



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:49 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

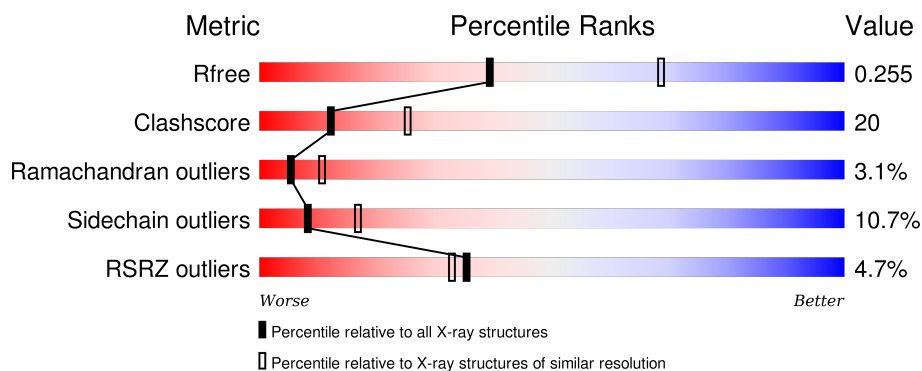
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	460	<div> <div>3%</div> <div>64% 25% 6% 5%</div> </div>
1	B	460	<div> <div>4%</div> <div>57% 31% 6% 5%</div> </div>
1	X	460	<div> <div>%</div> <div>64% 25% • • 5%</div> </div>
1	Y	460	<div> <div>8%</div> <div>53% 31% 5% 11%</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLI	Y	442	-	-	-	X
3	EDO	Y	443	-	-	-	X
4	SO4	X	441	-	-	-	X
5	COA	Y	441	-	-	-	X

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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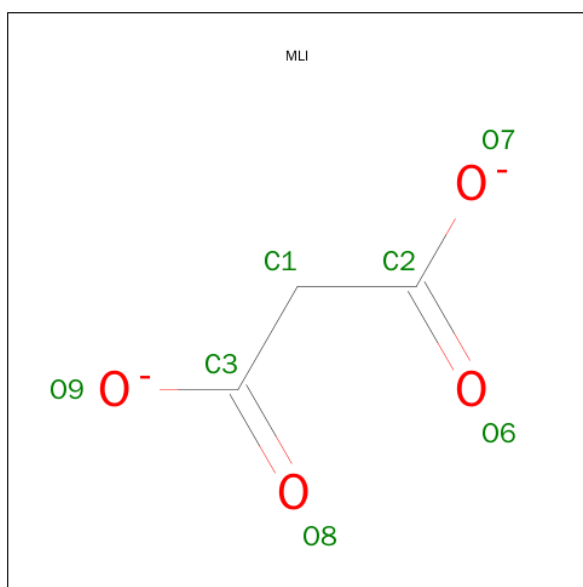
Chain	Residue	Modelled	Actual	Comment	Reference
A	294	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
A	376	MSE	LEU	ENGINEERED MUTATION	UNP Q0ASS9
B	-19	MSE	-	EXPRESSION TAG	UNP Q0ASS9
B	-18	GLY	-	EXPRESSION TAG	UNP Q0ASS9
B	-17	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	-16	SER	-	EXPRESSION TAG	UNP Q0ASS9
B	-15	HIS	-	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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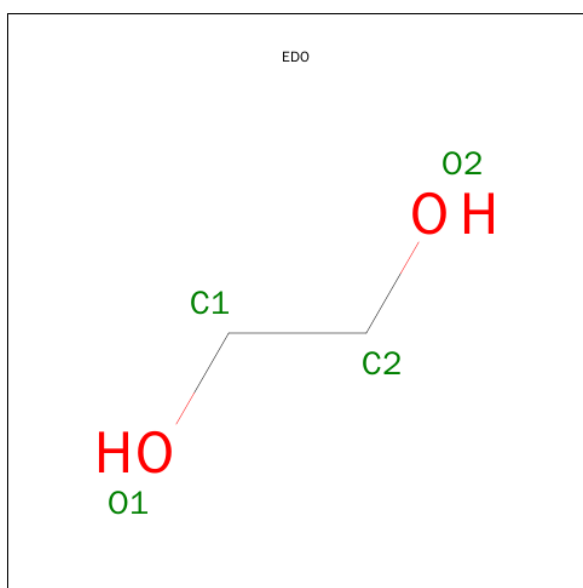
Chain	Residue	Modelled	Actual	Comment	Reference
X	-2	GLY	-	EXPRESSION TAG	UNP Q0ASS9
X	-1	SER	-	EXPRESSION TAG	UNP Q0ASS9
X	0	HIS	-	EXPRESSION TAG	UNP Q0ASS9
X	106	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
X	294	MSE	ILE	ENGINEERED MUTATION	UNP Q0ASS9
X	376	MSE	LEU	ENGINEERED MUTATION	UNP Q0ASS9
Y	-19	MSE	-	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: C₃H₂O₄).



