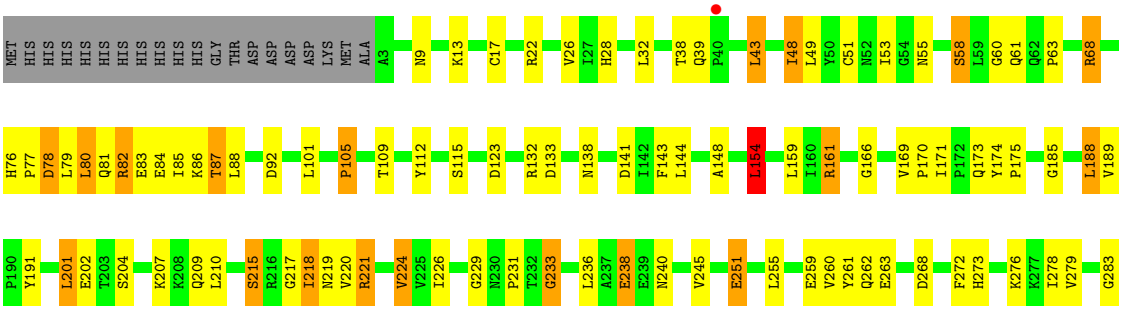
• Molecule 1: Alanine aminotransferase 2

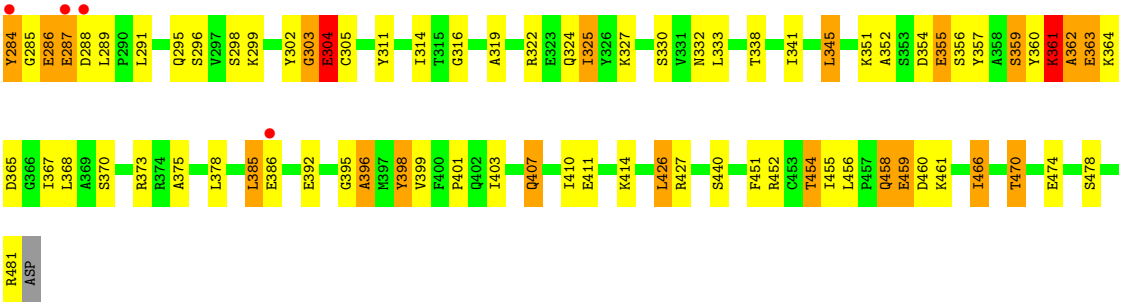
Chain A:



• Molecule 1: Alanine aminotransferase 2

Chain B:




Y284
G285
E286
E287
D288
L289
P290
L291
Q295
S296
V297
S298
K299
Y302
G303
E304
C305
Y311
I314
T315
G316
A319
R322
E323
Q324
I325
Y326
K327
S330
V331
N332
L333
T338
I341
L345
K351
A352
S353
D354
E355
S356
Y357
A358
S359
Y360
K361
A362
E363
K364
D365
G366
I367
L368
A369
S370
R373
R374
A375
L378
L385
E386
E392
G395
A396
M397
Y398
V399
F400
P401
Q402
I403
Q407
I410
E411
K414
L426
R427
S440
F451
R452
C453
T454
I455
L456
P457
Q458
E459
D460
K461
I466
T470
E474
S478
R481
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.86Å 126.97Å 75.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.16 – 2.71 36.26 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.8 (87.16-2.71) 96.9 (36.26-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.215 , 0.279 0.212 , 0.273	Depositor DCC
R_{free} test set	1582 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	46.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 30.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7514	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: DCS

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	1.07	2/3788 (0.1%)	1.06	18/5135 (0.4%)
1	B	1.13	4/3782 (0.1%)	1.10	21/5127 (0.4%)
All	All	1.10	6/7570 (0.1%)	1.08	39/10262 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	GLU	CG-CD	6.00	1.60	1.51
1	B	398	TYR	CE1-CZ	-5.84	1.30	1.38
1	A	297	VAL	CB-CG1	-5.51	1.41	1.52
1	B	407	GLN	CD-OE1	5.38	1.35	1.24
1	B	411	GLU	CG-CD	5.30	1.59	1.51
1	A	301	TYR	CD1-CE1	-5.09	1.31	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	361	LYS	N-CA-CB	-17.20	79.64	110.60
1	A	303	GLY	N-CA-C	9.19	136.07	113.10
1	A	289	LEU	N-CA-C	-9.18	86.22	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303	GLY	C-N-CA	9.09	144.42	121.70
1	B	285	GLY	N-CA-C	8.71	134.88	113.10
1	B	363	GLU	C-N-CA	-8.71	99.92	121.70
1	B	302	TYR	N-CA-C	8.27	133.32	111.00
1	A	303	GLY	CA-C-N	8.01	134.81	117.20
1	A	122	ARG	NE-CZ-NH2	-7.71	116.45	120.30
1	B	43	LEU	CA-CB-CG	-7.52	98.01	115.30
1	B	303	GLY	N-CA-C	7.26	131.25	113.10
1	A	373	ARG	N-CA-C	-7.13	91.75	111.00
1	A	104	ILE	N-CA-C	-6.99	92.13	111.00
1	A	289	LEU	CA-CB-CG	6.91	131.20	115.30
1	A	374	ARG	C-N-CA	-6.47	105.53	121.70
1	B	319	ALA	C-N-CD	-6.44	106.43	120.60
1	B	154	LEU	CA-CB-CG	6.41	130.05	115.30
1	B	221	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	60	GLY	N-CA-C	6.24	128.70	113.10
1	B	287	GLU	C-N-CA	-6.17	106.27	121.70
1	B	284	TYR	CB-CA-C	-5.86	98.67	110.40
1	A	287	GLU	N-CA-C	-5.70	95.61	111.00
1	B	284	TYR	CA-C-N	5.64	127.49	116.20
1	A	36	LEU	CA-CB-CG	5.46	127.87	115.30
1	B	362	ALA	N-CA-C	-5.45	96.29	111.00
1	A	278	ILE	CG1-CB-CG2	-5.43	99.46	111.40
1	A	399	VAL	CB-CA-C	5.42	121.70	111.40
1	B	233	GLY	N-CA-C	5.42	126.65	113.10
1	B	238	GLU	CB-CA-C	-5.41	99.58	110.40
1	A	303	GLY	CA-C-O	-5.35	110.97	120.60
1	A	303	GLY	O-C-N	-5.31	114.21	122.70
1	B	398	TYR	N-CA-C	5.31	125.33	111.00
1	A	60	GLY	N-CA-C	5.28	126.30	113.10
1	B	440	SER	N-CA-C	-5.27	96.77	111.00
1	A	105	PRO	N-CA-C	5.23	125.69	112.10
1	B	398	TYR	CB-CA-C	-5.17	100.06	110.40
1	B	61	GLN	N-CA-C	5.11	124.80	111.00
1	A	96	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	319	ALA	N-CA-C	-5.05	97.36	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	318	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	441	GLY	Peptide
1	B	161	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3706	0	3696	177	0
1	B	3703	0	3694	182	0
2	A	22	0	13	6	0
2	B	22	0	14	3	0
3	A	29	0	0	3	0
3	B	32	0	0	2	0
All	All	7514	0	7417	345	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 23.

