Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:41 pm BST

PDB ID	:	3S6G
Title	:	Crystal structures of Seleno-substituted mutant mmNAGS in space group P212121
Authors	:	Shi, D.; Li, Y.; Cabrera-Luque, J.; Jin, Z.; Yu, X.; Allewell, N.M.; Tuchman, M.
Deposited on	:	2011-05-25
Resolution	:	2.67 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 following versions of software and data (see references ⓘ) were used in the production of this report:

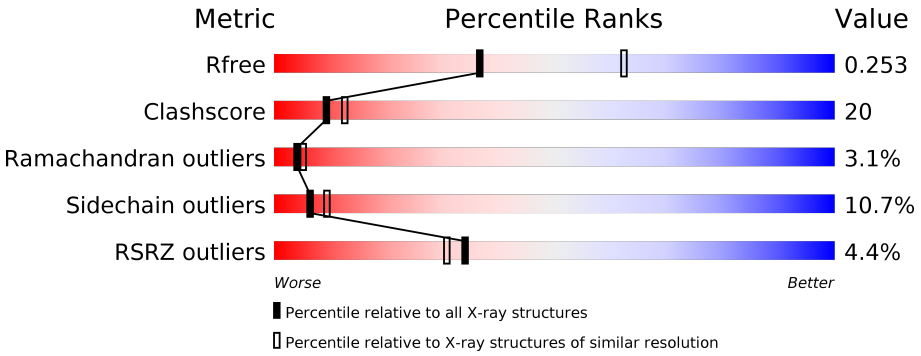
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.67 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	460	3% 64% 25% 6% 5%
1	B	460	4% 57% 31% 6% 5%
1	X	460	% 64% 25% • • 5%
1	Y	460	8% 53% 31% 5% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13303 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 N-acetylglutamate kinase / N-acetylglutamate synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	436	Total	C	N	O	S	Se	0	1	0
			3349	2104	605	631	2	7			
1	B	435	Total	C	N	O	S	Se	0	0	0
			3334	2094	601	630	2	7			
1	X	435	Total	C	N	O	S	Se	0	0	0
			3334	2094	601	630	2	7			
1	Y	408	Total	C	N	O	S	Se	0	0	0
			3127	1969	560	589	2	7			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	EXPRESSION TAG	UNP Q0ASS9
A	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
A	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-15	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	-9	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-8	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	-7	GLY	-	EXPRESSION TAG	UNP Q0ASS9
A	-6	LEU	-	EXPRESSION TAG	UNP Q0ASS9
A	-5	VAL	-	EXPRESSION TAG	UNP Q0ASS9
A	-4	PRO	-	EXPRESSION TAG	UNP Q0ASS9
A	-3	ARG	-	EXPRESSION TAG	UNP Q0ASS9
A	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
A	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
A	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9
A	106	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	294	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
A	376	MSE	LEU	ENGINEERED MUTATION	UNP Q0ASS9
B	-19	MSE	-	EXPRESSION TAG	UNP Q0ASS9
B	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
B	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	-15	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	-9	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	-8	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	-7	GLY	-	EXPRESSION TAG	UNP Q0ASS9
B	-6	LEU	-	EXPRESSION TAG	UNP Q0ASS9
B	-5	VAL	-	EXPRESSION TAG	UNP Q0ASS9
B	-4	PRO	-	EXPRESSION TAG	UNP Q0ASS9
B	-3	ARG	-	EXPRESSION TAG	UNP Q0ASS9
B	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
B	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9
B	106	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
B	294	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
B	376	MSE	LEU	ENGINEERED MUTATION	UNP Q0ASS9
X	-19	MSE	-	EXPRESSION TAG	UNP Q0ASS9
X	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-15	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	-9	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-8	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	-7	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-6	LEU	-	EXPRESSION TAG	UNP Q0ASS9
X	-5	VAL	-	EXPRESSION TAG	UNP Q0ASS9
X	-4	PRO	-	EXPRESSION TAG	UNP Q0ASS9
X	-3	ARG	-	EXPRESSION TAG	UNP Q0ASS9

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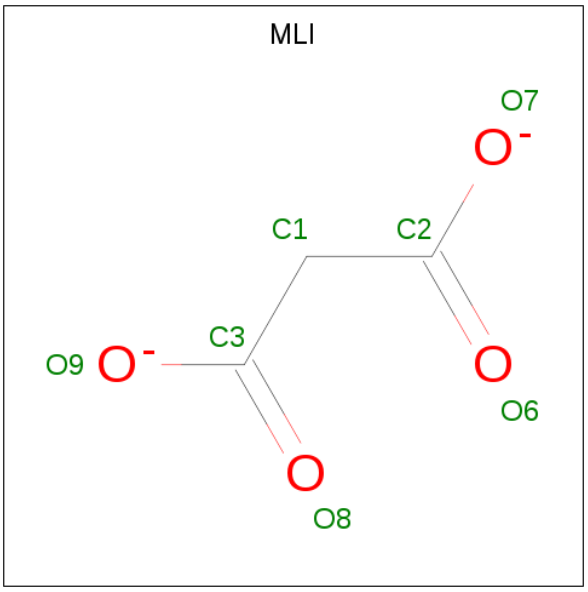
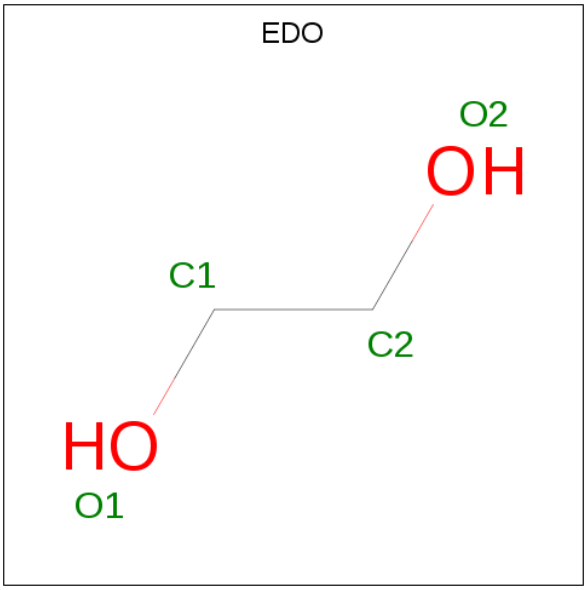
Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	106	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
X	294	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
X	376	MSE	LEU	ENGINEERED MUTATION	UNP Q0ASS9
Y	-19	MSE	-	EXPRESSION TAG	UNP Q0ASS9
Y	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
Y	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
Y	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
Y	-15	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	-14	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	-13	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	-12	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	-11	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	-10	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	-9	SER	-	EXPRESSION TAG	UNP Q0ASS9
Y	-8	SER	-	EXPRESSION TAG	UNP Q0ASS9
Y	-7	GLY	-	EXPRESSION TAG	UNP Q0ASS9
Y	-6	LEU	-	EXPRESSION TAG	UNP Q0ASS9
Y	-5	VAL	-	EXPRESSION TAG	UNP Q0ASS9
Y	-4	PRO	-	EXPRESSION TAG	UNP Q0ASS9
Y	-3	ARG	-	EXPRESSION TAG	UNP Q0ASS9
Y	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
Y	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
Y	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9
Y	106	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
Y	294	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
Y	376	MSE	LEU	ENGINEERED MUTATION	UNP Q0ASS9

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



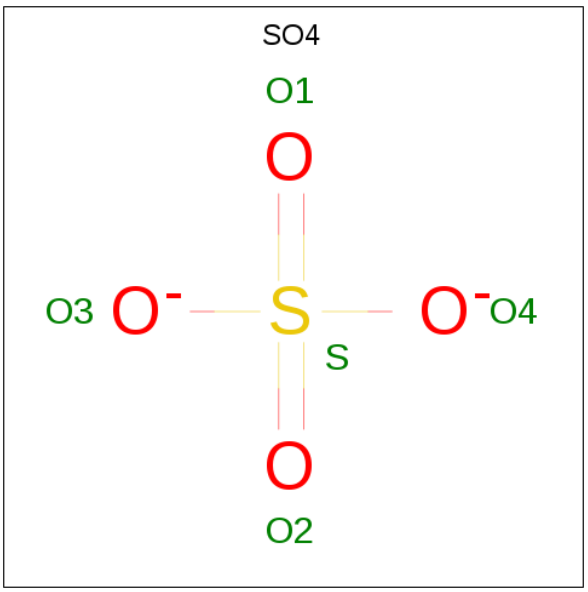
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 3 4	0	0
2	Y	1	Total C O 7 3 4	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



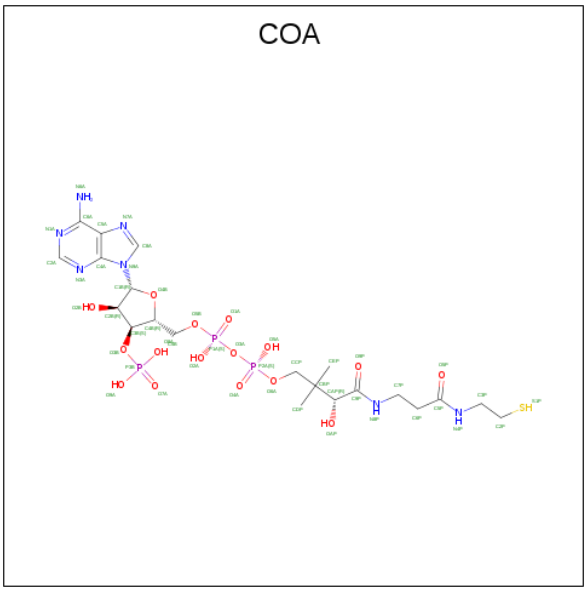
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	X	1	Total O S 5 4 1	0	0

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Y	1	Total C N O P S 48 21 7 16 3 1	0	0

- Molecule 6 is water.