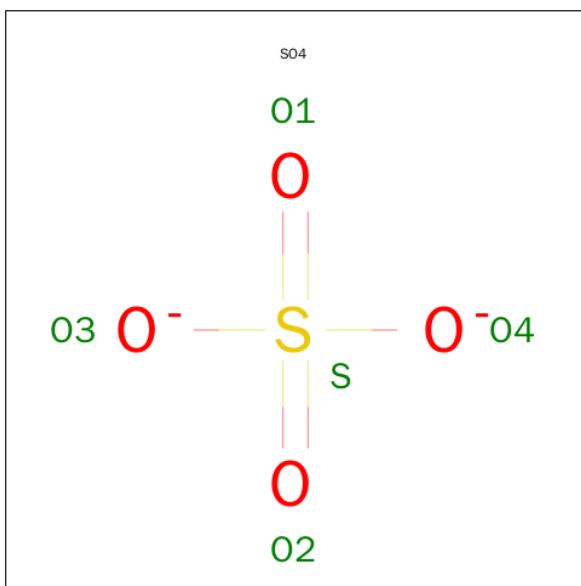
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	Y	1	Total	C	O	0	0
			7	3	4		

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



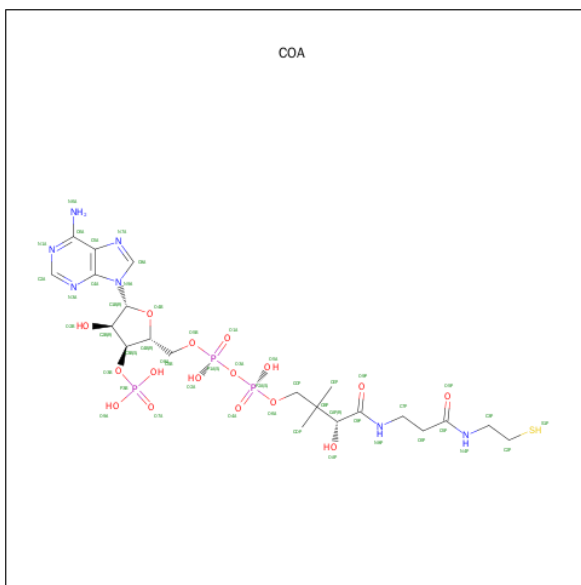
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	Y	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).

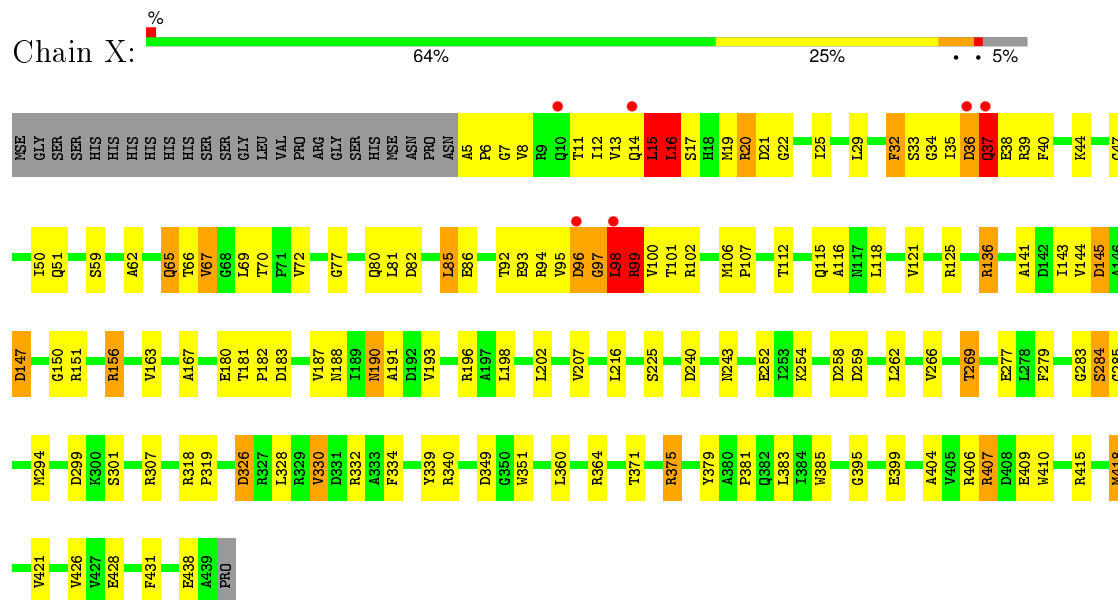


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	Y	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