All (345) 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:82:ARG:HH11	1:B:82:ARG:CB	1.43	1.29
1:B:284:TYR:CD1	1:B:288:ASP:OD1	1.90	1.24
1:B:284:TYR:CG	1:B:288:ASP:CG	2.12	1.23
1:B:303:GLY:HA2	1:B:304:GLU:CB	1.56	1.21
1:B:92:ASP:OD1	1:B:356:SER:HB2	1.42	1.18
1:A:354:ASP:OD1	1:A:355:GLU:N	1.76	1.18
1:B:84:GLU:O	1:B:87:THR:HG23	1.48	1.14
1:B:82:ARG:HH11	1:B:82:ARG:HB2	0.97	1.07
1:B:82:ARG:HB2	1:B:82:ARG:NH1	1.70	1.05
1:B:303:GLY:HA2	1:B:304:GLU:HB2	1.09	1.05
1:B:284:TYR:CD1	1:B:288:ASP:CG	2.29	1.04
1:B:141:ASP:OD1	1:B:322:ARG:NH1	1.90	1.04
1:B:284:TYR:CG	1:B:288:ASP:OD2	2.11	1.04
1:B:284:TYR:HB3	1:B:288:ASP:CB	1.88	1.03
1:A:49:LEU:CD2	1:A:51[B]:CYS:SG	2.49	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASP:O	1:A:357:TYR:HB3	1.60	1.01
1:A:373:ARG:HD2	1:A:459:GLU:OE2	1.59	1.01
1:B:303:GLY:CA	1:B:304:GLU:HB2	1.89	1.01
1:B:238:GLU:OE2	1:B:273:HIS:CG	2.18	0.96
1:B:284:TYR:CB	1:B:288:ASP:OD2	2.14	0.96
1:B:284:TYR:CE1	1:B:288:ASP:OD1	2.20	0.94
1:B:284:TYR:HB3	1:B:288:ASP:CG	1.88	0.94
1:B:378:LEU:HD12	1:B:455:ILE:HD12	1.49	0.93
1:B:82:ARG:CB	1:B:82:ARG:NH1	2.29	0.93
1:B:82:ARG:HH11	1:B:82:ARG:CG	1.81	0.92
1:A:407:GLN:HA	1:A:410:ILE:HG12	1.52	0.92
1:A:43:LEU:HD12	1:A:44:PRO:HD2	1.50	0.92
1:A:49:LEU:HD21	1:A:51[B]:CYS:SG	2.10	0.92
1:B:238:GLU:OE2	1:B:273:HIS:CD2	2.23	0.91
1:B:466:ILE:O	1:B:470:THR:HG22	1.73	0.89
1:B:49:LEU:HD23	1:B:51:CYS:SG	2.13	0.89
1:B:284:TYR:CB	1:B:288:ASP:CG	2.40	0.89
1:A:320:PRO:HB3	3:A:489:HOH:O	1.71	0.89
1:A:466:ILE:O	1:A:470:THR:HG23	1.74	0.88
1:B:260:VAL:HG22	1:B:296:SER:HB3	1.56	0.88
1:B:373:ARG:NH1	1:B:459:GLU:OE2	2.06	0.88
1:A:355:GLU:OE2	1:A:355:GLU:HA	1.73	0.88
1:B:92:ASP:OD1	1:B:354:ASP:HB3	1.74	0.87
1:A:288:ASP:O	1:A:289:LEU:HD23	1.76	0.85
1:B:303:GLY:CA	1:B:304:GLU:CB	2.49	0.85
1:A:349:PRO:O	1:A:351:LYS:HE2	1.76	0.85
1:B:284:TYR:HB3	1:B:288:ASP:HB2	1.59	0.85
1:B:466:ILE:O	1:B:470:THR:CG2	2.24	0.84
1:B:83:GLU:O	1:B:86:LYS:HG3	1.79	0.83
1:A:174:TYR:CE2	2:A:501:DCS:HA	2.13	0.83
1:A:454:THR:HG23	1:A:456:LEU:H	1.43	0.83
1:B:218:ILE:HD11	1:B:220:VAL:HG22	1.59	0.83
1:B:49:LEU:CD2	1:B:51:CYS:SG	2.67	0.83
1:A:68:ARG:HH21	1:B:109:THR:HG23	1.44	0.82
1:A:68:ARG:HH11	1:A:68:ARG:HG2	1.43	0.82
1:A:288:ASP:O	1:A:289:LEU:CG	2.27	0.81
1:A:354:ASP:O	1:A:357:TYR:CB	2.28	0.81
1:B:259:GLU:O	1:B:262:GLN:HG3	1.81	0.81
1:A:288:ASP:O	1:A:289:LEU:HG	1.80	0.80
1:A:68:ARG:HH11	1:A:68:ARG:CG	1.94	0.80
1:A:304:GLU:HG3	1:A:342:LEU:HD21	1.62	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:TYR:HB3	1:B:288:ASP:OD2	1.81	0.80
1:A:288:ASP:O	1:A:289:LEU:CD2	2.30	0.79
1:B:284:TYR:CD2	1:B:288:ASP:OD2	2.36	0.78
1:A:71:LEU:HD11	1:A:342:LEU:HD13	1.64	0.78
1:A:366:GLY:O	1:A:370:SER:HB2	1.83	0.78
1:A:351:LYS:O	1:A:352:ALA:HB3	1.81	0.78
1:A:242:TYR:CD1	1:A:282:LEU:HD13	2.17	0.78
1:A:249:LYS:HD2	1:A:284:TYR:CE1	2.19	0.78
1:B:245:VAL:HG21	1:B:278:ILE:HG22	1.65	0.77
1:A:351:LYS:O	1:A:352:ALA:CB	2.30	0.77
1:B:82:ARG:NH1	1:B:82:ARG:CG	2.43	0.77
1:B:407:GLN:O	1:B:410:ILE:HG12	1.84	0.76
1:B:286:GLU:O	1:B:287:GLU:CB	2.30	0.76
1:B:68:ARG:HG2	1:B:68:ARG:HH11	1.52	0.75
1:A:275:PHE:O	1:A:279:VAL:HG23	1.87	0.75
1:B:303:GLY:HA2	1:B:304:GLU:HB3	1.61	0.74
1:A:290:PRO:HB3	1:A:317:PHE:CZ	2.23	0.73
1:B:92:ASP:CG	1:B:354:ASP:HB3	2.08	0.73
1:A:288:ASP:C	1:A:289:LEU:HD23	2.08	0.73
1:B:330:SER:O	1:B:333:LEU:HA	1.89	0.73
1:B:238:GLU:OE2	1:B:273:HIS:CE1	2.41	0.73
1:B:63:PRO:HB2	1:B:68:ARG:HD2	1.72	0.72
1:B:83:GLU:HB3	1:B:86:LYS:HE3	1.70	0.72
1:A:68:ARG:HG2	1:A:68:ARG:NH1	2.04	0.72
1:A:354:ASP:OD1	1:A:356:SER:N	2.23	0.71
1:A:269:ASN:OD1	1:A:269:ASN:C	2.29	0.71
1:B:261:TYR:CE1	1:B:299:LYS:HG2	2.25	0.71
1:B:68:ARG:HG2	1:B:68:ARG:NH1	2.05	0.70
1:A:454:THR:HG22	1:A:457:PRO:HD3	1.72	0.70
1:A:197:THR:HG22	1:A:197:THR:O	1.91	0.70
1:A:421:ASP:HB3	1:A:438:PRO:HB2	1.73	0.70