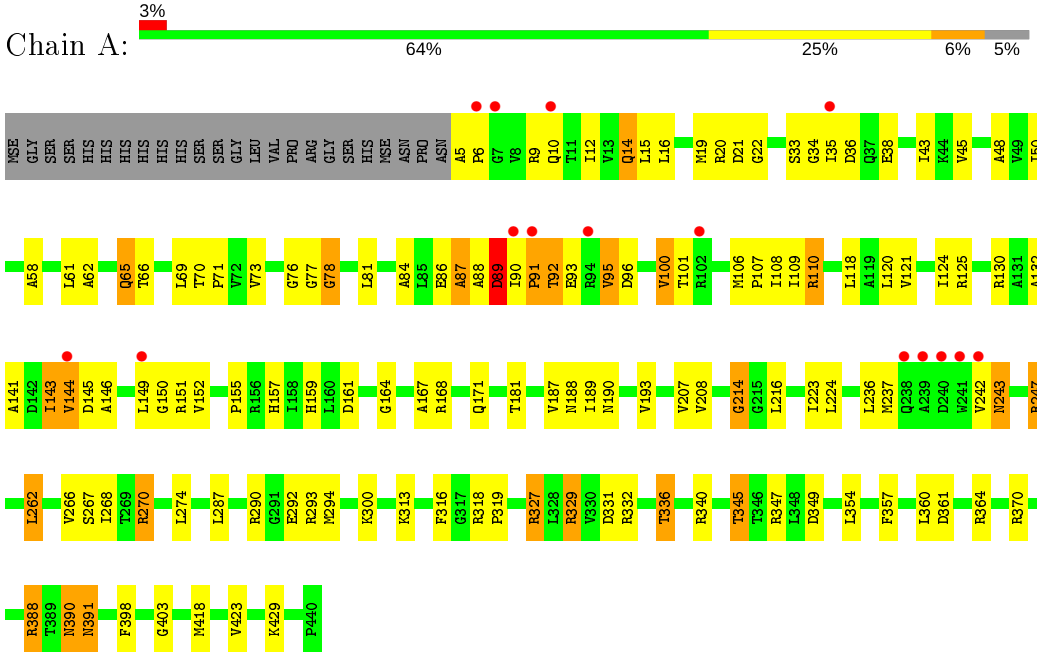
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	23	Total O 23 23	0	0
6	B	14	Total O 14 14	0	0
6	X	33	Total O 33 33	0	0
6	Y	14	Total O 14 14	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

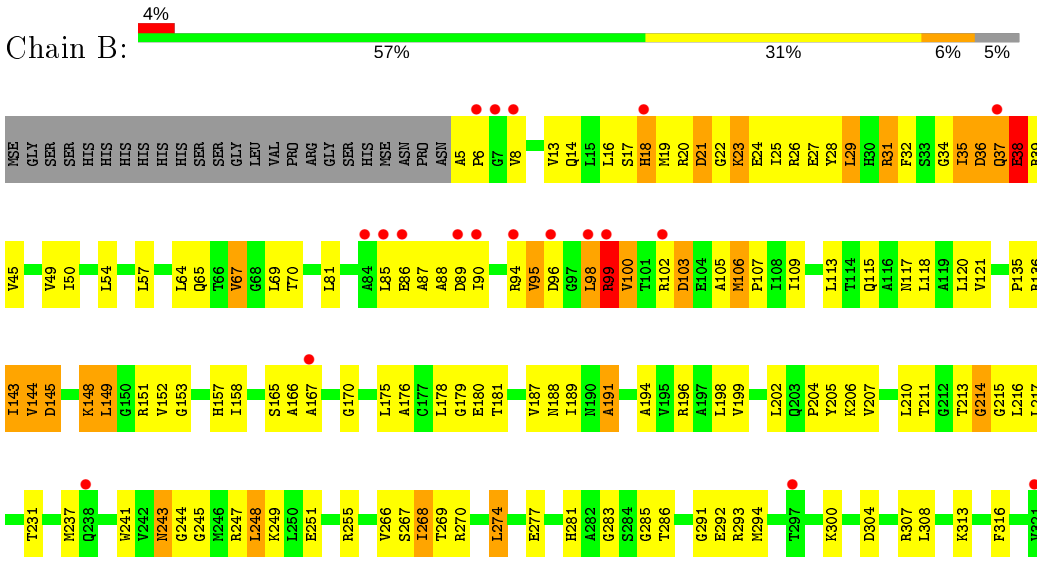
- Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase

Chain A:



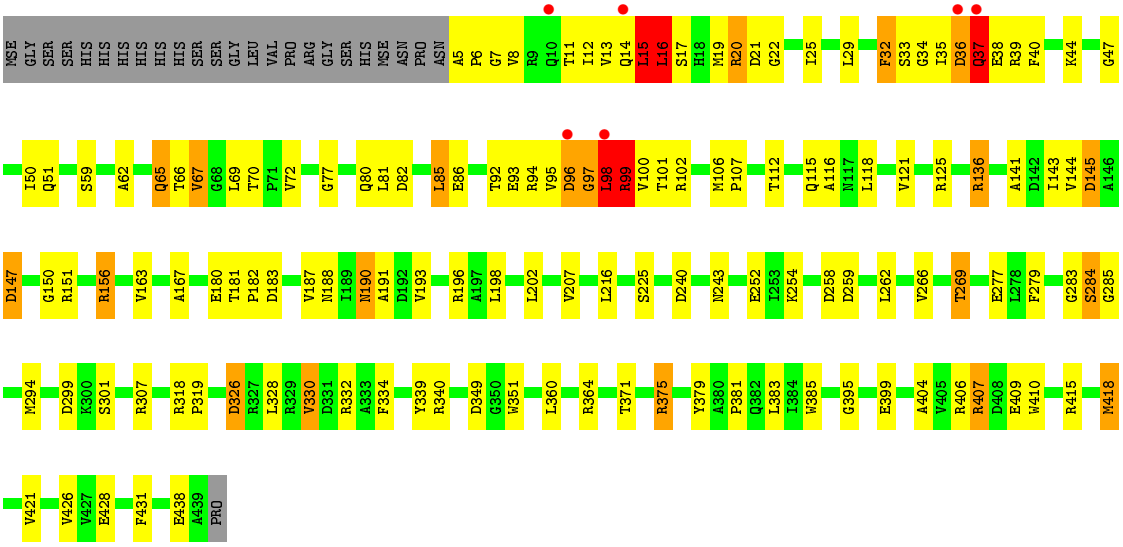
- Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase

Chain B:



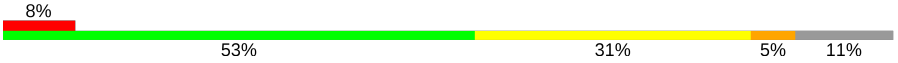
• Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase

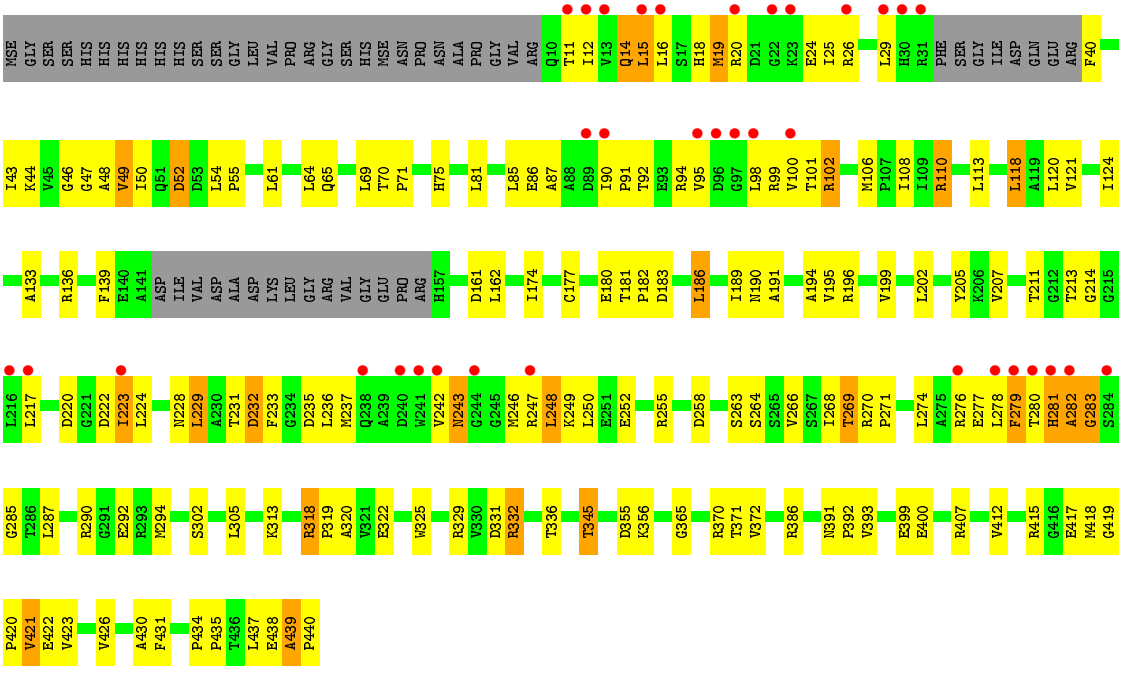
Chain X:



• Molecule 1: N-acetylglutamate kinase / N-acetylglutamate synthase

Chain Y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.43Å 117.47Å 149.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.97 – 2.67 37.97 – 2.67	Depositor EDS
% Data completeness (in resolution range)	95.4 (37.97-2.67) 95.2 (37.97-2.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.183 , 0.256 0.176 , 0.253	Depositor DCC
R_{free} test set	2006 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å^2)	59.4	Xtriage
Anisotropy	0.383	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13303	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 6.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MLI, SO4, EDO

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	0.45	0/3405	0.63	0/4615
1	B	0.36	0/3386	0.55	0/4589
1	X	0.47	0/3386	0.65	0/4589
1	Y	0.41	0/3175	0.60	0/4303
All	All	0.43	0/13352	0.61	0/18096

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

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	3349	0	3346	112	0
1	B	3334	0	3326	141	0
1	X	3334	0	3326	142	0
1	Y	3127	0	3120	143	0
2	A	7	0	2	0	0
2	Y	7	0	2	0	0
3	A	4	0	6	2	0
3	Y	4	0	6	0	0
4	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	Y	48	0	30	5	0
6	A	23	0	0	1	0
6	B	14	0	0	0	0
6	X	33	0	0	2	0
6	Y	14	0	0	1	0
All	All	13303	0	13164	522	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 20.