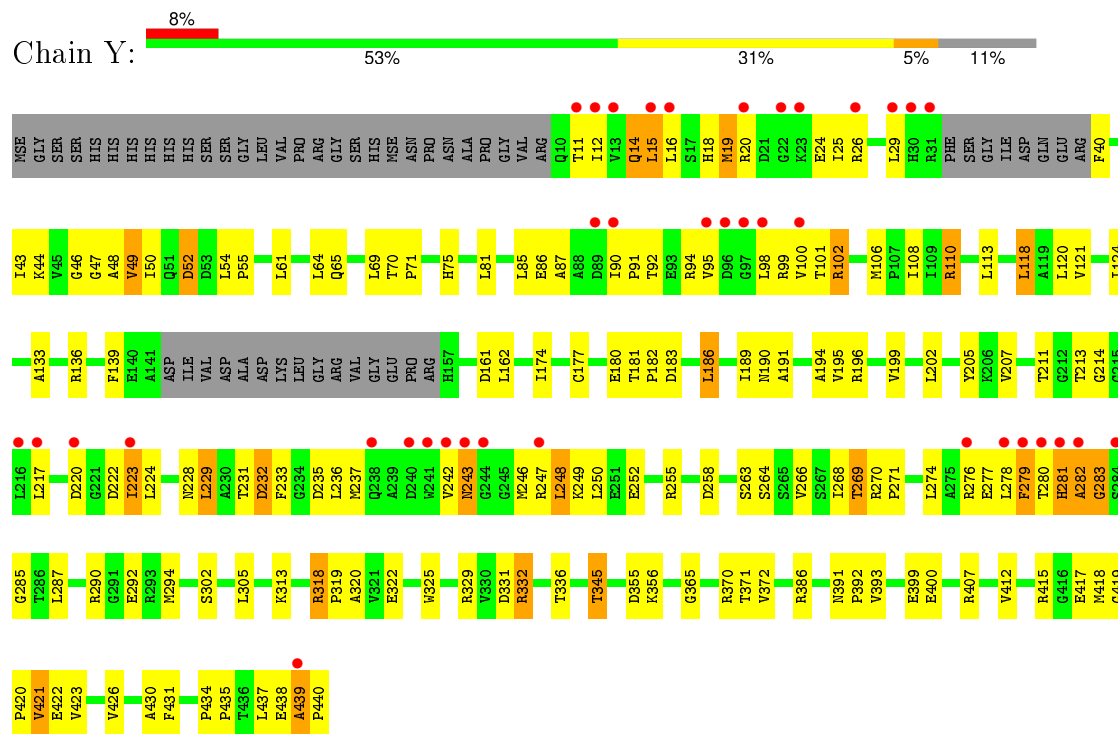
- Molecule 6 is water.