1:B:351:LYS:O	1:B:352:ALA:HB3	1.90	0.70
1:A:355:GLU:O	1:A:356:SER:C	2.30	0.69
1:A:173:GLN:NE2	1:A:178:SER:HB3	2.07	0.69
1:A:282:LEU:HD23	1:A:284:TYR:HE2	1.56	0.69
1:A:302:TYR:N	1:A:302:TYR:CD1	2.61	0.69
1:A:38:THR:HG22	1:A:39:GLN:HG3	1.75	0.69
1:A:83:GLU:CD	1:A:83:GLU:H	1.96	0.68
1:A:286:GLU:C	1:A:288:ASP:N	2.41	0.67
1:A:218:ILE:HD11	1:A:220:VAL:HG22	1.76	0.67
1:A:354:ASP:OD1	1:A:354:ASP:C	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:ILE:HD11	3:A:506:HOH:O	1.94	0.67
1:A:290:PRO:HB3	1:A:317:PHE:CE2	2.29	0.67
1:B:28:HIS:HD2	1:B:426:LEU:HD21	1.58	0.67
1:B:284:TYR:CG	1:B:288:ASP:OD1	2.32	0.67
1:B:78:ASP:O	1:B:81:GLN:HB2	1.95	0.67
1:B:68:ARG:HH11	1:B:68:ARG:CG	2.07	0.67
1:A:59:LEU:HD12	1:A:456:LEU:HB2	1.77	0.67
1:A:268:ASP:N	1:A:268:ASP:OD1	2.29	0.66
1:A:242:TYR:CD1	1:A:282:LEU:CD1	2.78	0.66
1:A:205:ASP:O	1:A:209:GLN:HG2	1.96	0.65
1:B:84:GLU:OE2	1:B:84:GLU:N	2.29	0.64
1:B:454:THR:HG23	1:B:456:LEU:H	1.62	0.64
1:B:298:SER:HB3	1:B:305:CYS:SG	2.38	0.64
1:B:287:GLU:O	1:B:288:ASP:C	2.30	0.64
1:B:401:PRO:HD2	1:B:451:PHE:O	1.98	0.64
1:B:322:ARG:HA	1:B:325:ILE:HG13	1.79	0.64
1:B:238:GLU:OE2	1:B:273:HIS:ND1	2.30	0.63
1:A:332:ASN:O	1:A:333:LEU:HB2	1.97	0.63
1:B:284:TYR:CB	1:B:288:ASP:CB	2.74	0.62
1:A:305:CYS:HB3	1:B:112:TYR:CE2	2.34	0.62
1:B:55:ASN:O	1:B:58:SER:HB2	1.98	0.62
1:B:357:TYR:O	1:B:361:LYS:HB2	2.00	0.62
1:A:174:TYR:CE1	1:A:176:LEU:HB3	2.34	0.62
1:A:249:LYS:CD	1:A:284:TYR:CE1	2.83	0.62
1:A:298:SER:HB3	1:A:305:CYS:SG	2.39	0.62
1:B:373:ARG:NH1	1:B:459:GLU:CD	2.53	0.61
1:A:174:TYR:CZ	2:A:501:DCS:HA	2.35	0.61
1:B:332:ASN:O	1:B:333:LEU:HB2	2.00	0.61
1:A:54:GLY:H	2:A:501:DCS:HND	1.48	0.61
1:B:260:VAL:HG22	1:B:296:SER:CB	2.30	0.61
1:A:288:ASP:C	1:A:289:LEU:O	2.34	0.60
1:B:85:ILE:HG13	1:B:86:LYS:N	2.14	0.60
1:A:454:THR:CG2	1:A:456:LEU:H	2.14	0.60
1:B:49:LEU:HD21	1:B:51:CYS:SG	2.42	0.59
1:A:349:PRO:O	1:A:351:LYS:CE	2.48	0.59
1:A:371:LEU:O	1:A:375:ALA:N	2.35	0.59
1:A:242:TYR:CE1	1:A:282:LEU:HD13	2.36	0.59
1:B:354:ASP:OD1	1:B:355:GLU:N	2.29	0.59
1:A:132:ARG:HD2	1:A:133:ASP:OD1	2.03	0.59
1:A:49:LEU:HD22	1:A:51[B]:CYS:SG	2.38	0.59
1:A:261:TYR:CE1	1:A:299:LYS:HG3	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:THR:OG1	1:A:434:ILE:HG13	2.03	0.58
1:B:84:GLU:O	1:B:87:THR:CG2	2.39	0.58
1:A:242:TYR:HD1	1:A:282:LEU:HD13	1.66	0.58
1:B:169:VAL:HB	1:B:188:LEU:CD1	2.33	0.58
1:A:373:ARG:HH11	1:A:459:GLU:CD	2.07	0.58
1:B:286:GLU:O	1:B:287:GLU:HB3	2.03	0.58
1:B:261:TYR:CE1	1:B:299:LYS:CG	2.87	0.58
1:B:22:ARG:HA	1:B:26:VAL:HG21	1.86	0.57
1:B:407:GLN:HB2	1:B:410:ILE:HD11	1.86	0.57
1:A:249:LYS:HD2	1:A:284:TYR:HE1	1.69	0.57
1:A:112:TYR:CZ	1:B:305:CYS:HB3	2.40	0.57
1:A:295:GLN:OE1	1:A:296:SER:N	2.34	0.57
1:B:48:ILE:CG2	1:B:48:ILE:O	2.52	0.57
1:B:132:ARG:HD2	1:B:133:ASP:OD1	2.04	0.57
1:A:109:THR:CG2	1:B:68:ARG:HH21	2.17	0.57
1:A:112:TYR:CE2	1:B:305:CYS:HB3	2.40	0.57
1:B:82:ARG:NH1	1:B:82:ARG:HG3	2.19	0.56
1:A:297:VAL:HG11	1:A:342:LEU:HD23	1.87	0.56
1:B:201:LEU:O	1:B:201:LEU:HD23	2.06	0.56
1:A:231:PRO:HB3	1:A:452:ARG:HD3	1.88	0.56
1:A:354:ASP:OD1	1:A:355:GLU:CA	2.52	0.56
1:B:209:GLN:OE1	3:B:497:HOH:O	2.17	0.56
1:B:238:GLU:OE2	1:B:273:HIS:NE2	2.39	0.56
1:B:327:LYS:O	1:B:330:SER:OG	2.20	0.56
1:A:109:THR:HG22	1:B:68:ARG:HH21	1.70	0.56
1:A:298:SER:O	1:A:303:GLY:HA2	2.05	0.56
1:A:333:LEU:O	1:A:334:CYS:HB3	2.06	0.55
1:B:298:SER:O	1:B:303:GLY:HA3	2.07	0.55
1:B:210:LEU:HD21	1:B:251:GLU:HG3	1.88	0.55
1:B:361:LYS:HA	1:B:364:LYS:HB3	1.88	0.55
1:B:375:ALA:HA	1:B:455:ILE:HD11	1.88	0.54
1:B:378:LEU:HD12	1:B:455:ILE:CD1	2.30	0.54
1:B:144:LEU:CD1	1:B:144:LEU:N	2.71	0.54
1:A:280:ARG:HH22	1:A:315:THR:HG21	1.72	0.54
1:A:354:ASP:O	1:A:357:TYR:N	2.40	0.54
1:A:144:LEU:HD12	1:A:311:TYR:HB3	1.90	0.54
1:A:82:ARG:HD2	1:B:88:LEU:HD22	1.90	0.53