All (522) 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:Y:418:MSE:HG3	1:Y:423:VAL:HG13	1.39	1.04
1:Y:332:ARG:H	1:Y:345:THR:HG22	1.23	1.03
1:B:405:VAL:HG13	5:Y:441:COA:H132	1.39	1.02
1:A:327:ARG:HG2	1:A:327:ARG:HH11	1.24	1.02
1:X:36:ASP:HB2	1:X:39:ARG:HG3	1.41	1.01
1:Y:110:ARG:HH11	1:Y:110:ARG:HG2	1.26	0.98
1:X:136:ARG:HH11	1:X:136:ARG:HG2	1.35	0.91
1:B:196:ARG:HD3	1:B:255:ARG:NH1	1.87	0.90
1:X:409:GLU:HG2	1:X:410:TRP:CD1	2.07	0.89
1:X:415:ARG:HH11	1:X:415:ARG:HG3	1.37	0.88
1:Y:439:ALA:HB1	1:Y:440:PRO:HD2	1.54	0.88
1:B:38:GLU:HA	1:B:38:GLU:OE2	1.76	0.85
1:A:14:GLN:HE21	1:A:14:GLN:HA	1.41	0.85
1:A:144:VAL:HG13	1:A:145:ASP:H	1.43	0.83
1:Y:421:VAL:HG13	1:Y:422:GLU:H	1.44	0.83
1:B:269:THR:HG22	1:B:285:GLY:HA3	1.61	0.81
1:B:293:ARG:HH11	1:B:294:MSE:H	1.24	0.81
1:Y:318:ARG:HG2	1:Y:439:ALA:HB3	1.61	0.81
1:B:293:ARG:HH12	1:B:294:MSE:HG3	1.45	0.80
1:Y:101:THR:O	1:Y:102:ARG:HB2	1.81	0.80
1:X:409:GLU:HG2	1:X:410:TRP:HD1	1.46	0.79
1:A:90:ILE:N	1:A:91:PRO:HD3	1.98	0.78
1:A:327:ARG:CG	1:A:327:ARG:HH11	1.96	0.78
1:Y:258:ASP:OD1	1:Y:290:ARG:HD2	1.84	0.78
1:B:21:ASP:HB2	1:Y:19:MSE:HE2	1.66	0.78
1:X:35:ILE:HG23	1:X:40:PHE:CZ	2.19	0.77
1:A:332:ARG:H	1:A:345:THR:HG22	1.49	0.77
1:X:16:LEU:HA	1:X:19:MSE:HG2	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:319:PRO:HD2	1:X:438:GLU:HG2	1.64	0.77
1:X:32:PHE:O	1:X:32:PHE:HD1	1.67	0.77
1:X:375:ARG:HH11	1:X:375:ARG:HB2	1.49	0.77
1:X:156:ARG:HH21	1:X:182:PRO:HG3	1.47	0.77
1:Y:248:LEU:O	1:Y:252:GLU:HG3	1.84	0.76
1:X:11:THR:O	1:X:15:LEU:HB2	1.86	0.75
1:X:415:ARG:NH1	1:X:415:ARG:HG3	1.99	0.75
1:B:405:VAL:HG13	5:Y:441:COA:CDP	2.16	0.75
1:A:100:VAL:HB	1:A:149:LEU:HA	1.69	0.74
1:Y:110:ARG:HH11	1:Y:110:ARG:CG	1.98	0.74
1:X:32:PHE:HE1	1:X:40:PHE:HA	1.50	0.74
1:A:143:ILE:HD11	1:A:150:GLY:O	1.87	0.74
1:Y:12:ILE:HG13	1:Y:15:LEU:HD21	1.68	0.74
1:Y:268:ILE:HG22	1:Y:268:ILE:O	1.87	0.74
1:X:32:PHE:CE1	1:X:40:PHE:HA	2.23	0.73
1:B:293:ARG:NH1	1:B:294:MSE:HG3	2.03	0.73
1:B:106:MSE:HE1	1:B:188:ASN:HB2	1.70	0.72
1:Y:121:VAL:HG21	1:Y:133:ALA:HB2	1.71	0.72
1:A:16:LEU:O	1:A:22:GLY:HA3	1.88	0.72
1:X:407:ARG:HG3	1:X:431:PHE:CZ	2.24	0.72
1:X:93:GLU:HB2	1:X:100:VAL:HG22	1.71	0.72
1:A:136:ARG:NE	1:A:137:GLY:H	1.86	0.72
1:B:14:GLN:HA	1:B:17:SER:HB3	1.71	0.72
1:X:136:ARG:NH1	1:X:136:ARG:HG2	2.00	0.72
1:X:35:ILE:HG22	1:X:37:GLN:H	1.54	0.71
1:Y:16:LEU:HD11	1:Y:26:ARG:HB2	1.72	0.71
1:Y:86:GLU:HG3	1:Y:91:PRO:HA	1.72	0.71
1:B:248:LEU:HG	1:B:249:LYS:N	2.04	0.71
1:Y:106:MSE:HE2	1:Y:186:LEU:HD13	1.72	0.71
1:Y:318:ARG:H	1:Y:318:ARG:HD2	1.56	0.70
1:A:243:ASN:HD22	1:A:243:ASN:H	1.38	0.70
1:B:323:GLY:O	1:B:327:ARG:HG2	1.91	0.70
1:X:94:ARG:HA	1:X:99:ARG:HA	1.74	0.70
1:X:81:LEU:O	1:X:85:LEU:HB2	1.92	0.69
1:X:407:ARG:HG3	1:X:431:PHE:CE1	2.26	0.69
1:Y:223:ILE:HD12	1:Y:223:ILE:H	1.57	0.69
1:B:38:GLU:HG2	1:B:167:ALA:HB2	1.75	0.69
1:X:156:ARG:NH2	1:X:182:PRO:HG3	2.07	0.68
1:B:102:ARG:HG3	1:B:103:ASP:H	1.58	0.68
1:Y:269:THR:HG22	1:Y:285:GLY:HA3	1.75	0.68
1:X:50:ILE:HD12	1:X:116:ALA:HB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:233:PHE:CE1	1:Y:237:MSE:HE3	2.28	0.68
1:B:106:MSE:HB3	1:B:107:PRO:HD3	1.75	0.68
1:A:332:ARG:N	1:A:345:THR:HG22	2.09	0.68
1:X:294:MSE:HE2	1:X:371:THR:HG22	1.74	0.68
1:A:120:LEU:O	1:A:124:ILE:HG12	1.94	0.67
1:Y:331:ASP:HB3	1:Y:345:THR:CG2	2.23	0.67
1:B:106:MSE:HG2	1:B:151:ARG:HH21	1.59	0.67
1:Y:439:ALA:HB1	1:Y:440:PRO:CD	2.24	0.67
1:X:190:ASN:HD21	1:X:193:VAL:HG13	1.59	0.67
6:A:448:HOH:O	1:X:19:MSE:HE3	1.94	0.67
1:X:38:GLU:OE2	1:X:38:GLU:HA	1.95	0.67
1:Y:49:VAL:HA	1:Y:52:ASP:HB3	1.77	0.66
1:Y:99:ARG:O	1:Y:100:VAL:HG22	1.96	0.66
1:X:39:ARG:HD3	1:X:202:LEU:O	1.96	0.66
1:Y:118:LEU:HD13	1:Y:118:LEU:O	1.96	0.66
1:B:293:ARG:NH1	1:B:294:MSE:H	1.94	0.65
1:A:214:GLY:HA3	1:A:270:ARG:HG3	1.79	0.65
1:Y:391:ASN:OD1	1:Y:393:VAL:HG23	1.97	0.65
1:Y:305:LEU:HD13	1:Y:325:TRP:HB3	1.78	0.65
1:Y:196:ARG:NH1	1:Y:255:ARG:HH12	1.93	0.65
1:Y:332:ARG:N	1:Y:345:THR:HG22	2.05	0.65
1:Y:294:MSE:HE1	1:Y:372:VAL:HA	1.78	0.65
1:Y:417:GLU:HA	5:Y:441:COA:H143	1.80	0.64
1:B:331:ASP:HB3	1:B:345:THR:HG23	1.79	0.64
1:Y:12:ILE:HG13	1:Y:15:LEU:CD2	2.27	0.64
1:X:29:LEU:HD21	1:X:67:VAL:HG13	1.79	0.64
1:X:136:ARG:HH11	1:X:136:ARG:CG	2.08	0.64
1:A:84:ALA:O	1:A:87:ALA:HB3	1.96	0.64
1:X:40:PHE:N	6:X:468:HOH:O	2.31	0.63
1:A:65:GLN:HG2	1:A:130:ARG:H	1.62	0.63
1:B:405:VAL:CG1	5:Y:441:COA:H132	2.24	0.63
1:Y:69:LEU:O	1:Y:71:PRO:HD3	1.98	0.63
1:Y:269:THR:HG23	1:Y:277:GLU:HG2	1.81	0.63
1:X:319:PRO:HD2	1:X:438:GLU:CG	2.29	0.63
1:A:237:MSE:CE	1:A:251:GLU:HG3	2.29	0.63
1:Y:100:VAL:HG23	1:Y:100:VAL:O	1.98	0.62
1:Y:232:ASP:O	1:Y:236:LEU:HD12	1.99	0.62
1:B:37:GLN:O	1:B:38:GLU:HB2	1.98	0.62
1:B:5:ALA:HB3	1:B:6:PRO:HD3	1.82	0.62
1:B:35:ILE:HG12	1:B:39:ARG:HD3	1.81	0.62
1:X:14:GLN:HG3	6:X:473:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:379:TYR:O	1:X:381:PRO:HD3	2.00	0.62
1:A:157:HIS:CD2	1:A:159:HIS:CE1	2.88	0.61
1:B:89:ASP:HB2	1:B:102:ARG:NH2	2.15	0.61
1:X:106:MSE:HE1	1:X:188:ASN:HB2	1.81	0.61
1:X:32:PHE:O	1:X:34:GLY:N	2.29	0.61
1:A:5:ALA:HB3	1:A:6:PRO:HD3	1.82	0.61
1:B:29:LEU:HD11	1:B:67:VAL:HG22	1.82	0.61
1:A:418:MSE:HE2	1:A:423:VAL:HG22	1.82	0.61
1:A:106:MSE:HE2	1:A:151:ARG:HB3	1.83	0.61
1:A:106:MSE:O	1:A:109:ILE:HG22	2.00	0.60
1:A:54:LEU:HB3	1:A:55:PRO:HD3	1.82	0.60
1:A:58:ALA:HA	1:A:124:ILE:HD13	1.83	0.60
1:A:357:PHE:H	3:A:442:EDO:H11	1.66	0.60
1:B:332:ARG:H	1:B:345:THR:HG22	1.64	0.60
1:Y:400:GLU:O	1:Y:415:ARG:HD2	2.01	0.60
1:A:382:GLN:HE22	1:A:418:MSE:HG3	1.67	0.60
1:A:243:ASN:ND2	1:A:243:ASN:H	1.99	0.59
1:Y:98:LEU:HD22	1:Y:190:ASN:HD21	1.67	0.59
1:B:196:ARG:HD3	1:B:255:ARG:CZ	2.32	0.59
1:A:106:MSE:HB3	1:A:107:PRO:HD3	1.85	0.59
1:B:243:ASN:H	1:B:243:ASN:HD22	1.49	0.59
1:Y:95:VAL:HB	1:Y:101:THR:CG2	2.33	0.58
1:B:332:ARG:HH11	1:B:332:ARG:HG2	1.68	0.58
1:X:340:ARG:HG2	1:X:360:LEU:HD12	1.85	0.58
1:Y:95:VAL:HB	1:Y:101:THR:HG21	1.84	0.58
1:A:88:ALA:O	1:A:89:ASP:HB2	2.03	0.58
1:Y:412:VAL:HG23	1:Y:431:PHE:CE1	2.39	0.58
1:A:14:GLN:NE2	1:A:14:GLN:HA	2.16	0.58
1:A:106:MSE:HA	1:A:109:ILE:HG22	1.86	0.58
1:A:106:MSE:HE3	1:A:187:VAL:HA	1.85	0.58
1:Y:40:PHE:HB2	1:Y:70:THR:H	1.69	0.58
1:A:144:VAL:HG13	1:A:145:ASP:N	2.15	0.57
1:A:9:ARG:CZ	1:A:33:SER:HB2	2.33	0.57
1:X:95:VAL:O	1:X:97:GLY:N	2.37	0.57
1:A:382:GLN:HE22	1:A:418:MSE:CG	2.18	0.57
1:X:98:LEU:O	1:X:99:ARG:CB	2.53	0.57
1:A:43:ILE:HD12	1:A:71:PRO:HB3	1.86	0.57
1:A:390:ASN:ND2	1:A:390:ASN:H	2.02	0.57
1:X:50:ILE:CD1	1:X:116:ALA:HB1	2.35	0.57
1:X:207:VAL:HB	1:X:266:VAL:HG22	1.86	0.57
1:X:351:TRP:CZ3	1:X:418:MSE:HE3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:331:ASP:HB3	1:Y:345:THR:HG23	1.86	0.57
1:B:23:LYS:O	1:B:27:GLU:HG3	2.05	0.56
1:Y:233:PHE:CZ	1:Y:237:MSE:HE3	2.40	0.56
1:A:144:VAL:HG12	1:A:152:VAL:O	2.04	0.56
1:A:106:MSE:CE	1:A:187:VAL:HA	2.34	0.56
1:B:31:ARG:HA	1:B:31:ARG:NE	2.21	0.56
1:Y:418:MSE:HB2	1:Y:422:GLU:OE1	2.05	0.56
1:Y:418:MSE:HG3	1:Y:423:VAL:CG1	2.26	0.56
1:X:332:ARG:HG2	1:X:334:PHE:CZ	2.40	0.56
1:X:5:ALA:N	1:X:6:PRO:HD2	2.21	0.56
1:Y:269:THR:CG2	1:Y:285:GLY:HA3	2.34	0.56
1:A:106:MSE:HE2	1:A:151:ARG:CB	2.35	0.56
1:B:105:ALA:O	1:B:109:ILE:HG12	2.06	0.56
1:X:143:ILE:O	1:X:143:ILE:HG13	2.04	0.56
1:Y:12:ILE:HG22	1:Y:12:ILE:O	2.06	0.56
1:Y:294:MSE:HE2	1:Y:371:THR:HG22	1.86	0.56
1:Y:98:LEU:HD22	1:Y:190:ASN:ND2	2.20	0.56
1:A:106:MSE:CE	1:A:151:ARG:HB3	2.36	0.55
1:X:67:VAL:O	1:X:67:VAL:HG13	2.06	0.55
1:A:237:MSE:HE1	1:A:251:GLU:HG3	1.86	0.55
1:Y:14:GLN:HA	1:Y:14:GLN:HE21	1.71	0.55
1:Y:94:ARG:O	1:Y:95:VAL:HG12	2.05	0.55
1:B:354:LEU:HB2	1:B:383:LEU:HD21	1.87	0.55