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

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



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



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.183 , 0.256 0.187 , 0.255	Depositor DCC
R_{free} test set	2006 reflections (3.77%)	DCC
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 , 62.6	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57148 reflections	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 [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	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:X:32:PHE:O	1:X:32:PHE:HD1	1.67	0.77
1:X:319:PRO:HD2	1:X:438:GLU:HG2	1.64	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:16:LEU:HA	1:X:19:MSE:HG2	1.65	0.77
1:A:332:ARG:H	1:A:345:THR:HG22	1.49	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:415:ARG:NH1	1:X:415:ARG:HG3	1.99	0.75
1:X:11:THR:O	1:X:15:LEU:HB2	1.86	0.75
1:B:405:VAL:HG13	5:Y:441:COA:CDP	2.16	0.75
1:Y:110:ARG:HH11	1:Y:110:ARG:CG	1.98	0.74
1:A:100:VAL:HB	1:A:149:LEU:HA	1.69	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:Y:121:VAL:HG21	1:Y:133:ALA:HB2	1.71	0.72
1:B:106:MSE:HE1	1:B:188:ASN:HB2	1.70	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:H	1:Y:223:ILE:HD12	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:Y:269:THR:HG22	1:Y:285:GLY:HA3	1.75	0.68
1:B:102:ARG:HG3	1:B:103:ASP:H	1.58	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:Y:331:ASP:HB3	1:Y:345:THR:CG2	2.23	0.67
1:A:120:LEU:O	1:A:124:ILE:HG12	1.94	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
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:X:190:ASN:HD21	1:X:193:VAL:HG13	1.59	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:332:ARG:N	1:Y:345:THR:HG22	2.05	0.65
1:Y:196:ARG:NH1	1:Y:255:ARG:HH12	1.93	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:Y:12:ILE:HG13	1:Y:15:LEU:CD2	2.27	0.64
1:B:331:ASP:HB3	1:B:345:THR:HG23	1.79	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:X:32:PHE:O	1:X:34:GLY:N	2.29	0.61
1:X:106:MSE:HE1	1:X:188:ASN:HB2	1.81	0.61
1:B:89:ASP:HB2	1:B:102:ARG:NH2	2.15	0.61
1:B:29:LEU:HD11	1:B:67:VAL:HG22	1.82	0.61
1:A:5:ALA:HB3	1:A:6:PRO:HD3	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:58:ALA:HA	1:A:124:ILE:HD13	1.83	0.60
1:A:54:LEU:HB3	1:A:55:PRO:HD3	1.82	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:357:PHE:H	3:A:442:EDO:H11	1.66	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:HD22	1:B:243:ASN:H	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:HE3	1:A:187:VAL:HA	1.85	0.58
1:A:106:MSE:HA	1:A:109:ILE:HG22	1.86	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:X:50:ILE:CD1	1:X:116:ALA:HB1	2.35	0.57
1:A:390:ASN:ND2	1:A:390:ASN:H	2.02	0.57
1:Y:331:ASP:HB3	1:Y:345:THR:HG23	1.86	0.57
1:X:207:VAL:HB	1:X:266:VAL:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:351:TRP:CZ3	1:X:418:MSE:HE3	2.40	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:Y:418:MSE:HG3	1:Y:423:VAL:CG1	2.26	0.56
1:Y:418:MSE:HB2	1:Y:422:GLU:OE1	2.05	0.56
1:B:31:ARG:HA	1:B:31:ARG:NE	2.21	0.56
1:X:332:ARG:HG2	1:X:334:PHE:CZ	2.40	0.56
1:Y:269:THR:CG2	1:Y:285:GLY:HA3	2.34	0.56
1:X:5:ALA:N	1:X:6:PRO:HD2	2.21	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:A:106:MSE:HE2	1:A:151:ARG:CB	2.35	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:X:67:VAL:O	1:X:67:VAL:HG13	2.06	0.55
1:A:106:MSE:CE	1:A:151:ARG:HB3	2.36	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: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:B:354:LEU:HB2	1:B:383:LEU:HD21	1.87	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:Y:110:ARG:HG2	1:Y:110:ARG:NH1	2.05	0.54
1:B:13:VAL:HG13	1:B:26:ARG:HD2	1.90	0.54
1:A:76:GLY:O	1:A:78:GLY:N	2.41	0.54