1:B:284:TYR:CB	1:B:288:ASP:HB2	2.33	0.53
1:B:360:TYR:CG	1:B:360:TYR:O	2.61	0.53
1:A:297:VAL:O	1:A:297:VAL:CG1	2.55	0.53
1:A:352:ALA:HA	1:A:357:TYR:CG	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ILE:O	1:B:48:ILE:HG23	2.08	0.53
1:A:286:GLU:O	1:A:287:GLU:C	2.44	0.53
1:A:298:SER:C	1:A:299:LYS:HD3	2.29	0.53
1:B:357:TYR:O	1:B:360:TYR:HB3	2.08	0.53
1:B:218:ILE:C	1:B:218:ILE:HD12	2.29	0.53
1:B:341:ILE:HG22	1:B:345:LEU:CD2	2.39	0.53
1:A:305:CYS:O	1:A:308:ARG:HD2	2.09	0.52
1:B:478:SER:HA	1:B:481:ARG:HG3	1.91	0.52
1:B:226:ILE:HG22	1:B:229:GLY:HA2	1.91	0.52
1:B:311:TYR:C	1:B:311:TYR:CD2	2.83	0.52
1:B:115:SER:OG	1:B:330:SER:HA	2.10	0.52
1:B:154:LEU:HD11	1:B:325:ILE:HG23	1.92	0.52
1:B:304:GLU:OE2	1:B:304:GLU:HA	2.09	0.52
1:A:373:ARG:NH1	1:A:459:GLU:OE1	2.42	0.52
1:A:254:VAL:HG13	1:A:290:PRO:HB2	1.91	0.52
1:B:169:VAL:HG13	1:B:170:PRO:HD2	1.92	0.52
1:B:407:GLN:HA	1:B:410:ILE:HG12	1.92	0.52
1:A:76:HIS:HB3	1:A:79:LEU:HD22	1.91	0.52
1:B:385:LEU:HD11	1:B:470:THR:HB	1.92	0.51
1:B:286:GLU:O	1:B:287:GLU:HB2	2.07	0.51
1:B:279:VAL:HG13	1:B:288:ASP:OD2	2.10	0.51
1:B:361:LYS:O	1:B:362:ALA:C	2.45	0.51
1:A:282:LEU:HD23	1:A:284:TYR:CE2	2.44	0.51
1:A:88:LEU:HD23	1:A:88:LEU:H	1.75	0.51
1:B:218:ILE:HD11	1:B:220:VAL:CG2	2.38	0.51
1:A:9:ASN:O	1:B:221:ARG:NH2	2.44	0.51
1:B:92:ASP:CG	1:B:354:ASP:CB	2.79	0.51
1:A:113:SER:HB2	1:A:118:ILE:HG13	1.92	0.50
1:B:466:ILE:O	1:B:470:THR:HG23	2.06	0.50
1:A:269:ASN:OD1	1:A:269:ASN:O	2.29	0.50
1:A:304:GLU:CG	1:A:342:LEU:HD21	2.37	0.50
1:B:351:LYS:O	1:B:352:ALA:CB	2.56	0.50
1:A:158:LEU:HD13	1:A:325:ILE:HD13	1.93	0.50
1:B:166:GLY:HA3	1:B:218:ILE:HD13	1.94	0.50
1:B:174:TYR:CZ	2:B:502:DCS:HA	2.46	0.50
1:B:245:VAL:HG21	1:B:278:ILE:CG2	2.40	0.50
1:B:53:ILE:HG13	2:B:502:DCS:OG	2.11	0.50
1:B:144:LEU:N	1:B:144:LEU:HD12	2.27	0.50
1:B:287:GLU:O	1:B:287:GLU:OE1	2.30	0.49
1:A:357:TYR:CD2	1:A:357:TYR:C	2.85	0.49
1:A:299:LYS:HD3	1:A:299:LYS:N	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:O	1:A:173:GLN:HB3	2.13	0.49
1:A:354:ASP:CG	1:A:355:GLU:N	2.58	0.49
1:A:49:LEU:C	1:A:49:LEU:HD23	2.33	0.49
1:A:88:LEU:H	1:A:88:LEU:CD2	2.26	0.49
1:A:154:LEU:HD11	1:A:325:ILE:HG23	1.94	0.48
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.58	0.48
1:B:78:ASP:O	1:B:81:GLN:CB	2.60	0.48
1:B:81:GLN:HA	1:B:81:GLN:OE1	2.12	0.48
1:A:355:GLU:C	1:A:357:TYR:N	2.60	0.48
1:B:81:GLN:OE1	1:B:81:GLN:CA	2.57	0.48
1:A:173:GLN:HG2	1:A:174:TYR:O	2.13	0.48
1:A:218:ILE:C	1:A:218:ILE:HD12	2.34	0.48
1:B:169:VAL:HB	1:B:188:LEU:HD13	1.94	0.48
1:A:55:ASN:O	1:A:58:SER:HB2	2.14	0.48
1:B:330:SER:O	1:B:333:LEU:CA	2.62	0.48
1:B:148:ALA:HB2	1:B:296:SER:HB2	1.96	0.48
1:A:59:LEU:CD1	1:A:456:LEU:HB2	2.43	0.48
1:A:260:VAL:HG22	1:A:296:SER:HB3	1.96	0.48
1:B:361:LYS:CA	1:B:364:LYS:H	2.26	0.48
1:B:395:GLY:O	1:B:396:ALA:HB3	2.13	0.48
1:A:407:GLN:H	1:A:407:GLN:HG2	1.59	0.47
1:B:367:ILE:O	1:B:368:LEU:C	2.50	0.47
1:A:466:ILE:CD1	3:A:506:HOH:O	2.57	0.47
1:A:399:VAL:HG13	1:A:401:PRO:HD3	1.96	0.47
1:B:360:TYR:O	1:B:364:LYS:N	2.47	0.47
1:A:221:ARG:NH2	1:B:9:ASN:O	2.48	0.47
1:A:308:ARG:NH2	2:A:501:DCS:O2P	2.48	0.47
1:A:214:ARG:NH2	1:A:251:GLU:OE1	2.46	0.46
1:B:174:TYR:CD2	1:B:175:PRO:HD2	2.50	0.46
1:A:288:ASP:HB3	1:A:289:LEU:O	2.16	0.46
1:A:274:SER:HB2	1:A:277:LYS:H	1.80	0.46
1:A:11:ASN:HA	1:B:161:ARG:HG2	1.98	0.46
1:A:218:ILE:HD11	1:A:220:VAL:CG2	2.44	0.46
1:A:281:SER:OG	1:A:282:LEU:N	2.47	0.46
1:A:355:GLU:O	1:A:358:ALA:N	2.48	0.46
1:A:197:THR:O	1:A:197:THR:CG2	2.62	0.46
1:A:83:GLU:CD	1:A:83:GLU:N	2.65	0.45
1:B:138:ASN:HB3	3:B:509:HOH:O	2.16	0.45
1:B:240:ASN:OD1	1:B:240:ASN:O	2.34	0.45
1:A:369:ALA:O	1:A:373:ARG:HB2	2.16	0.45
1:A:395:GLY:O	1:A:396:ALA:HB3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:GLN:HB2	1:B:410:ILE:CD1	2.46	0.45
1:A:304:GLU:OE2	1:A:304:GLU:HA	2.16	0.45