1:B:38:GLU:OE2	1:B:70:THR:O	2.23	0.55
1:X:351:TRP:CD1	1:X:426:VAL:HG21	2.41	0.55
1:X:395:GLY:O	1:X:399:GLU:HG3	2.06	0.55
1:Y:270:ARG:HB2	1:Y:271:PRO:HD2	1.89	0.55
1:B:86:GLU:C	1:B:88:ALA:H	2.11	0.55
1:X:38:GLU:HG2	1:X:167:ALA:HB2	1.89	0.54
1:X:72:VAL:HG11	1:X:198:LEU:HD21	1.88	0.54
1:X:16:LEU:O	1:X:22:GLY:HA3	2.07	0.54
1:Y:196:ARG:CZ	1:Y:255:ARG:HH12	2.20	0.54
1:Y:46:GLY:O	1:Y:49:VAL:HG13	2.07	0.54
1:A:132:ALA:HB2	1:A:171:GLN:OE1	2.07	0.54
1:A:76:GLY:O	1:A:78:GLY:N	2.41	0.54
1:B:13:VAL:HG13	1:B:26:ARG:HD2	1.90	0.54
1:X:326:ASP:N	1:X:326:ASP:OD1	2.41	0.54
1:X:44:LYS:HE3	1:X:191:ALA:HB1	1.88	0.54
1:Y:110:ARG:HG2	1:Y:110:ARG:NH1	2.05	0.54
1:X:156:ARG:CZ	1:X:156:ARG:HB3	2.38	0.54
1:B:102:ARG:O	1:B:103:ASP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:ASP:HA	1:A:364[B]:ARG:NH1	2.23	0.53
1:Y:110:ARG:NH1	1:Y:110:ARG:CG	2.68	0.53
1:A:144:VAL:HG22	1:A:145:ASP:N	2.23	0.53
1:X:7:GLY:O	1:X:11:THR:HG23	2.08	0.53
1:A:331:ASP:HB3	1:A:345:THR:HG23	1.90	0.53
1:X:72:VAL:CG1	1:X:198:LEU:HD21	2.37	0.53
1:B:293:ARG:NH1	1:B:294:MSE:O	2.41	0.53
1:B:32:PHE:HB3	1:B:69:LEU:HD21	1.89	0.53
1:Y:25:ILE:O	1:Y:29:LEU:HB2	2.08	0.53
1:Y:418:MSE:CG	1:Y:423:VAL:HG13	2.25	0.53
1:A:157:HIS:HD2	1:A:159:HIS:CE1	2.26	0.53
1:A:382:GLN:NE2	1:A:418:MSE:HG3	2.24	0.53
1:B:24:GLU:OE1	1:B:281:HIS:CD2	2.62	0.53
1:B:64:LEU:O	1:B:67:VAL:HG12	2.09	0.53
1:X:38:GLU:CG	1:X:167:ALA:HB2	2.38	0.53
1:Y:211:THR:O	1:Y:270:ARG:HB3	2.08	0.53
1:Y:331:ASP:HB3	1:Y:345:THR:HG22	1.89	0.53
1:A:294:MSE:HE1	1:A:375:ARG:HG2	1.91	0.52
1:B:293:ARG:HH11	1:B:294:MSE:N	2.01	0.52
1:B:304:ASP:HB3	1:B:307:ARG:HB2	1.90	0.52
1:B:39:ARG:HG2	1:B:202:LEU:O	2.08	0.52
1:Y:50:ILE:HD11	1:Y:75:HIS:HB2	1.91	0.52
1:B:331:ASP:HB3	1:B:345:THR:O	2.09	0.52
1:X:294:MSE:HE2	1:X:371:THR:CG2	2.40	0.52
1:B:338:SER:O	1:B:339:TYR:HB2	2.09	0.52
1:A:21:ASP:OD2	1:X:20:ARG:NH1	2.43	0.52
1:B:213:THR:HG23	1:B:213:THR:O	2.09	0.52
1:X:51:GLN:HB2	1:X:80:GLN:NE2	2.25	0.52
1:A:354:LEU:HD13	1:A:376:MSE:HE2	1.92	0.52
1:B:148:LYS:HD2	1:B:149:LEU:HD23	1.92	0.52
1:Y:313:LYS:HD3	1:Y:319:PRO:HB3	1.91	0.52
1:A:327:ARG:CG	1:A:327:ARG:NH1	2.63	0.52
1:X:143:ILE:HD11	1:X:151:ARG:HA	1.91	0.52
1:B:384:ILE:O	1:B:385:TRP:HB3	2.10	0.52
1:X:95:VAL:HG12	1:X:96:ASP:N	2.26	0.52
1:X:99:ARG:HD3	1:X:101:THR:HG22	1.91	0.51
1:Y:292:GLU:HG3	1:Y:336:THR:OG1	2.10	0.51
1:X:47:GLY:O	1:X:50:ILE:HG12	2.10	0.51
1:Y:189:ILE:HD12	1:Y:194:ALA:HB2	1.93	0.51
1:X:29:LEU:CD2	1:X:67:VAL:HG13	2.41	0.51
1:Y:246:MSE:HA	1:Y:249:LYS:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LEU:HD22	1:B:22:GLY:HA2	1.92	0.51
1:B:244:GLY:HA2	1:B:247:ARG:HD2	1.92	0.51
1:B:332:ARG:HG2	1:B:332:ARG:NH1	2.26	0.51
1:Y:54:LEU:N	1:Y:55:PRO:HD2	2.25	0.51
1:A:136:ARG:CD	1:A:137:GLY:H	2.23	0.51
1:B:106:MSE:CE	1:B:109:ILE:HG13	2.41	0.51
1:B:269:THR:CG2	1:B:285:GLY:HA3	2.34	0.51
1:X:16:LEU:HA	1:X:19:MSE:CG	2.36	0.51
1:A:161:ASP:HB3	1:B:118:LEU:CD1	2.41	0.51
1:Y:421:VAL:HG13	1:Y:422:GLU:N	2.21	0.51
1:B:106:MSE:HE3	1:B:106:MSE:HA	1.92	0.51
1:Y:243:ASN:H	1:Y:243:ASN:HD22	1.59	0.51
1:B:294:MSE:HE1	1:B:334:PHE:HB3	1.93	0.51
1:A:121:VAL:O	1:A:125:ARG:HG3	2.11	0.50
1:B:106:MSE:HB3	1:B:107:PRO:CD	2.41	0.50
1:B:213:THR:O	1:B:215:GLY:N	2.37	0.50
1:B:332:ARG:N	1:B:345:THR:HG22	2.26	0.50
1:Y:85:LEU:HD13	1:Y:92:THR:CG2	2.42	0.50
1:B:20:ARG:C	1:B:22:GLY:H	2.15	0.50
1:X:38:GLU:OE2	1:X:70:THR:HB	2.10	0.50
1:B:207:VAL:O	1:B:266:VAL:HA	2.12	0.50
1:X:93:GLU:HB2	1:X:100:VAL:CG2	2.41	0.50
1:Y:47:GLY:C	1:Y:49:VAL:H	2.14	0.50
1:A:143:ILE:HD13	1:A:144:VAL:N	2.27	0.50
1:B:32:PHE:HE2	1:B:205:TYR:HE2	1.60	0.50
1:A:141:ALA:O	1:A:181:THR:HA	2.11	0.50
1:Y:277:GLU:OE1	1:Y:283:GLY:HA3	2.12	0.50
1:Y:419:GLY:O	1:Y:423:VAL:HG22	2.11	0.50
1:B:354:LEU:HB3	1:B:385:TRP:HB3	1.93	0.50
1:Y:16:LEU:CD1	1:Y:26:ARG:HB2	2.41	0.50
1:Y:268:ILE:O	1:Y:268:ILE:CG2	2.56	0.49
1:Y:90:ILE:N	1:Y:91:PRO:HD3	2.27	0.49
1:A:313:LYS:O	1:A:316:PHE:O	2.29	0.49
1:X:35:ILE:HG23	1:X:40:PHE:CE2	2.48	0.49
1:Y:44:LYS:HD2	1:Y:195:VAL:HG21	1.94	0.49
1:Y:24:GLU:CD	1:Y:365:GLY:HA2	2.32	0.49
1:A:190:ASN:O	1:A:193:VAL:HG22	2.11	0.49
1:Y:64:LEU:HD11	1:Y:278:LEU:CD1	2.43	0.49
1:A:62:ALA:O	1:A:66:THR:HG23	2.12	0.49
1:A:331:ASP:HB3	1:A:345:THR:CG2	2.43	0.49
1:A:34:GLY:O	1:A:36:ASP:OD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LEU:O	1:A:71:PRO:HD3	2.13	0.49
1:A:242:VAL:HG12	1:A:247:ARG:HG3	1.94	0.49
1:A:398:PHE:CE1	1:X:406:ARG:HD3	2.48	0.49
1:B:81:LEU:O	1:B:85:LEU:HB2	2.12	0.49
1:X:107:PRO:HG3	1:Y:182:PRO:O	2.12	0.49
1:Y:12:ILE:HG23	1:Y:15:LEU:HD21	1.94	0.49
1:B:245:GLY:O	1:B:248:LEU:HD23	2.12	0.49
1:B:294:MSE:HB3	1:B:336:THR:HA	1.95	0.49
1:X:38:GLU:HG3	1:X:163:VAL:HG12	1.94	0.49
1:Y:320:ALA:HA	1:Y:437:LEU:HD23	1.95	0.49
1:Y:224:LEU:HD23	1:Y:224:LEU:C	2.34	0.49
1:A:43:ILE:HG12	1:A:208:VAL:HB	1.94	0.48
1:B:102:ARG:HG3	1:B:103:ASP:N	2.27	0.48
1:X:15:LEU:O	1:X:17:SER:N	2.46	0.48
1:A:125:ARG:NH1	1:B:165:SER:O	2.40	0.48
1:B:17:SER:O	1:B:18:HIS:HB2	2.13	0.48
1:B:36:ASP:O	1:B:38:GLU:N	2.46	0.48
1:B:214:GLY:H	1:B:270:ARG:NH2	2.11	0.48
1:X:16:LEU:HD12	1:X:17:SER:N	2.28	0.48
1:A:95:VAL:HG23	1:A:100:VAL:HG11	1.96	0.48
1:B:16:LEU:HD22	1:B:22:GLY:CA	2.43	0.48
1:Y:64:LEU:HD11	1:Y:278:LEU:HD12	1.96	0.48
1:A:262:LEU:HD13	1:A:290:ARG:NH2	2.28	0.48
1:B:18:HIS:O	1:B:19:MSE:SE	2.82	0.48
1:B:362:ASP:O	1:B:366:GLU:HG2	2.13	0.48
1:X:62:ALA:O	1:X:66:THR:HG23	2.13	0.48
1:X:415:ARG:NH1	1:X:415:ARG:CG	2.70	0.48
1:A:292:GLU:OE1	1:A:336:THR:HG23	2.13	0.48
1:B:50:ILE:HG22	1:B:57:LEU:CD2	2.44	0.48
1:B:36:ASP:C	1:B:38:GLU:H	2.16	0.47
1:X:36:ASP:O	1:X:37:GLN:HB3	2.14	0.47
1:Y:207:VAL:HB	1:Y:266:VAL:HG22	1.96	0.47
1:B:179:GLY:C	1:B:187:VAL:HG12	2.35	0.47
1:Y:277:GLU:O	1:Y:277:GLU:HG3	2.12	0.47
1:B:20:ARG:HD3	1:Y:20:ARG:HD2	1.95	0.47
1:B:35:ILE:O	1:B:35:ILE:HG23	2.14	0.47
1:X:65:GLN:HA	1:X:69:LEU:O	2.15	0.47
1:B:217:LEU:HA	1:B:222:ASP:O	2.14	0.47
1:X:141:ALA:O	1:X:181:THR:HA	2.15	0.47
1:A:190:ASN:OD1	1:A:193:VAL:HG13	2.14	0.47
1:X:82:ASP:O	1:X:86:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:O	1:B:99:ARG:C	2.53	0.47
1:Y:214:GLY:H	1:Y:270:ARG:HD3	1.80	0.47
1:Y:399:GLU:OE2	1:Y:399:GLU:HA	2.14	0.47
1:B:407:ARG:HD3	1:B:431:PHE:CZ	2.48	0.47
1:A:340:ARG:HG2	1:A:360:LEU:HD12	1.97	0.47
1:X:32:PHE:CD1	1:X:32:PHE:O	2.56	0.47
1:Y:15:LEU:C	1:Y:15:LEU:HD12	2.35	0.47
1:A:109:ILE:HG23	1:A:110:ARG:N	2.30	0.47
1:Y:231:THR:O	1:Y:232:ASP:HB3	2.15	0.47
1:B:32:PHE:HE2	1:B:205:TYR:CE2	2.33	0.47
1:X:101:THR:HG21	1:X:188:ASN:ND2	2.30	0.47
1:Y:252:GLU:HG2	1:Y:255:ARG:NH2	2.30	0.47
1:B:113:LEU:HD12	1:B:178:LEU:HG	1.97	0.46
1:B:148:LYS:CD	1:B:149:LEU:HD23	2.45	0.46
1:B:44:LYS:NZ	1:B:191:ALA:HB1	2.31	0.46
1:B:45:VAL:HG23	1:B:45:VAL:O	2.14	0.46
1:A:101:THR:HG21	1:A:188:ASN:HD22	1.79	0.46
1:X:39:ARG:CD	1:X:202:LEU:O	2.62	0.46
1:X:29:LEU:HD21	1:X:67:VAL:CG1	2.45	0.46
1:B:144:VAL:HG13	1:B:152:VAL:O	2.16	0.46
1:X:15:LEU:HD12	1:X:16:LEU:N	2.31	0.46
1:Y:228:ASN:O	1:Y:229:LEU:C	2.54	0.46
1:Y:25:ILE:HD11	1:Y:279:PHE:HB2	1.97	0.46
1:X:259:ASP:CG	1:X:259:ASP:O	2.54	0.46
1:A:187:VAL:HG22	1:A:188:ASN:N	2.31	0.46
1:B:40:PHE:CE2	1:B:69:LEU:HB3	2.50	0.46
1:X:98:LEU:O	1:X:99:ARG:HB2	2.16	0.46
1:Y:14:GLN:O	1:Y:14:GLN:HG3	2.15	0.46
1:Y:229:LEU:O	1:Y:233:PHE:N	2.49	0.46
1:B:228:ASN:OD1	1:B:291:GLY:HA3	2.14	0.46
1:X:183:ASP:C	1:X:183:ASP:OD2	2.54	0.46
1:Y:332:ARG:HA	1:Y:332:ARG:HD3	1.71	0.46
1:A:390:ASN:H	1:A:390:ASN:HD22	1.62	0.46
1:A:90:ILE:N	1:A:91:PRO:CD	2.75	0.46
1:Y:217:LEU:HA	1:Y:222:ASP:O	2.15	0.46
1:X:12:ILE:O	1:X:16:LEU:HG	2.16	0.46
1:X:307:ARG:HG2	1:X:339:TYR:CD1	2.51	0.46
1:A:403:GLY:HA2	1:X:404:ALA:O	2.16	0.46