1:X:326:ASP:N	1:X:326:ASP:OD1	2.41	0.54
1:A:132:ALA:HB2	1:A:171:GLN:OE1	2.07	0.54
1:X:44:LYS:HE3	1:X:191:ALA:HB1	1.88	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:Y:110:ARG:NH1	1:Y:110:ARG:CG	2.68	0.53
1:A:361:ASP:HA	1:A:364[B]:ARG:NH1	2.23	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:Y:418:MSE:CG	1:Y:423:VAL:HG13	2.25	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:A:157:HIS:HD2	1:A:159:HIS:CE1	2.26	0.53
1:X:38:GLU:CG	1:X:167:ALA:HB2	2.38	0.53
1:B:64:LEU:O	1:B:67:VAL:HG12	2.09	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:Y:331:ASP:HB3	1:Y:345:THR:HG22	1.89	0.53
1:Y:211:THR:O	1:Y:270:ARG:HB3	2.08	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: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:304:ASP:HB3	1:B:307:ARG:HB2	1.90	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:A:21:ASP:OD2	1:X:20:ARG:NH1	2.43	0.52
1:B:338:SER:O	1:B:339:TYR:HB2	2.09	0.52
1:X:51:GLN:HB2	1:X:80:GLN:NE2	2.25	0.52
1:B:213:THR:O	1:B:213:THR:HG23	2.09	0.52
1:Y:313:LYS:HD3	1:Y:319:PRO:HB3	1.91	0.52
1:B:148:LYS:HD2	1:B:149:LEU:HD23	1.92	0.52
1:A:354:LEU:HD13	1:A:376:MSE:HE2	1.92	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:X:95:VAL:HG12	1:X:96:ASP:N	2.26	0.52
1:B:384:ILE:O	1:B:385:TRP:HB3	2.10	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:332:ARG:HG2	1:B:332:ARG:NH1	2.26	0.51
1:B:16:LEU:HD22	1:B:22:GLY:HA2	1.92	0.51
1:Y:54:LEU:N	1:Y:55:PRO:HD2	2.25	0.51
1:B:244:GLY:HA2	1:B:247:ARG:HD2	1.92	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:B:106:MSE:CE	1:B:109:ILE:HG13	2.41	0.51
1:A:136:ARG:CD	1:A:137:GLY:H	2.23	0.51
1:Y:421:VAL:HG13	1:Y:422:GLU:N	2.21	0.51
1:A:161:ASP:HB3	1:B:118:LEU:CD1	2.41	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:B:106:MSE:HB3	1:B:107:PRO:CD	2.41	0.50
1:A:121:VAL:O	1:A:125:ARG:HG3	2.11	0.50
1:B:332:ARG:N	1:B:345:THR:HG22	2.26	0.50
1:B:213:THR:O	1:B:215:GLY:N	2.37	0.50
1:Y:85:LEU:HD13	1:Y:92:THR:CG2	2.42	0.50
1:X:38:GLU:OE2	1:X:70:THR:HB	2.10	0.50
1:B:20:ARG:C	1:B:22:GLY:H	2.15	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:B:207:VAL:O	1:B:266:VAL:HA	2.12	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:Y:419:GLY:O	1:Y:423:VAL:HG22	2.11	0.50
1:Y:277:GLU:OE1	1:Y:283:GLY:HA3	2.12	0.50
1:A:141:ALA:O	1:A:181:THR:HA	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: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:A:313:LYS:O	1:A:316:PHE:O	2.29	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:69:LEU:O	1:A:71:PRO:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLY:O	1:A:36:ASP:OD1	2.31	0.49
1:Y:12:ILE:HG23	1:Y:15:LEU:HD21	1.94	0.49
1:X:107:PRO:HG3	1:Y:182:PRO:O	2.12	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:A:242:VAL:HG12	1:A:247:ARG:HG3	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:X:15:LEU:O	1:X:17:SER:N	2.46	0.48
1:B:102:ARG:HG3	1:B:103:ASP:N	2.27	0.48
1:A:43:ILE:HG12	1:A:208:VAL:HB	1.94	0.48
1:B:36:ASP:O	1:B:38:GLU:N	2.46	0.48
1:B:17:SER:O	1:B:18:HIS:HB2	2.13	0.48
1:A:125:ARG:NH1	1:B:165:SER:O	2.40	0.48
1:X:16:LEU:HD12	1:X:17:SER:N	2.28	0.48
1:B:214:GLY:H	1:B:270:ARG:NH2	2.11	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:X:62:ALA:O	1:X:66:THR:HG23	2.13	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:A:262:LEU:HD13	1:A:290:ARG:NH2	2.28	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:X:36:ASP:O	1:X:37:GLN:HB3	2.14	0.47
1:B:36:ASP:C	1:B:38:GLU:H	2.16	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:HG3	1:Y:277:GLU:O	2.12	0.47
1:B:35:ILE:HG23	1:B:35:ILE:O	2.14	0.47
1:B:20:ARG:HD3	1:Y:20:ARG:HD2	1.95	0.47
1:X:65:GLN:HA	1:X:69:LEU:O	2.15	0.47
1:X:141:ALA:O	1:X:181:THR:HA	2.15	0.47
1:B:217:LEU:HA	1:B:222:ASP:O	2.14	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:Y:214:GLY:H	1:Y:270:ARG:HD3	1.80	0.47