1:B:399:VAL:HG13	1:B:455:ILE:HD13	1.98	0.45
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.46	0.45
1:A:96:ARG:HG3	1:A:100:ILE:HD12	1.98	0.45
1:A:49:LEU:HD23	1:A:49:LEU:O	2.17	0.44
1:A:63:PRO:HB2	1:A:68:ARG:HD2	1.97	0.44
1:B:407:GLN:O	1:B:410:ILE:CG1	2.58	0.44
1:A:85:ILE:HA	1:A:88:LEU:CD2	2.47	0.44
1:B:77:PRO:HB3	1:B:101:LEU:HD11	1.98	0.44
1:A:239:GLU:O	1:A:243:ASP:OD1	2.35	0.44
1:A:249:LYS:HD3	1:A:284:TYR:OH	2.17	0.44
1:B:458:GLN:CG	1:B:461:LYS:HD3	2.48	0.44
1:A:82:ARG:NH1	1:A:82:ARG:HB2	2.33	0.44
1:A:362:ALA:O	1:A:365:ASP:O	2.35	0.44
1:B:287:GLU:O	1:B:288:ASP:O	2.35	0.44
1:A:242:TYR:HD1	1:A:282:LEU:CD1	2.27	0.44
1:A:336:ASN:OD1	1:A:338:THR:HG23	2.17	0.44
1:B:170:PRO:O	1:B:171:ILE:HD12	2.17	0.44
1:A:231:PRO:HG3	1:A:442:PHE:CD2	2.52	0.44
1:B:330:SER:O	1:B:333:LEU:N	2.50	0.44
1:A:297:VAL:O	1:A:302:TYR:HD2	2.01	0.44
1:B:262:GLN:HG2	1:B:272:PHE:CZ	2.53	0.44
1:A:112:TYR:CE1	1:B:305:CYS:SG	3.11	0.44
1:A:237:ALA:HB2	1:A:270:LYS:HE3	2.00	0.44
1:A:466:ILE:HD12	1:A:470:THR:CG2	2.48	0.44
1:B:284:TYR:CD2	1:B:288:ASP:CG	2.80	0.44
1:B:210:LEU:CD2	1:B:251:GLU:HG3	2.47	0.43
1:A:308:ARG:HE	1:A:308:ARG:HA	1.84	0.43
1:A:49:LEU:CD2	1:A:51[A]:CYS:HB2	2.48	0.43
1:B:361:LYS:HD2	1:B:365:ASP:OD2	2.19	0.43
1:A:212:ASP:OD1	1:A:216:ARG:NH2	2.46	0.43
1:A:228:PRO:HG2	1:A:261:TYR:O	2.19	0.43
1:A:84:GLU:OE2	1:A:84:GLU:N	2.51	0.43
1:A:263:GLU:HG3	1:A:302:TYR:OH	2.19	0.43
1:B:255:LEU:O	1:B:291:LEU:HD12	2.18	0.43
1:B:385:LEU:HD12	1:B:385:LEU:HA	1.74	0.43
1:A:85:ILE:HA	1:A:88:LEU:HD23	2.00	0.43
1:A:304:GLU:HG3	1:A:342:LEU:CD2	2.42	0.43
1:B:38:THR:HG22	1:B:39:GLN:HG2	2.00	0.43
1:B:78:ASP:OD1	1:B:78:ASP:N	2.50	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ASP:HB3	1:B:314:ILE:O	2.18	0.43
1:B:191:TYR:O	1:B:191:TYR:CD1	2.71	0.43
1:A:158:LEU:CD1	1:A:325:ILE:HD13	2.48	0.43
1:A:299:LYS:HZ1	2:A:501:DCS:H4A2	1.83	0.43
1:B:295:GLN:HB3	1:B:311:TYR:CZ	2.54	0.43
1:B:363:GLU:O	1:B:364:LYS:C	2.54	0.43
1:B:454:THR:HG23	1:B:456:LEU:HB2	2.00	0.43
1:B:359:SER:O	1:B:363:GLU:HB2	2.18	0.43
1:B:218:ILE:HD12	1:B:219:ASN:N	2.33	0.43
1:B:470:THR:O	1:B:474:GLU:HG2	2.19	0.43
1:A:408:LYS:HE2	1:A:408:LYS:HB3	1.70	0.42
1:A:345:LEU:HA	1:A:345:LEU:HD12	1.86	0.42
1:B:143:PHE:O	1:B:311:TYR:HA	2.19	0.42
1:A:307:LYS:HA	1:A:307:LYS:HD3	1.69	0.42
1:A:280:ARG:HD3	1:A:280:ARG:HA	1.55	0.42
1:A:381:ALA:HB1	1:A:466:ILE:HD13	2.01	0.42
1:B:296:SER:OG	2:B:502:DCS:O1P	2.26	0.42
1:A:166:GLY:HA3	1:A:218:ILE:CD1	2.49	0.42
1:B:13:LYS:HE2	1:B:185:GLY:HA3	2.01	0.41
1:B:170:PRO:HD3	1:B:224:VAL:O	2.20	0.41
1:A:258:ASP:OD2	2:A:501:DCS:N1	2.52	0.41
1:A:305:CYS:HB3	1:B:112:TYR:CD2	2.55	0.41
1:A:363:GLU:O	1:A:367:ILE:HB	2.20	0.41
1:A:171:ILE:HG13	1:A:190:PRO:HB3	2.03	0.41
1:A:28:HIS:CG	1:A:31:ARG:HH12	2.39	0.41
1:A:293:SER:O	1:A:312:PHE:HA	2.20	0.41
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.81	0.41
1:B:231:PRO:HB3	1:B:452:ARG:HD3	2.02	0.41
1:A:76:HIS:HB3	1:A:79:LEU:CD2	2.51	0.41
1:B:201:LEU:HD23	1:B:201:LEU:C	2.40	0.41
1:B:455:ILE:HD12	1:B:455:ILE:HA	1.93	0.41
1:A:68:ARG:NH2	1:B:109:THR:HG23	2.24	0.41
1:A:466:ILE:HD12	1:A:470:THR:HG23	2.03	0.41
1:B:188:LEU:HD12	1:B:189:VAL:N	2.36	0.41
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.98	0.41
1:A:43:LEU:HD13	1:A:43:LEU:HA	1.68	0.40
1:A:72:ALA:HB2	1:B:76:HIS:HB2	2.03	0.40
1:A:371:LEU:HD23	1:A:374:ARG:NH2	2.37	0.40
1:A:85:ILE:HG13	1:A:86:LYS:N	2.37	0.40
1:B:215:SER:C	1:B:217:GLY:H	2.23	0.40
1:A:249:LYS:HD3	1:A:284:TYR:CZ	2.57	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:O	1:A:408:LYS:C	2.59	0.40
1:B:287:GLU:H	1:B:316:GLY:HA2	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/500 (96%)	450 (94%)	24 (5%)	4 (1%)	19	41
1	B	477/500 (95%)	446 (94%)	26 (6%)	5 (1%)	15	35
All	All	955/1000 (96%)	896 (94%)	50 (5%)	9 (1%)	17	38