1:B:187:VAL:HG22	1:B:188:ASN:N	2.30	0.45
1:X:144:VAL:O	1:X:145:ASP:HB3	2.16	0.45
1:X:190:ASN:ND2	1:X:193:VAL:HG22	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:21:ASP:O	1:X:25:ILE:HG13	2.15	0.45
1:B:18:HIS:CE1	1:Y:276:ARG:HE	2.34	0.45
1:Y:90:ILE:HG22	1:Y:90:ILE:O	2.15	0.45
1:X:38:GLU:HG3	1:X:163:VAL:CG1	2.45	0.45
1:Y:400:GLU:O	1:Y:415:ARG:CD	2.64	0.45
1:A:390:ASN:ND2	1:A:390:ASN:N	2.63	0.45
1:X:38:GLU:HG2	1:X:167:ALA:CB	2.47	0.45
1:X:328:LEU:HG	1:X:330:VAL:HG23	1.97	0.45
1:A:143:ILE:HD13	1:A:143:ILE:C	2.36	0.45
1:B:308:LEU:HD13	1:B:344:ILE:HD11	1.99	0.45
1:X:121:VAL:O	1:X:125:ARG:HG3	2.17	0.45
1:X:269:THR:HG23	1:X:285:GLY:HA3	1.98	0.45
1:B:94:ARG:NH1	1:B:148:LYS:HA	2.31	0.45
1:B:139:PHE:HB3	1:B:189:ILE:CD1	2.47	0.45
1:B:157:HIS:O	1:B:158:ILE:HD12	2.17	0.45
1:B:143:ILE:HD13	1:B:181:THR:HG21	1.98	0.45
1:X:77:GLY:O	1:X:81:LEU:HG	2.16	0.45
1:Y:61:LEU:O	1:Y:65:GLN:HG3	2.17	0.45
1:A:155:PRO:HG3	1:A:189:ILE:HD12	1.99	0.45
1:B:293:ARG:NH2	1:B:375:ARG:HH22	2.15	0.45
1:A:357:PHE:N	3:A:442:EDO:H11	2.31	0.44
1:B:144:VAL:O	1:B:145:ASP:C	2.55	0.44
1:B:24:GLU:O	1:B:28:TYR:HD2	2.00	0.44
1:B:37:GLN:O	1:B:38:GLU:CB	2.63	0.44
1:X:80:GLN:HB3	1:X:112:THR:CG2	2.47	0.44
1:Y:407:ARG:NH1	1:Y:431:PHE:CD2	2.85	0.44
1:A:136:ARG:CZ	1:A:137:GLY:H	2.29	0.44
1:A:136:ARG:HG3	1:B:136:ARG:HD2	1.99	0.44
1:B:277:GLU:HA	1:B:283:GLY:HA2	2.00	0.44
1:B:354:LEU:HB3	1:B:385:TRP:CB	2.48	0.44
1:X:35:ILE:HG23	1:X:40:PHE:HZ	1.79	0.44
1:X:151:ARG:NH2	1:Y:183:ASP:HB2	2.33	0.44
1:Y:195:VAL:O	1:Y:199:VAL:HG23	2.17	0.44
1:Y:270:ARG:HB2	1:Y:271:PRO:CD	2.47	0.44
1:A:12:ILE:O	1:A:16:LEU:HG	2.17	0.44
1:X:35:ILE:HG22	1:X:37:GLN:N	2.26	0.44
1:B:403:GLY:HA3	1:B:414:TRP:CZ2	2.53	0.44
1:X:85:LEU:CD2	1:X:92:THR:HG22	2.48	0.44
1:Y:276:ARG:HA	1:Y:280:THR:HG22	1.99	0.44
1:B:21:ASP:O	1:B:25:ILE:HG13	2.18	0.44
1:B:31:ARG:HA	1:B:31:ARG:HE	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:441:COA:HN4	5:Y:441:COA:H71	1.58	0.44
1:Y:44:LYS:HE3	1:Y:191:ALA:HB1	2.00	0.44
1:X:299:ASP:OD2	1:X:301:SER:OG	2.36	0.43
1:A:61:LEU:HB2	1:A:124:ILE:HD12	1.99	0.43
1:A:237:MSE:HE2	1:A:251:GLU:HG3	1.99	0.43
1:Y:282:ALA:O	1:Y:283:GLY:C	2.56	0.43
1:X:51:GLN:HB2	1:X:80:GLN:HE22	1.83	0.43
1:Y:237:MSE:HE1	1:Y:247:ARG:O	2.18	0.43
1:A:331:ASP:OD2	1:A:345:THR:CG2	2.67	0.43
1:B:148:LYS:CE	1:B:149:LEU:HD23	2.49	0.43
1:B:237:MSE:HE2	1:B:251:GLU:HG2	2.00	0.43
1:Y:181:THR:HB	1:Y:182:PRO:HD2	2.00	0.43
1:Y:318:ARG:HB2	1:Y:319:PRO:HD2	2.00	0.43
1:A:329:ARG:HD3	1:A:329:ARG:HA	1.84	0.43
1:B:95:VAL:O	1:B:96:ASP:C	2.57	0.43
1:Y:19:MSE:HA	1:Y:19:MSE:HE3	2.00	0.43
1:Y:356:LYS:HE2	1:Y:356:LYS:HB2	1.72	0.43
1:B:95:VAL:CG2	1:B:149:LEU:HD11	2.49	0.43
1:X:12:ILE:O	1:X:15:LEU:HB3	2.18	0.43
1:A:48:ALA:O	1:A:51:GLN:N	2.50	0.43
1:B:95:VAL:CG2	1:B:98:LEU:HB2	2.49	0.43
1:X:25:ILE:HG12	1:X:279:PHE:HB3	2.00	0.43
1:X:277:GLU:HB2	1:X:284:SER:O	2.19	0.43
1:Y:434:PRO:HA	1:Y:435:PRO:HD3	1.92	0.43
1:X:100:VAL:HB	1:X:102:ARG:NH1	2.34	0.43
1:X:12:ILE:HD12	1:X:66:THR:O	2.19	0.43
1:X:277:GLU:HA	1:X:283:GLY:HA2	2.01	0.43
1:X:38:GLU:CD	1:X:167:ALA:HB2	2.39	0.43
1:Y:318:ARG:HD2	1:Y:318:ARG:N	2.31	0.43
1:B:41:ALA:HA	1:B:206:LYS:O	2.19	0.42
1:Y:423:VAL:HA	1:Y:426:VAL:HG12	2.00	0.42
1:A:14:GLN:CA	1:A:14:GLN:HE21	2.22	0.42
1:B:199:VAL:HG13	1:B:204:PRO:HD2	2.01	0.42
1:X:13:VAL:C	1:X:15:LEU:H	2.21	0.42
1:X:118:LEU:HD21	1:Y:162:LEU:HD23	2.01	0.42
1:A:207:VAL:HB	1:A:266:VAL:HG22	2.00	0.42
1:Y:16:LEU:C	1:Y:18:HIS:H	2.23	0.42
1:X:106:MSE:HE3	1:X:151:ARG:HB3	2.02	0.42
1:A:164:GLY:O	1:A:168:ARG:HB2	2.20	0.42
1:A:54:LEU:N	1:A:55:PRO:CD	2.81	0.42
1:Y:205:TYR:O	1:Y:264:SER:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:HB3	1:A:167:ALA:HB2	2.02	0.42
1:A:89:ASP:C	1:A:91:PRO:HD3	2.38	0.42
1:X:181:THR:HB	1:X:182:PRO:HD2	2.01	0.42
1:X:254:LYS:HD3	1:X:258:ASP:OD2	2.18	0.42
1:X:307:ARG:HG2	1:X:339:TYR:CG	2.54	0.42
1:B:117:ASN:O	1:B:121:VAL:HG23	2.20	0.42
1:Y:124:ILE:CD1	1:Y:174:ILE:HD11	2.49	0.42
1:Y:281:HIS:O	1:Y:282:ALA:HB2	2.19	0.42
1:A:136:ARG:NE	1:A:137:GLY:N	2.61	0.42
1:A:382:GLN:NE2	1:A:418:MSE:CG	2.80	0.42
1:Y:391:ASN:HA	1:Y:392:PRO:HD3	1.81	0.42
1:A:361:ASP:OD1	1:A:364[B]:ARG:NH1	2.53	0.42
1:B:383:LEU:C	1:B:384:ILE:HD12	2.40	0.42
1:B:191:ALA:O	1:B:194:ALA:HB3	2.20	0.42
1:B:32:PHE:C	1:B:34:GLY:H	2.23	0.42
1:X:428:GLU:HA	1:X:428:GLU:OE2	2.20	0.42
1:Y:106:MSE:HE3	1:Y:106:MSE:HA	2.01	0.42
1:Y:162:LEU:HG	6:Y:444:HOH:O	2.20	0.42
1:A:388:ARG:O	1:A:391:ASN:HB2	2.19	0.41
1:B:21:ASP:HB2	1:Y:19:MSE:CE	2.45	0.41
1:X:147:ASP:N	1:X:147:ASP:OD2	2.38	0.41
1:X:196:ARG:HH11	1:X:196:ARG:HG3	1.85	0.41
1:Y:113:LEU:HD23	1:Y:113:LEU:HA	1.85	0.41
1:Y:121:VAL:HG21	1:Y:133:ALA:CB	2.43	0.41
1:B:274:LEU:O	1:B:274:LEU:HD22	2.20	0.41
1:X:36:ASP:CB	1:X:39:ARG:HG3	2.29	0.41
1:X:95:VAL:HG12	1:X:96:ASP:H	1.85	0.41
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.79	0.41
1:X:332:ARG:HG2	1:X:334:PHE:CE2	2.55	0.41
1:Y:419:GLY:HA2	1:Y:420:PRO:HD3	1.96	0.41
1:B:196:ARG:HD3	1:B:255:ARG:HH12	1.74	0.41
1:X:101:THR:HG21	1:X:188:ASN:HD22	1.86	0.41
1:X:37:GLN:O	1:X:40:PHE:CE2	2.73	0.41
1:Y:139:PHE:CE1	1:Y:194:ALA:HB1	2.55	0.41
1:Y:294:MSE:CE	1:Y:371:THR:HG22	2.50	0.41
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.84	0.41
1:B:352:VAL:HG11	1:B:380:ALA:HB2	2.02	0.41
1:B:49:VAL:HG12	1:B:49:VAL:O	2.21	0.41
1:X:283:GLY:O	1:X:284:SER:HB2	2.21	0.41
1:X:383:LEU:HD23	1:X:385:TRP:CZ3	2.56	0.41
1:Y:191:ALA:O	1:Y:195:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:386:ARG:NH1	1:Y:430:ALA:O	2.52	0.41
1:B:142:ASP:O	1:B:153:GLY:HA2	2.21	0.41
1:B:23:LYS:HG3	1:B:24:GLU:N	2.34	0.41
1:A:19:MSE:HG3	1:X:19:MSE:HE2	2.03	0.41
1:A:58:ALA:HA	1:A:124:ILE:CD1	2.50	0.41
1:A:70:THR:HA	1:A:71:PRO:HD3	1.85	0.41
1:B:166:ALA:O	1:B:170:GLY:N	2.53	0.41
1:X:5:ALA:N	1:X:6:PRO:CD	2.83	0.41
1:Y:43:ILE:HD12	1:Y:43:ILE:N	2.36	0.41
1:A:349:ASP:OD2	1:A:429:LYS:HE3	2.21	0.41
1:B:135:PRO:HA	1:B:176:ALA:HB3	2.03	0.41
1:B:148:LYS:HG3	1:B:149:LEU:N	2.35	0.41
1:A:145:ASP:O	1:A:146:ALA:C	2.59	0.41
1:B:313:LYS:O	1:B:316:PHE:O	2.39	0.41
1:B:340:ARG:NH2	1:B:366:GLU:OE1	2.50	0.41
1:X:95:VAL:CG1	1:X:96:ASP:N	2.84	0.41
1:A:88:ALA:O	1:A:89:ASP:CB	2.69	0.41
1:B:149:LEU:HD22	1:B:149:LEU:HA	1.77	0.41
1:B:268:ILE:HG23	1:B:286:THR:HB	2.03	0.41
1:X:13:VAL:C	1:X:15:LEU:N	2.75	0.41
1:X:143:ILE:HD11	1:X:150:GLY:O	2.21	0.41
1:B:24:GLU:O	1:B:28:TYR:CD2	2.74	0.40
1:B:300:LYS:O	1:B:300:LYS:HG2	2.21	0.40
1:X:151:ARG:HH22	1:Y:183:ASP:HB2	1.86	0.40
1:Y:81:LEU:HD22	1:Y:81:LEU:O	2.21	0.40
1:A:19:MSE:HE2	1:X:19:MSE:HG3	2.03	0.40
1:Y:243:ASN:H	1:Y:243:ASN:ND2	2.19	0.40
1:B:94:ARG:HD2	1:B:148:LYS:O	2.22	0.40
1:B:175:LEU:HD22	1:B:198:LEU:HD21	2.02	0.40
1:B:45:VAL:HG12	1:B:210:LEU:HD12	2.02	0.40
1:X:409:GLU:CG	1:X:410:TRP:CD1	2.91	0.40
1:Y:242:VAL:O	1:Y:242:VAL:HG12	2.21	0.40
1:A:313:LYS:HD2	1:A:319:PRO:HG3	2.04	0.40
1:A:61:LEU:HD13	1:A:73:VAL:HG21	2.03	0.40
1:B:292:GLU:HG2	1:B:368:LEU:HD21	2.03	0.40
1:X:36:ASP:O	1:X:37:GLN:CB	2.70	0.40
1:Y:108:ILE:N	1:Y:108:ILE:HD12	2.36	0.40
1:Y:85:LEU:HD13	1:Y:92:THR:HG21	2.03	0.40
1:A:86:GLU:HA	1:A:91:PRO:HG3	2.04	0.40
1:B:106:MSE:HE3	1:B:109:ILE:HG13	2.02	0.40
1:X:44:LYS:CE	1:X:191:ALA:HB1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:118:LEU:HD12	1:Y:161:ASP:HB3	2.04	0.40
1:Y:318:ARG:CG	1:Y:439:ALA:HB3	2.43	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	435/460 (95%)	394 (91%)	29 (7%)	12 (3%)	5 6
1	B	433/460 (94%)	378 (87%)	39 (9%)	16 (4%)	3 4
1	X	433/460 (94%)	394 (91%)	26 (6%)	13 (3%)	4 5
1	Y	402/460 (87%)	352 (88%)	39 (10%)	11 (3%)	5 6
All	All	1703/1840 (93%)	1518 (89%)	133 (8%)	52 (3%)	4 5