1:B:98:LEU:O	1:B:99:ARG:C	2.53	0.47
1:Y:399:GLU:HA	1:Y:399:GLU:OE2	2.14	0.47
1:B:407:ARG:HD3	1:B:431:PHE:CZ	2.48	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:340:ARG:HG2	1:A:360:LEU:HD12	1.97	0.47
1:Y:231:THR:O	1:Y:232:ASP:HB3	2.15	0.47
1:A:109:ILE:HG23	1:A:110:ARG:N	2.30	0.47
1:Y:252:GLU:HG2	1:Y:255:ARG:NH2	2.30	0.47
1:X:101:THR:HG21	1:X:188:ASN:ND2	2.30	0.47
1:B:32:PHE:HE2	1:B:205:TYR:CE2	2.33	0.47
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:113:LEU:HD12	1:B:178:LEU:HG	1.97	0.46
1:B:45:VAL:HG23	1:B:45:VAL:O	2.14	0.46
1:X:39:ARG:CD	1:X:202:LEU:O	2.62	0.46
1:A:101:THR:HG21	1:A:188:ASN:HD22	1.79	0.46
1:X:29:LEU:HD21	1:X:67:VAL:CG1	2.45	0.46
1:X:15:LEU:HD12	1:X:16:LEU:N	2.31	0.46
1:B:144:VAL:HG13	1:B:152:VAL:O	2.16	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:O	1:X:259:ASP:CG	2.54	0.46
1:X:98:LEU:O	1:X:99:ARG:HB2	2.16	0.46
1:Y:229:LEU:O	1:Y:233:PHE:N	2.49	0.46
1:A:187:VAL:HG22	1:A:188:ASN:N	2.31	0.46
1:Y:14:GLN:O	1:Y:14:GLN:HG3	2.15	0.46
1:B:40:PHE:CE2	1:B:69:LEU:HB3	2.50	0.46
1:Y:332:ARG:HA	1:Y:332:ARG:HD3	1.71	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:A:90:ILE:N	1:A:91:PRO:CD	2.75	0.46
1:A:390:ASN:H	1:A:390:ASN:HD22	1.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:190:ASN:ND2	1:X:193:VAL:HG22	2.31	0.45
1:X:144:VAL:O	1:X:145:ASP:HB3	2.16	0.45
1:X:21:ASP:O	1:X:25:ILE:HG13	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:X:38:GLU:HG2	1:X:167:ALA:CB	2.47	0.45
1:A:390:ASN:ND2	1:A:390:ASN:N	2.63	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:X:77:GLY:O	1:X:81:LEU:HG	2.16	0.45
1:B:143:ILE:HD13	1:B:181:THR:HG21	1.98	0.45
1:Y:61:LEU:O	1:Y:65:GLN:HG3	2.17	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: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:B:37:GLN:O	1:B:38:GLU:CB	2.63	0.44
1:A:357:PHE:N	3:A:442:EDO:H11	2.31	0.44
1:Y:407:ARG:NH1	1:Y:431:PHE:CD2	2.85	0.44
1:B:24:GLU:O	1:B:28:TYR:HD2	2.00	0.44
1:X:80:GLN:HB3	1:X:112:THR:CG2	2.47	0.44
1:B:144:VAL:O	1:B:145:ASP:C	2.55	0.44
1:A:136:ARG:HG3	1:B:136:ARG:HD2	1.99	0.44
1:A:136:ARG:CZ	1:A:137:GLY:H	2.29	0.44
1:B:277:GLU:HA	1:B:283:GLY:HA2	2.00	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:B:354:LEU:HB3	1:B:385:TRP:CB	2.48	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:X:35:ILE:HG22	1:X:37:GLN:N	2.26	0.44
1:A:12:ILE:O	1:A:16:LEU:HG	2.17	0.44
1:Y:276:ARG:HA	1:Y:280:THR:HG22	1.99	0.44
1:X:85:LEU:CD2	1:X:92:THR:HG22	2.48	0.44
1:B:403:GLY:HA3	1:B:414:TRP:CZ2	2.53	0.44
5:Y:441:COA:HN4	5:Y:441:COA:H71	1.58	0.44
1:B:21:ASP:O	1:B:25:ILE:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ARG:HA	1:B:31:ARG:HE	1.83	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:Y:282:ALA:O	1:Y:283:GLY:C	2.56	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:237:MSE:HE1	1:Y:247:ARG:O	2.18	0.43
1:X:51:GLN:HB2	1:X:80:GLN:HE22	1.83	0.43
1:A:331:ASP:OD2	1:A:345:THR:CG2	2.67	0.43
1:Y:318:ARG:HB2	1:Y:319:PRO:HD2	2.00	0.43
1:B:148:LYS:CE	1:B:149:LEU:HD23	2.49	0.43
1:Y:181:THR:HB	1:Y:182:PRO:HD2	2.00	0.43
1:B:237:MSE:HE2	1:B:251:GLU:HG2	2.00	0.43
1:Y:19:MSE:HA	1:Y:19:MSE:HE3	2.00	0.43
1:B:95:VAL:O	1:B:96:ASP:C	2.57	0.43
1:A:329:ARG:HD3	1:A:329:ARG:HA	1.84	0.43
1:Y:356:LYS:HE2	1:Y:356:LYS:HB2	1.72	0.43
1:X:12:ILE:O	1:X:15:LEU:HB3	2.18	0.43
1:B:95:VAL:CG2	1:B:149:LEU:HD11	2.49	0.43
1:B:95:VAL:CG2	1:B:98:LEU:HB2	2.49	0.43
1:A:48:ALA:O	1:A:51:GLN:N	2.50	0.43
1:X:25:ILE:HG12	1:X:279:PHE:HB3	2.00	0.43
1:Y:434:PRO:HA	1:Y:435:PRO:HD3	1.92	0.43
1:X:277:GLU:HB2	1:X:284:SER:O	2.19	0.43
1:Y:318:ARG:N	1:Y:318:ARG:HD2	2.31	0.43
1:X:12:ILE:HD12	1:X:66:THR:O	2.19	0.43
1:X:100:VAL:HB	1:X:102:ARG:NH1	2.34	0.43
1:X:38:GLU:CD	1:X:167:ALA:HB2	2.39	0.43
1:X:277:GLU:HA	1:X:283:GLY:HA2	2.01	0.43
1:Y:423:VAL:HA	1:Y:426:VAL:HG12	2.00	0.42