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	GLU
1	B	283	GLY
1	B	304	GLU
1	A	352	ALA
1	A	396	ALA
1	B	105	PRO
1	B	396	ALA
1	B	233	GLY
1	A	456	LEU

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	396/414 (96%)	339 (86%)	57 (14%)	3 7
1	B	395/414 (95%)	343 (87%)	52 (13%)	4 8
All	All	791/828 (96%)	682 (86%)	109 (14%)	3 7

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	8	ASP
1	A	32	LEU
1	A	36	LEU
1	A	37	LYS
1	A	43	LEU
1	A	46	ASP
1	A	47	GLU
1	A	58	SER
1	A	65	THR
1	A	68	ARG
1	A	78	ASP
1	A	79	LEU
1	A	80	LEU
1	A	88	LEU
1	A	90	SER
1	A	103	MET
1	A	109	THR
1	A	144	LEU
1	A	154	LEU
1	A	155	MET
1	A	159	LEU
1	A	162	ASN
1	A	176	LEU
1	A	196	SER
1	A	203	THR
1	A	204	SER
1	A	218	ILE
1	A	250	ASN
1	A	263	GLU
1	A	268	ASP
1	A	281	SER
1	A	288	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	289	LEU
1	A	290	PRO
1	A	295	GLN
1	A	302	TYR
1	A	304	GLU
1	A	308	ARG
1	A	313	GLU
1	A	323	GLU
1	A	336	ASN
1	A	338	THR
1	A	345	LEU
1	A	355	GLU
1	A	370	SER
1	A	392	GLU
1	A	399	VAL
1	A	403	ILE
1	A	408	LYS
1	A	426	LEU
1	A	445	VAL
1	A	453	CYS
1	A	454	THR
1	A	455	ILE
1	A	461	LYS
1	A	466	ILE
1	B	17	CYS
1	B	32	LEU
1	B	48	ILE
1	B	58	SER
1	B	68	ARG
1	B	78	ASP
1	B	79	LEU
1	B	80	LEU
1	B	82	ARG
1	B	87	THR
1	B	105	PRO
1	B	123	ASP
1	B	154	LEU
1	B	159	LEU
1	B	173	GLN
1	B	188	LEU
1	B	201	LEU
1	B	202	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	204	SER
1	B	207	LYS
1	B	215	SER
1	B	218	ILE
1	B	224	VAL
1	B	236	LEU
1	B	251	GLU
1	B	263	GLU
1	B	268	ASP
1	B	276	LYS
1	B	286	GLU
1	B	289	LEU
1	B	304	GLU
1	B	324	GLN
1	B	325	ILE
1	B	338	THR
1	B	345	LEU
1	B	355	GLU
1	B	359	SER
1	B	361	LYS
1	B	370	SER
1	B	385	LEU
1	B	386	GLU
1	B	398	TYR
1	B	403	ILE
1	B	414	LYS
1	B	426	LEU
1	B	427	ARG
1	B	454	THR
1	B	458	GLN
1	B	459	GLU
1	B	460	ASP
1	B	466	ILE
1	B	470	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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	DCS	B	502	-	22,23,23	2.73	4 (18%)	25,33,33	2.52	11 (44%)
2	DCS	A	501	-	22,23,23	2.75	6 (27%)	25,33,33	1.81	5 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DCS	B	502	-	-	6/10/21/21	0/2/2/2
2	DCS	A	501	-	-	6/10/21/21	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	DCS	C3-C2	7.89	1.48	1.40
2	A	501	DCS	CA-C	-7.82	1.46	1.52
2	B	502	DCS	C5-C4	6.67	1.49	1.40
2	A	501	DCS	C3-C2	6.60	1.47	1.40
2	B	502	DCS	C3-C4	6.37	1.49	1.40
2	A	501	DCS	C5-C4	5.04	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	DCS	C3-C4	4.31	1.46	1.40
2	B	502	DCS	C-ND	-2.57	1.31	1.34
2	A	501	DCS	C-ND	-2.57	1.31	1.34
2	A	501	DCS	O-C	-2.28	1.18	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	DCS	CB-OG-ND	6.48	115.61	105.72
2	B	502	DCS	C4A-N-CA	5.81	124.93	113.92
2	A	501	DCS	C4A-C4-C3	4.57	124.94	120.04
2	A	501	DCS	O-C-CA	-4.28	123.09	126.18
2	B	502	DCS	C6-C5-C4	3.77	120.79	118.12
2	B	502	DCS	C4-C3-C2	-3.08	115.35	120.06
2	A	501	DCS	CB-OG-ND	3.05	110.36	105.72
2	B	502	DCS	O3P-P-O4P	-2.95	98.90	106.73
2	A	501	DCS	O3P-P-O2P	2.43	116.91	107.64
2	B	502	DCS	O-C-CA	-2.40	124.45	126.18
2	B	502	DCS	O3-C3-C4	2.31	124.91	118.13
2	B	502	DCS	O3P-P-O2P	2.26	116.27	107.64
2	B	502	DCS	C3-C4-C5	-2.25	116.56	118.72
2	B	502	DCS	C6-N1-C2	2.25	123.34	119.17
2	A	501	DCS	C3-C4-C5	-2.18	116.63	118.72
2	B	502	DCS	C4A-C4-C3	2.07	122.26	120.04