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	77	GLY
1	A	95	VAL
1	A	96	ASP
1	A	144	VAL
1	B	38	GLU
1	B	103	ASP
1	B	438	GLU
1	X	33	SER
1	X	36	ASP
1	X	96	ASP
1	X	99	ARG
1	X	145	ASP
1	Y	87	ALA

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Mol	Chain	Res	Type
1	Y	229	LEU
1	Y	232	ASP
1	Y	269	THR
1	A	78	GLY
1	A	89	ASP
1	A	91	PRO
1	A	214	GLY
1	B	18	HIS
1	B	35	ILE
1	B	37	GLN
1	B	98	LEU
1	B	99	ARG
1	B	100	VAL
1	B	145	ASP
1	B	191	ALA
1	X	16	LEU
1	X	37	GLN
1	Y	282	ALA
1	Y	283	GLY
1	A	87	ALA
1	A	92	THR
1	B	214	GLY
1	Y	19	MSE
1	Y	48	ALA
1	Y	102	ARG
1	B	21	ASP
1	B	87	ALA
1	X	15	LEU
1	X	98	LEU
1	X	284	SER
1	Y	52	ASP
1	Y	439	ALA
1	A	93	GLU
1	A	110	ARG
1	B	241	TRP
1	X	330	VAL
1	B	8	VAL
1	X	8	VAL
1	X	97	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	346/357 (97%)	303 (88%)	43 (12%)	4 6
1	B	344/357 (96%)	309 (90%)	35 (10%)	7 10
1	X	344/357 (96%)	311 (90%)	33 (10%)	8 12
1	Y	323/357 (90%)	289 (90%)	34 (10%)	7 10
All	All	1357/1428 (95%)	1212 (89%)	145 (11%)	6 9