1:B:41:ALA:HA	1:B:206:LYS:O	2.19	0.42
1:A:14:GLN:CA	1:A:14:GLN:HE21	2.22	0.42
1:X:13:VAL:C	1:X:15:LEU:H	2.21	0.42
1:B:199:VAL:HG13	1:B:204:PRO:HD2	2.01	0.42
1:X:118:LEU:HD21	1:Y:162:LEU:HD23	2.01	0.42
1:Y:16:LEU:C	1:Y:18:HIS:H	2.23	0.42
1:A:207:VAL:HB	1:A:266:VAL:HG22	2.00	0.42
1:X:106:MSE:HE3	1:X:151:ARG:HB3	2.02	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
1:A:164:GLY:O	1:A:168:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:307:ARG:HG2	1:X:339:TYR:CG	2.54	0.42
1:X:254:LYS:HD3	1:X:258:ASP:OD2	2.18	0.42
1:A:38:GLU:HB3	1:A:167:ALA:HB2	2.02	0.42
1:Y:281:HIS:O	1:Y:282:ALA:HB2	2.19	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:A:136:ARG:NE	1:A:137:GLY:N	2.61	0.42
1:Y:391:ASN:HA	1:Y:392:PRO:HD3	1.81	0.42
1:A:382:GLN:NE2	1:A:418:MSE:CG	2.80	0.42
1:B:383:LEU:C	1:B:384:ILE:HD12	2.40	0.42
1:A:361:ASP:OD1	1:A:364[B]:ARG:NH1	2.53	0.42
1:Y:106:MSE:HE3	1:Y:106:MSE:HA	2.01	0.42
1:B:32:PHE:C	1:B:34:GLY:H	2.23	0.42
1:B:191:ALA:O	1:B:194:ALA:HB3	2.20	0.42
1:Y:162:LEU:HG	6:Y:444:HOH:O	2.20	0.42
1:X:428:GLU:HA	1:X:428:GLU:OE2	2.20	0.42
1:B:21:ASP:HB2	1:Y:19:MSE:CE	2.45	0.41
1:Y:121:VAL:HG21	1:Y:133:ALA:CB	2.43	0.41
1:A:388:ARG:O	1:A:391:ASN:HB2	2.19	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:X:147:ASP:N	1:X:147:ASP:OD2	2.38	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:274:LEU:O	1:B:274:LEU:HD22	2.20	0.41
1:Y:419:GLY:HA2	1:Y:420:PRO:HD3	1.96	0.41
1:X:332:ARG:HG2	1:X:334:PHE:CE2	2.55	0.41
1:B:198:LEU:HA	1:B:198:LEU:HD12	1.79	0.41
1:X:37:GLN:O	1:X:40:PHE:CE2	2.73	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:Y:294:MSE:CE	1:Y:371:THR:HG22	2.50	0.41
1:Y:139:PHE:CE1	1:Y:194:ALA:HB1	2.55	0.41
1:Y:191:ALA:O	1:Y:195:VAL:HG23	2.20	0.41
1:X:283:GLY:O	1:X:284:SER:HB2	2.21	0.41
1:Y:386:ARG:NH1	1:Y:430:ALA:O	2.52	0.41
1:B:352:VAL:HG11	1:B:380:ALA:HB2	2.02	0.41
1:A:224:LEU:HD12	1:A:224:LEU:HA	1.84	0.41
1:B:49:VAL:O	1:B:49:VAL:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:383:LEU:HD23	1:X:385:TRP:CZ3	2.56	0.41
1:B:23:LYS:HG3	1:B:24:GLU:N	2.34	0.41
1:B:142:ASP:O	1:B:153:GLY:HA2	2.21	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:X:5:ALA:N	1:X:6:PRO:CD	2.83	0.41
1:B:166:ALA:O	1:B:170:GLY:N	2.53	0.41
1:Y:43:ILE:HD12	1:Y:43:ILE:N	2.36	0.41
1:A:145:ASP:O	1:A:146:ALA:C	2.59	0.41
1:X:95:VAL:CG1	1:X:96:ASP:N	2.84	0.41
1:B:148:LYS:HG3	1:B:149:LEU:N	2.35	0.41
1:B:340:ARG:NH2	1:B:366:GLU:OE1	2.50	0.41
1:B:135:PRO:HA	1:B:176:ALA:HB3	2.03	0.41
1:A:349:ASP:OD2	1:A:429:LYS:HE3	2.21	0.41
1:B:313:LYS:O	1:B:316:PHE:O	2.39	0.41
1:A:88:ALA:O	1:A:89:ASP:CB	2.69	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: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:151:ARG:HH22	1:Y:183:ASP:HB2	1.86	0.40
1:B:24:GLU:O	1:B:28:TYR:CD2	2.74	0.40
1:Y:81:LEU:HD22	1:Y:81:LEU:O	2.21	0.40
1:B:300:LYS:O	1:B:300:LYS:HG2	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:X:409:GLU:CG	1:X:410:TRP:CD1	2.91	0.40
1:B:94:ARG:HD2	1:B:148:LYS:O	2.22	0.40
1:B:45:VAL:HG12	1:B:210:LEU:HD12	2.02	0.40
1:B:175:LEU:HD22	1:B:198:LEU:HD21	2.02	0.40
1:Y:242:VAL:O	1:Y:242:VAL:HG12	2.21	0.40
1:X:36:ASP:O	1:X:37:GLN:CB	2.70	0.40
1:A:61:LEU:HD13	1:A:73:VAL:HG21	2.03	0.40
1:Y:85:LEU:HD13	1:Y:92:THR:HG21	2.03	0.40
1:A:313:LYS:HD2	1:A:319:PRO:HG3	2.04	0.40
1:B:292:GLU:HG2	1:B:368:LEU:HD21	2.03	0.40
1:Y:108:ILE:N	1:Y:108:ILE:HD12	2.36	0.40
1:Y:318:ARG:CG	1:Y:439:ALA:HB3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:44:LYS:CE	1:X:191:ALA:HB1	2.51	0.40
1:X:118:LEU:HD12	1:Y:161:ASP:HB3	2.04	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%)	6	13
1	B	433/460 (94%)	378 (87%)	39 (9%)	16 (4%)	4	8
1	X	433/460 (94%)	394 (91%)	26 (6%)	13 (3%)	5	11
1	Y	402/460 (87%)	352 (88%)	39 (10%)	11 (3%)	6	13
All	All	1703/1840 (93%)	1518 (89%)	133 (8%)	52 (3%)	5	11