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	DCS	C3-C4-C4A-N
2	A	501	DCS	C5-C4-C4A-N
2	A	501	DCS	C5A-O4P-P-O2P
2	A	501	DCS	C5A-O4P-P-O3P
2	B	502	DCS	C3-C4-C4A-N
2	B	502	DCS	C5-C4-C4A-N
2	B	502	DCS	C5A-O4P-P-O1P
2	B	502	DCS	C5A-O4P-P-O2P
2	B	502	DCS	C5A-O4P-P-O3P
2	B	502	DCS	C4-C4A-N-CA
2	A	501	DCS	C5A-O4P-P-O1P
2	A	501	DCS	C4-C4A-N-CA

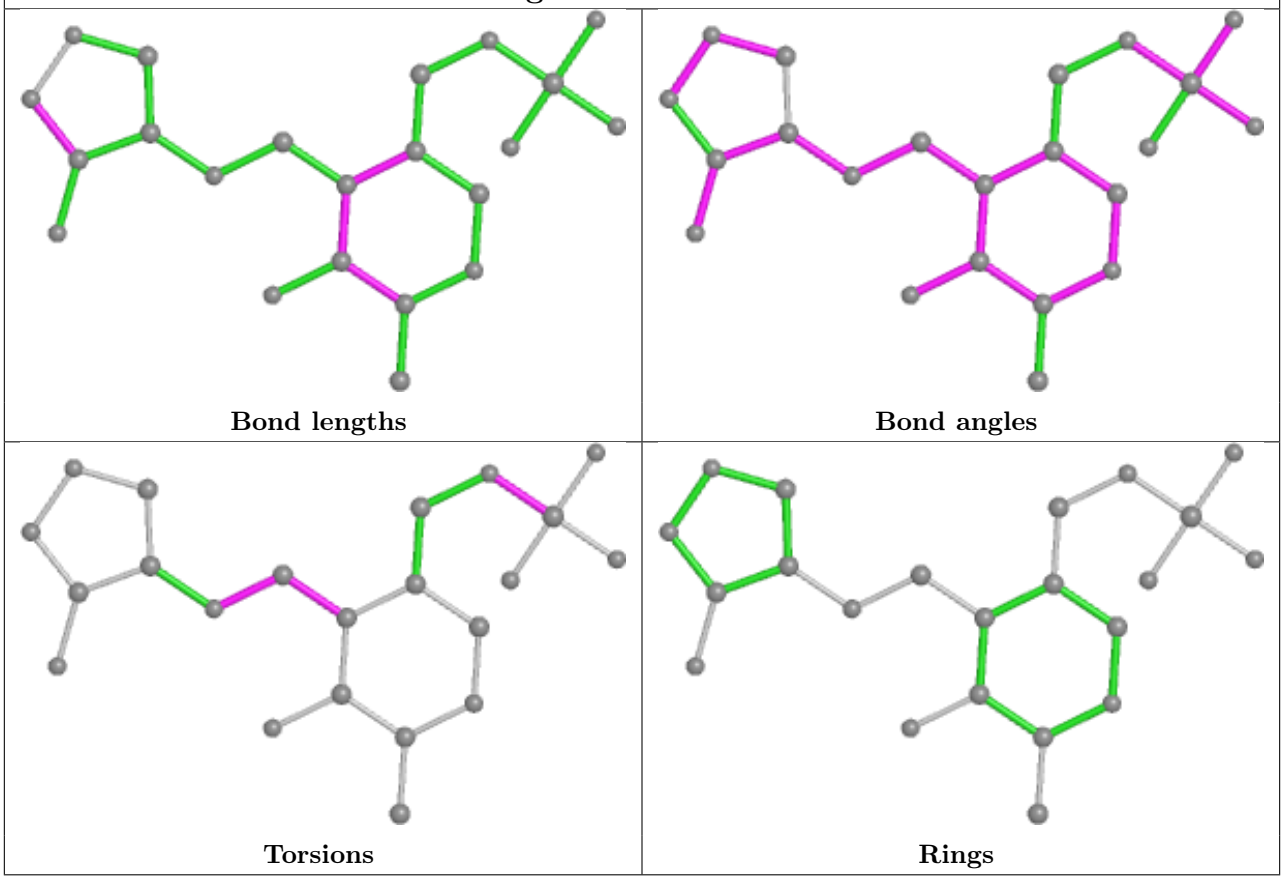
There are no ring outliers.

2 monomers are involved in 9 short contacts:

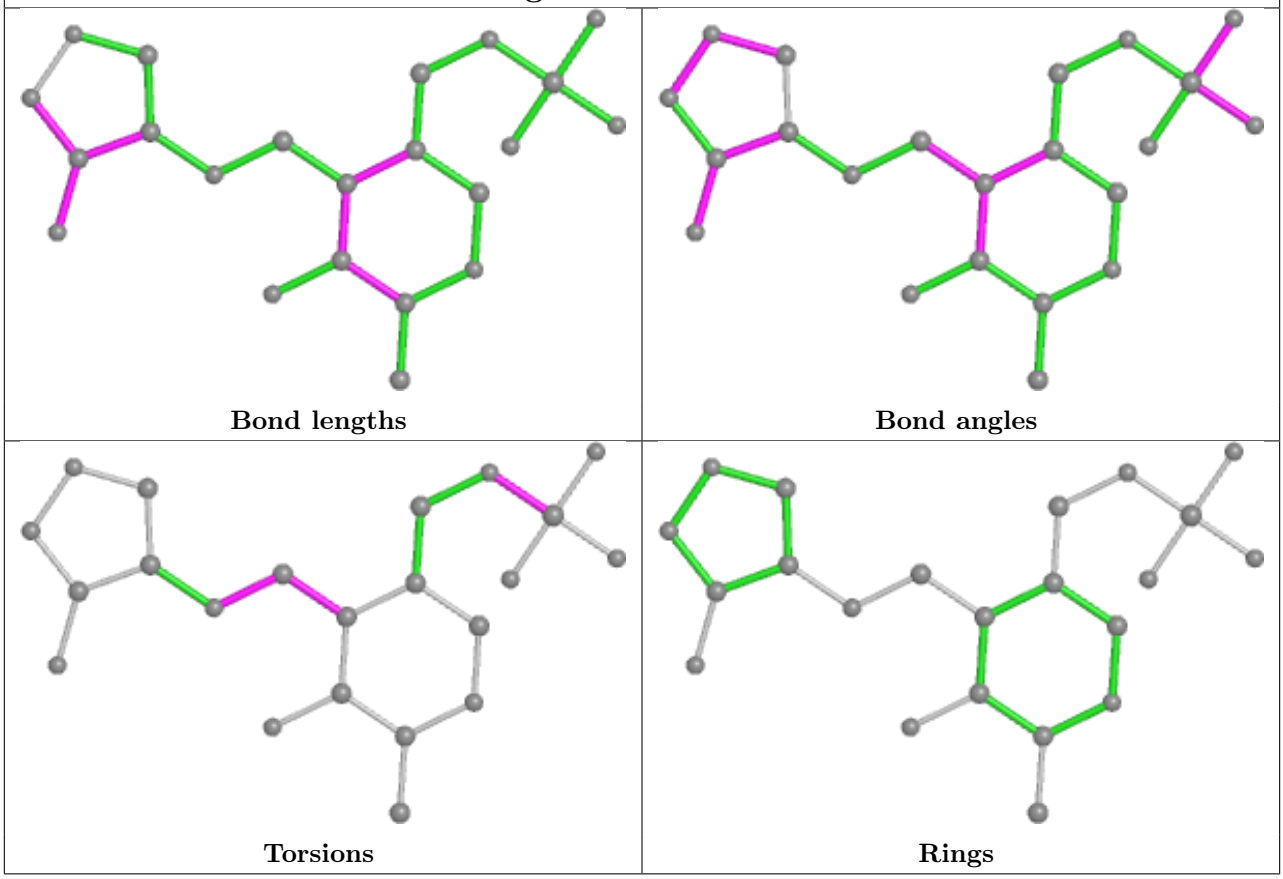
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	DCS	3	0
2	A	501	DCS	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 DCS B 502