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	14	GLN
1	A	15	LEU
1	A	20	ARG
1	A	35	ILE
1	A	45	VAL
1	A	50	ILE
1	A	54	LEU
1	A	65	GLN
1	A	81	LEU
1	A	89	ASP
1	A	92	THR
1	A	100	VAL
1	A	108	ILE
1	A	118	LEU
1	A	136	ARG
1	A	143	ILE
1	A	216	LEU
1	A	223	ILE
1	A	236	LEU
1	A	243	ASN
1	A	247	ARG
1	A	248	LEU
1	A	249	LYS

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Mol	Chain	Res	Type
1	A	262	LEU
1	A	267	SER
1	A	268	ILE
1	A	270	ARG
1	A	274	LEU
1	A	287	LEU
1	A	293	ARG
1	A	300	LYS
1	A	318	ARG
1	A	327	ARG
1	A	329	ARG
1	A	336	THR
1	A	345	THR
1	A	347	ARG
1	A	370	ARG
1	A	375	ARG
1	A	388	ARG
1	A	390	ASN
1	A	391	ASN
1	B	23	LYS
1	B	29	LEU
1	B	31	ARG
1	B	36	ASP
1	B	38	GLU
1	B	54	LEU
1	B	65	GLN
1	B	67	VAL
1	B	90	ILE
1	B	95	VAL
1	B	99	ARG
1	B	100	VAL
1	B	106	MSE
1	B	115	GLN
1	B	120	LEU
1	B	143	ILE
1	B	144	VAL
1	B	148	LYS
1	B	149	LEU
1	B	180	GLU
1	B	211	THR
1	B	216	LEU
1	B	231	THR

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Mol	Chain	Res	Type
1	B	243	ASN
1	B	248	LEU
1	B	267	SER
1	B	268	ILE
1	B	274	LEU
1	B	332	ARG
1	B	336	THR
1	B	345	THR
1	B	378	ASP
1	B	382	GLN
1	B	406	ARG
1	B	407	ARG
1	X	15	LEU
1	X	16	LEU
1	X	20	ARG
1	X	32	PHE
1	X	37	GLN
1	X	59	SER
1	X	65	GLN
1	X	67	VAL
1	X	85	LEU
1	X	98	LEU
1	X	99	ARG
1	X	115	GLN
1	X	136	ARG
1	X	147	ASP
1	X	156	ARG
1	X	180	GLU
1	X	187	VAL
1	X	190	ASN
1	X	216	LEU
1	X	225	SER
1	X	240	ASP
1	X	243	ASN
1	X	252	GLU
1	X	262	LEU
1	X	269	THR
1	X	318	ARG
1	X	326	ASP
1	X	349	ASP
1	X	364	ARG
1	X	375	ARG

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Mol	Chain	Res	Type
1	X	407	ARG
1	X	418	MSE
1	X	421	VAL
1	Y	11	THR
1	Y	14	GLN
1	Y	15	LEU
1	Y	49	VAL
1	Y	110	ARG
1	Y	118	LEU
1	Y	120	LEU
1	Y	136	ARG
1	Y	177	CYS
1	Y	180	GLU
1	Y	186	LEU
1	Y	202	LEU
1	Y	213	THR
1	Y	220	ASP
1	Y	223	ILE
1	Y	235	ASP
1	Y	243	ASN
1	Y	248	LEU
1	Y	250	LEU
1	Y	263	SER
1	Y	274	LEU
1	Y	279	PHE
1	Y	281	HIS
1	Y	287	LEU
1	Y	302	SER
1	Y	318	ARG
1	Y	322	GLU
1	Y	329	ARG
1	Y	332	ARG
1	Y	345	THR
1	Y	355	ASP
1	Y	370	ARG
1	Y	421	VAL
1	Y	438	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN

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Mol	Chain	Res	Type
1	A	51	GLN
1	A	65	GLN
1	A	115	GLN
1	A	157	HIS
1	A	159	HIS
1	A	188	ASN
1	A	203	GLN
1	A	243	ASN
1	A	382	GLN
1	A	390	ASN
1	B	18	HIS
1	B	51	GLN
1	B	188	ASN
1	B	190	ASN
1	B	243	ASN
1	X	14	GLN
1	X	188	ASN
1	X	190	ASN
1	Y	14	GLN
1	Y	18	HIS
1	Y	243	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	EDO	A	442	-	3,3,3	0.49	0	2,2,2	0.37	0
2	MLI	A	441	-	0,6,6	0.00	-	0,7,7	0.00	-
3	EDO	Y	443	-	3,3,3	0.46	0	2,2,2	0.36	0
5	COA	Y	441	-	41,50,50	2.71	11 (26%)	52,75,75	1.80	10 (19%)
4	SO4	X	441	-	4,4,4	0.16	0	6,6,6	0.17	0
2	MLI	Y	442	-	0,6,6	0.00	-	0,7,7	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	Y	443	-	-	1/1/1/1	-
2	MLI	Y	442	-	-	0/0/4/4	-
5	COA	Y	441	-	-	22/44/64/64	0/3/3/3
2	MLI	A	441	-	-	0/0/4/4	-
3	EDO	A	442	-	-	1/1/1/1	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	441	COA	C2A-N3A	9.30	1.47	1.32
5	Y	441	COA	C9P-N8P	7.32	1.49	1.33
5	Y	441	COA	C5P-N4P	6.20	1.47	1.33
5	Y	441	COA	C2A-N1A	4.20	1.41	1.33
5	Y	441	COA	O4B-C1B	4.06	1.46	1.41
5	Y	441	COA	C6A-N6A	3.47	1.46	1.34
5	Y	441	COA	C4A-N3A	3.31	1.40	1.35
5	Y	441	COA	C8A-N7A	3.27	1.40	1.34
5	Y	441	COA	C2B-C1B	3.24	1.58	1.53
5	Y	441	COA	C5A-N7A	2.62	1.49	1.39
5	Y	441	COA	P1A-O1A	2.12	1.58	1.50

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	Y	441	COA	N3A-C2A-N1A	-5.82	119.59	128.68
5	Y	441	COA	O6A-CCP-CBP	5.38	119.20	110.55
5	Y	441	COA	O2B-C2B-C3B	4.01	122.55	111.17
5	Y	441	COA	O4B-C4B-C5B	3.27	120.12	109.37
5	Y	441	COA	O3B-C3B-C2B	3.14	123.06	111.68
5	Y	441	COA	P2A-O3A-P1A	-2.84	123.09	132.83
5	Y	441	COA	O5B-C5B-C4B	2.46	117.47	108.99
5	Y	441	COA	C6P-C7P-N8P	2.39	116.72	111.90
5	Y	441	COA	C2P-C3P-N4P	2.34	117.65	112.31
5	Y	441	COA	O2B-C2B-C1B	2.32	119.41	110.85

There are no chirality outliers.