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 ⓘ

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%)	6	12
1	B	344/357 (96%)	309 (90%)	35 (10%)	9	19
1	X	344/357 (96%)	311 (90%)	33 (10%)	10	21
1	Y	323/357 (90%)	289 (90%)	34 (10%)	8	17
All	All	1357/1428 (95%)	1212 (89%)	145 (11%)	8	17

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 [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLI	A	441	-	0,6,6	0.00	-	0,7,7	0.00	-
3	EDO	A	442	-	3,3,3	0.49	0	2,2,2	0.46	0
4	SO4	X	441	-	4,4,4	0.21	0	6,6,6	0.12	0
5	COA	Y	441	-	40,50,50	2.64	10 (25%)	50,75,75	2.92	14 (28%)
2	MLI	Y	442	-	0,6,6	0.00	-	0,7,7	0.00	-
3	EDO	Y	443	-	3,3,3	0.47	0	2,2,2	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MLI	A	441	-	-	0/0/4/4	0/0/0/0
3	EDO	A	442	-	-	0/1/1/1	0/0/0/0
4	SO4	X	441	-	-	0/0/0/0	0/0/0/0
5	COA	Y	441	-	-	0/44/64/64	0/3/3/3
2	MLI	Y	442	-	-	0/0/4/4	0/0/0/0
3	EDO	Y	443	-	-	0/1/1/1	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	441	COA	C5A-C4A	2.08	1.45	1.40
5	Y	441	COA	C5A-N7A	2.89	1.49	1.39
5	Y	441	COA	C8A-N7A	3.09	1.40	1.34
5	Y	441	COA	C4A-N3A	3.12	1.40	1.35
5	Y	441	COA	C6A-N6A	3.82	1.46	1.34
5	Y	441	COA	C2A-N1A	4.12	1.41	1.33
5	Y	441	COA	O4B-C1B	4.38	1.46	1.41
5	Y	441	COA	C5P-N4P	5.88	1.47	1.33
5	Y	441	COA	C9P-N8P	7.63	1.49	1.33
5	Y	441	COA	C2A-N3A	8.44	1.47	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	441	COA	N3A-C2A-N1A	-12.15	119.59	128.89
5	Y	441	COA	C4B-O4B-C1B	-5.80	103.35	109.72
5	Y	441	COA	P2A-O3A-P1A	-3.43	123.09	132.73
5	Y	441	COA	C6P-C7P-N8P	2.21	116.72	111.88
5	Y	441	COA	O5B-C5B-C4B	2.27	117.47	109.12
5	Y	441	COA	C2B-C1B-N9A	2.54	118.17	114.29
5	Y	441	COA	C2P-C3P-N4P	2.67	117.65	112.37
5	Y	441	COA	O3B-C3B-C2B	2.97	123.06	111.51
5	Y	441	COA	O4B-C4B-C5B	3.02	120.12	109.32
5	Y	441	COA	O3A-P1A-O5B	3.05	111.02	102.94
5	Y	441	COA	O3A-P2A-O6A	3.06	111.06	102.94
5	Y	441	COA	O2B-C2B-C3B	3.95	122.55	111.16
5	Y	441	COA	O6A-CCP-CBP	5.38	119.20	110.55
5	Y	441	COA	O4B-C1B-N9A	9.64	128.29	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	429/460 (93%)	-0.05	15 (3%) 48 46	36, 64, 125, 185	0
1	B	428/460 (93%)	0.15	20 (4%) 35 33	48, 88, 165, 210	0
1	X	428/460 (93%)	-0.11	6 (1%) 78 76	39, 64, 108, 185	0
1	Y	401/460 (87%)	0.25	38 (9%) 10 8	41, 76, 174, 250	0
All	All	1686/1840 (91%)	0.06	79 (4%) 35 33	36, 74, 149, 250	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	ASP	9.4
1	Y	281	HIS	9.3
1	B	7	GLY	8.3
1	Y	97	GLY	8.3
1	Y	23	LYS	6.5
1	Y	20	ARG	6.3
1	Y	96	ASP	6.2
1	A	242	VAL	5.6
1	B	8	VAL	5.5
1	B	94	ARG	5.4
1	Y	242	VAL	5.3
1	Y	98	LEU	5.3
1	A	239	ALA	5.1
1	A	10	GLN	5.0
1	Y	279	PHE	4.9
1	A	7	GLY	4.8
1	B	321	VAL	4.8
1	Y	22	GLY	4.7
1	A	94	ARG	4.6
1	Y	11	THR	4.5
1	A	6	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	Y	278	LEU	4.3
1	X	14	GLN	4.3
1	Y	100	VAL	4.2
1	X	36	ASP	4.2
1	B	84	ALA	4.2
1	Y	95	VAL	4.1
1	Y	217	LEU	4.0
1	X	96	ASP	4.0
1	Y	12	ILE	3.9
1	A	240	ASP	3.9
1	B	98	LEU	3.8
1	B	37	GLN	3.8
1	B	90	ILE	3.7
1	Y	30	HIS	3.7
1	Y	282	ALA	3.7
1	X	10	GLN	3.6
1	B	85	LEU	3.6
1	Y	13	VAL	3.5
1	X	37	GLN	3.5
1	A	91	PRO	3.5
1	B	238	GLN	3.4
1	B	89	ASP	3.2
1	Y	238	GLN	3.2
1	B	102	ARG	3.1
1	B	297	THR	3.1
1	Y	247	ARG	3.0
1	Y	240	ASP	3.0
1	Y	284	SER	3.0
1	A	238	GLN	2.9
1	B	6	PRO	2.9
1	Y	31	ARG	2.8
1	B	99	ARG	2.7
1	Y	15	LEU	2.7
1	Y	280	THR	2.7
1	Y	223	ILE	2.6
1	A	90	ILE	2.5
1	Y	90	ILE	2.5
1	B	18	HIS	2.4
1	Y	244	GLY	2.4
1	A	241	TRP	2.4
1	Y	241	TRP	2.3
1	Y	16	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	86	GLU	2.3
1	A	35	ILE	2.2
1	A	102	ARG	2.2
1	Y	216	LEU	2.2
1	Y	89	ASP	2.2
1	A	149	LEU	2.1
1	Y	276	ARG	2.1
1	Y	26	ARG	2.1
1	B	167	ALA	2.1
1	X	98	LEU	2.1
1	A	144	VAL	2.1
1	B	93	GLU	2.0
1	Y	243	ASN	2.0
1	Y	220	ASP	2.0
1	Y	29	LEU	2.0
1	Y	439	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	SO4	X	441	5/5	0.77	0.27	3.65	140,141,150,152	0
2	MLI	Y	442	7/7	0.87	0.27	3.11	86,91,107,110	0
3	EDO	Y	443	4/4	0.93	0.18	2.31	86,90,91,95	0
5	COA	Y	441	48/48	0.86	0.27	2.17	62,119,217,293	0
3	EDO	A	442	4/4	0.93	0.17	1.38	60,69,77,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MLI	A	441	7/7	0.84	0.18	0.95	61,78,96,102	0

6.5 Other polymers [i](#)

There are no such residues in this entry.