Ligand DCS A 501



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	479/500 (95%)	-0.15	5 (1%)	82	83	24, 40, 61, 76	0
1	B	479/500 (95%)	-0.02	5 (1%)	82	83	24, 39, 61, 76	0
All	All	958/1000 (95%)	-0.09	10 (1%)	82	83	24, 40, 61, 76	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ASP	6.8
1	A	355	GLU	3.9
1	A	288	ASP	3.7
1	B	284	TYR	3.4
1	A	375	ALA	2.7
1	B	287	GLU	2.5
1	B	40	PRO	2.4
1	A	46	ASP	2.4
1	A	268	ASP	2.2
1	B	386	GLU	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)

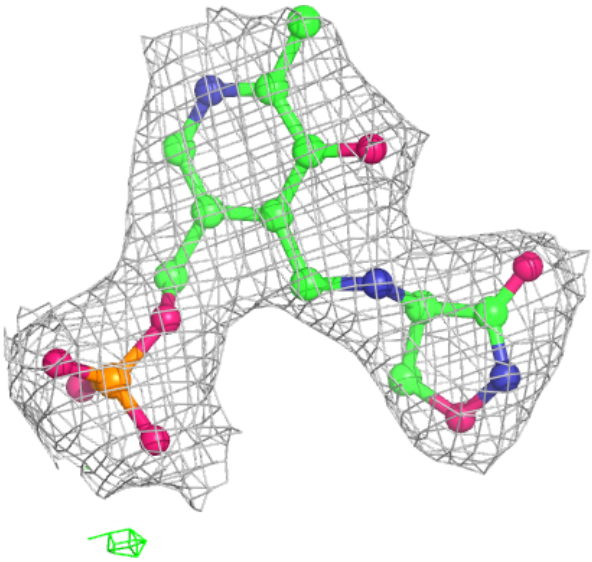
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

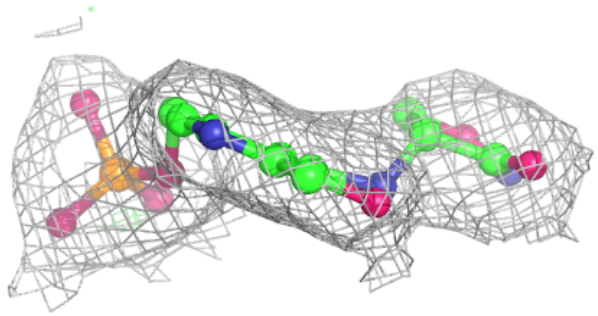
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DCS	A	501	22/22	0.98	0.19	27,32,38,39	0
2	DCS	B	502	22/22	0.98	0.24	26,33,42,44	0

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 DCS A 501:

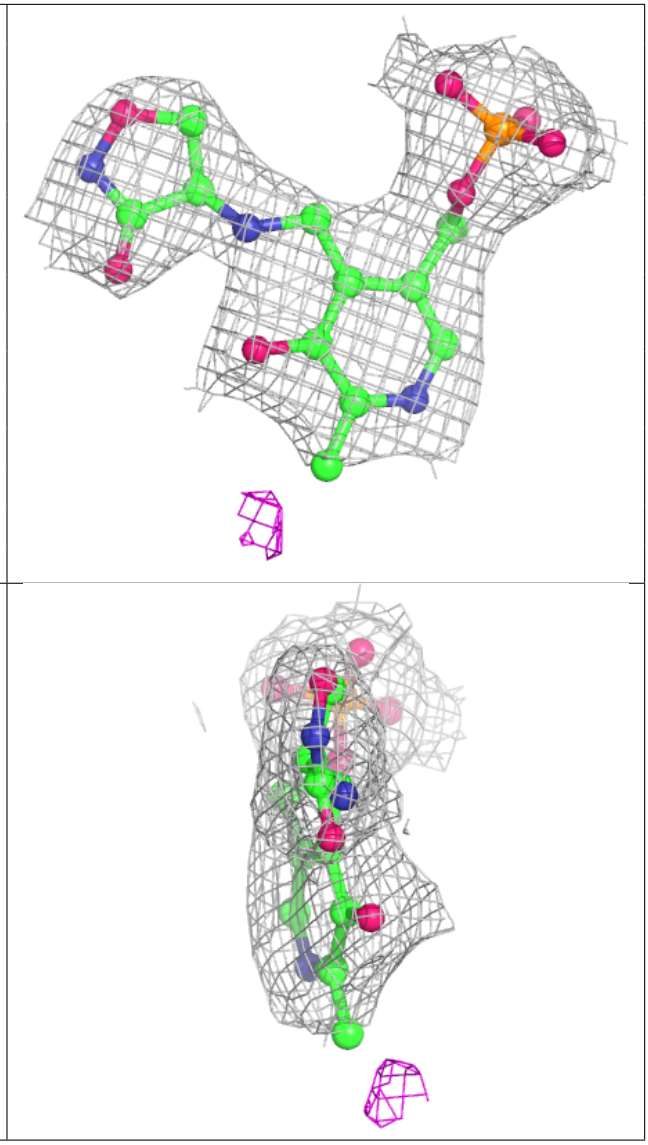
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)





Electron density around DCS B 502:

$2mF_o$-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.