All (24) torsion outliers are listed below:

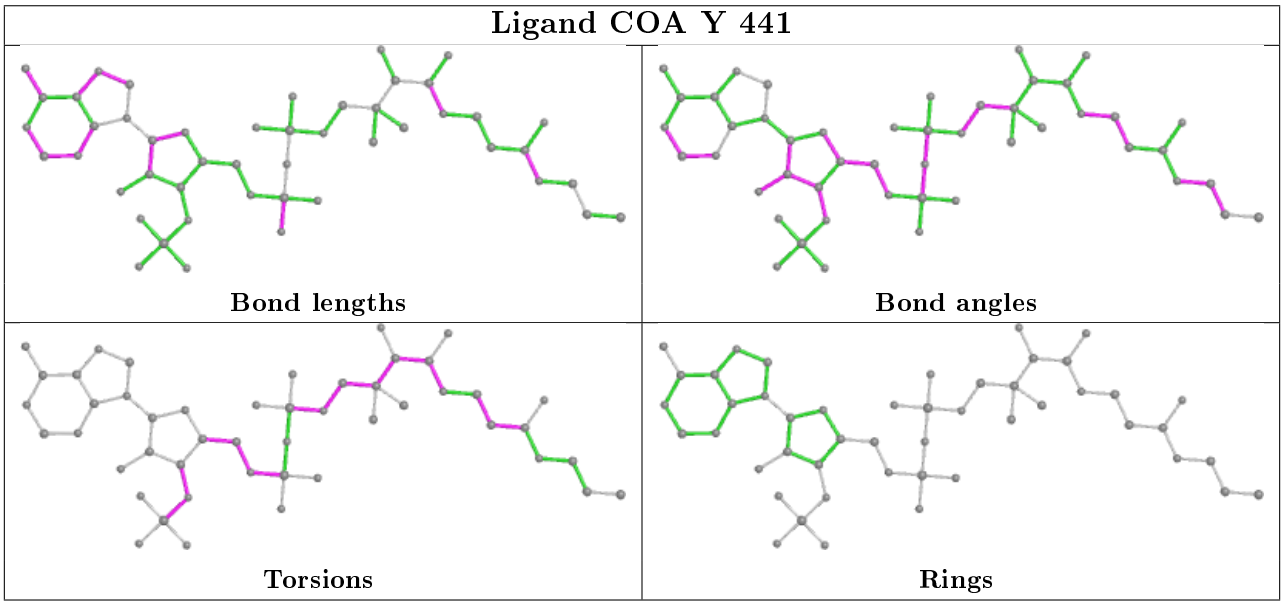
Mol	Chain	Res	Type	Atoms
5	Y	441	COA	C2B-C3B-O3B-P3B
5	Y	441	COA	C3B-O3B-P3B-O9A
5	Y	441	COA	C5B-O5B-P1A-O1A
5	Y	441	COA	CAP-CBP-CCP-O6A
5	Y	441	COA	O9P-C9P-CAP-CBP
5	Y	441	COA	CAP-C9P-N8P-C7P
5	Y	441	COA	C5P-C6P-C7P-N8P
5	Y	441	COA	O9P-C9P-N8P-C7P
5	Y	441	COA	C4B-C5B-O5B-P1A
5	Y	441	COA	N4P-C5P-C6P-C7P
5	Y	441	COA	C4B-C3B-O3B-P3B
3	A	442	EDO	O1-C1-C2-O2
5	Y	441	COA	CEP-CBP-CCP-O6A
5	Y	441	COA	C9P-CAP-CBP-CDP
5	Y	441	COA	C5B-O5B-P1A-O3A
5	Y	441	COA	CBP-CCP-O6A-P2A
5	Y	441	COA	C5B-O5B-P1A-O2A
5	Y	441	COA	CDP-CBP-CCP-O6A
5	Y	441	COA	O5P-C5P-C6P-C7P
5	Y	441	COA	C3B-C4B-C5B-O5B
5	Y	441	COA	C9P-CAP-CBP-CEP
5	Y	441	COA	CCP-O6A-P2A-O4A
3	Y	443	EDO	O1-C1-C2-O2
5	Y	441	COA	C9P-CAP-CBP-CCP

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	442	EDO	2	0
5	Y	441	COA	5	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.



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, 95^{th} 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	429/460 (93%)	-0.09	15 (3%) 44 40	36, 64, 125, 185	0
1	B	428/460 (93%)	0.11	19 (4%) 34 31	48, 88, 165, 210	0
1	X	428/460 (93%)	-0.14	6 (1%) 75 73	39, 64, 108, 185	0
1	Y	401/460 (87%)	0.22	35 (8%) 10 8	41, 76, 174, 250	0
All	All	1686/1840 (91%)	0.02	75 (4%) 34 31	36, 74, 149, 250	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	281	HIS	9.3
1	B	96	ASP	9.2
1	Y	97	GLY	8.3
1	B	7	GLY	8.2
1	Y	23	LYS	6.2
1	Y	96	ASP	6.2
1	Y	20	ARG	6.1
1	B	8	VAL	5.5
1	A	242	VAL	5.4
1	Y	98	LEU	5.4
1	B	94	ARG	5.3
1	Y	242	VAL	5.1
1	A	239	ALA	5.1
1	Y	279	PHE	4.9
1	A	10	GLN	4.9
1	B	321	VAL	4.8
1	A	7	GLY	4.7
1	A	94	ARG	4.7
1	Y	22	GLY	4.5
1	A	6	PRO	4.4
1	Y	11	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	Y	100	VAL	4.3
1	Y	278	LEU	4.2
1	X	14	GLN	4.2
1	X	36	ASP	4.2
1	B	84	ALA	4.1
1	Y	95	VAL	4.1
1	Y	217	LEU	3.9
1	X	96	ASP	3.9
1	A	240	ASP	3.7
1	Y	12	ILE	3.7
1	Y	30	HIS	3.7
1	B	90	ILE	3.7
1	B	98	LEU	3.7
1	B	37	GLN	3.7
1	B	85	LEU	3.6
1	X	10	GLN	3.6
1	Y	282	ALA	3.6
1	A	91	PRO	3.5
1	X	37	GLN	3.5
1	Y	13	VAL	3.3
1	B	238	GLN	3.2
1	B	89	ASP	3.1
1	B	102	ARG	3.1
1	Y	238	GLN	3.0
1	B	297	THR	3.0
1	Y	247	ARG	3.0
1	B	6	PRO	2.9
1	Y	284	SER	2.9
1	Y	240	ASP	2.9
1	A	238	GLN	2.9
1	Y	31	ARG	2.8
1	B	99	ARG	2.7
1	Y	280	THR	2.7
1	Y	90	ILE	2.6
1	Y	15	LEU	2.5
1	A	90	ILE	2.5
1	Y	223	ILE	2.5
1	B	18	HIS	2.3
1	Y	244	GLY	2.3
1	A	241	TRP	2.3
1	B	86	GLU	2.2
1	Y	241	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	35	ILE	2.2
1	A	102	ARG	2.2
1	Y	216	LEU	2.2
1	Y	16	LEU	2.1
1	Y	89	ASP	2.1
1	Y	276	ARG	2.1
1	A	149	LEU	2.1
1	X	98	LEU	2.1
1	Y	26	ARG	2.0
1	Y	29	LEU	2.0
1	B	167	ALA	2.0
1	A	144	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

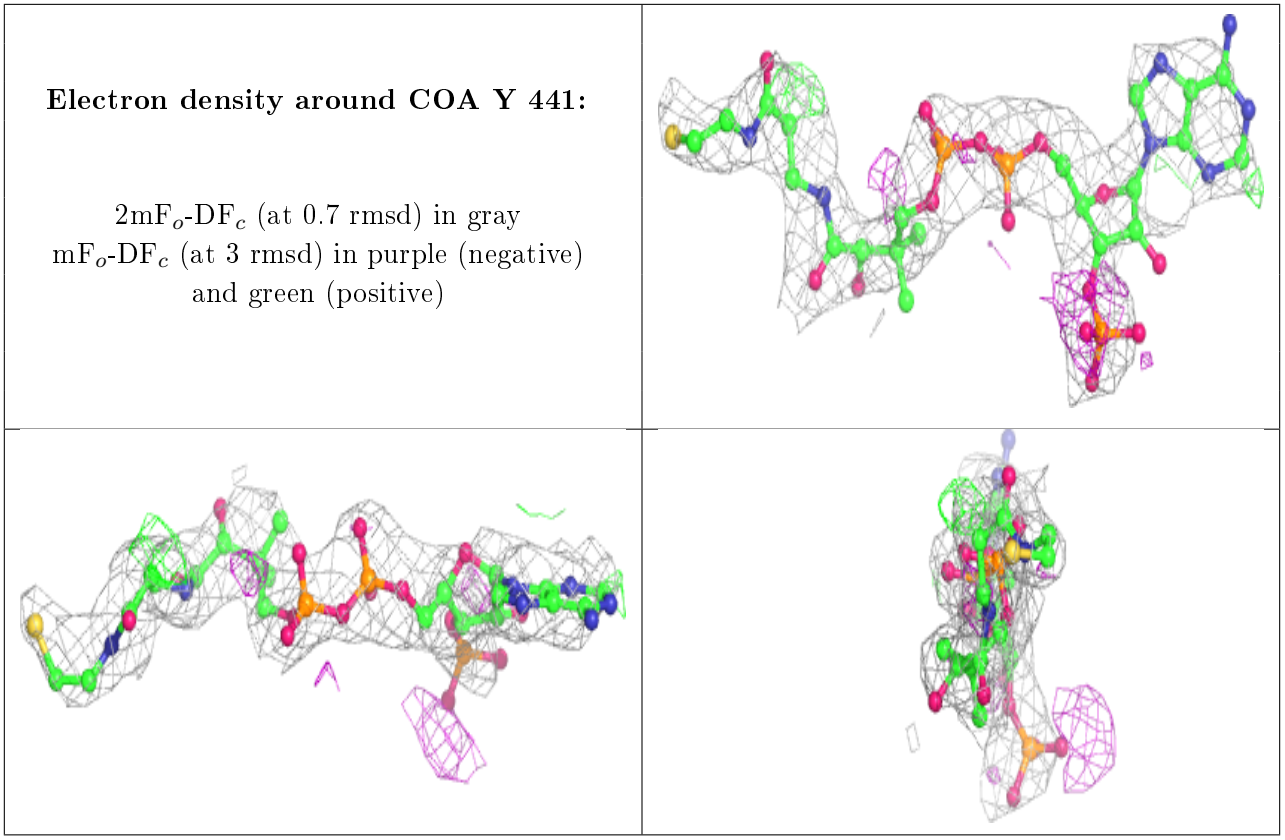
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	SO4	X	441	5/5	0.77	0.27	140,141,150,152	0
2	MLI	A	441	7/7	0.84	0.18	61,78,96,102	0
5	COA	Y	441	48/48	0.86	0.27	62,119,217,293	0
2	MLI	Y	442	7/7	0.87	0.27	86,91,107,110	0
3	EDO	Y	443	4/4	0.93	0.18	86,90,91,95	0
3	EDO	A	442	4/4	0.93	0.17	60,69,77,79	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 COA Y 441:

$2mF_o$-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

There are no such residues in this entry.