Full wwPDB X-ray Structure Validation Report (i)

Sep 6, 2016 – 09:09 PM EDT

PDB ID	:	5DQL
Title	:	Crystal Structure of 2-vinyl glyoxylate modified isocitrate lyase from Mycobacterium tuberculosis
Authors	:	Huang, H.-L.; Meek, T.D.
Deposited on	:	2015-09-14
Resolution	:	1.78 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

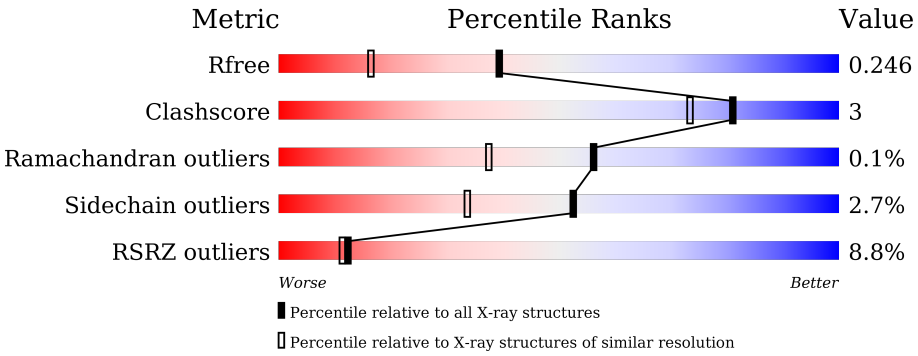
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 1.78 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	6655 (1.80-1.76)
Clashscore	102246	7658 (1.80-1.76)
Ramachandran outliers	100387	7570 (1.80-1.76)
Sidechain outliers	100360	7569 (1.80-1.76)
RSRZ outliers	91569	6671 (1.80-1.76)

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 <=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	428	9% 91% 8%
1	B	428	8% 93% 7%
1	C	428	6% 88% 11%
1	D	428	12% 90% 9%

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
3	VGX	C	502	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14521 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.

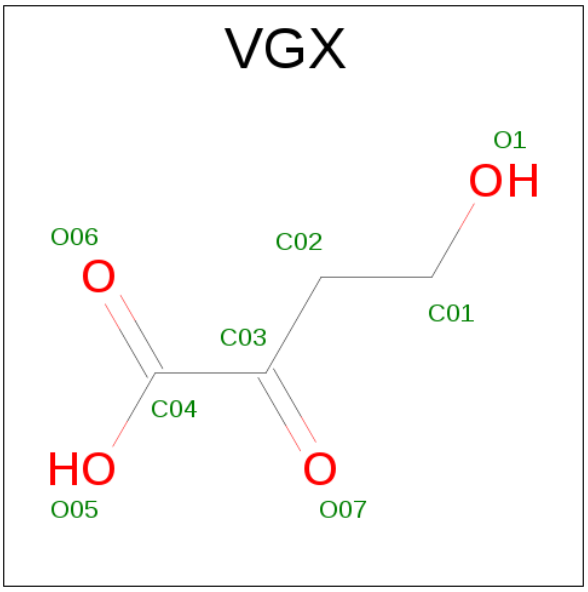
- Molecule 1 is a protein called Isocitrate lyase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	1	0	0
			3308	2078	575	646	9			
1	B	427	Total	C	N	O	S	2	0	0
			3308	2078	575	646	9			
1	C	427	Total	C	N	O	S	2	2	0
			3324	2088	581	646	9			
1	D	427	Total	C	N	O	S	0	0	0
			3308	2078	575	646	9			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	2	Total	Mg	0	0
			2	2		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 4-hydroxy-2-oxobutanoic acid (three-letter code: VGX) (formula: $C_4H_6O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	1	0
3	D	1	Total C O 7 4 3	1	0

- Molecule 4 is water.

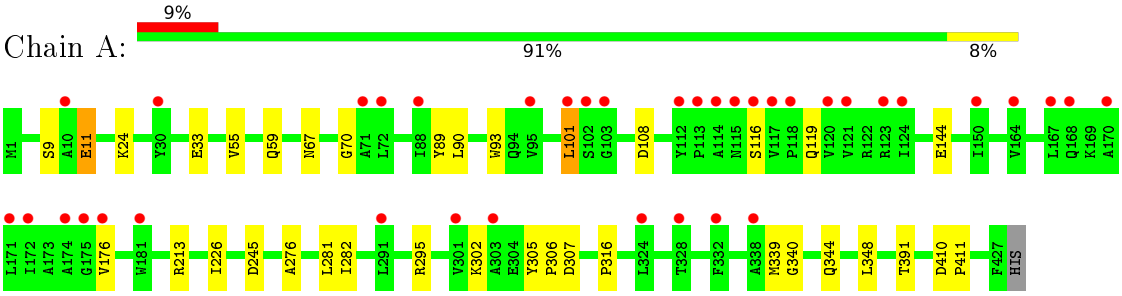
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	330	Total O 330 330	0	0
4	B	332	Total O 332 332	0	0
4	C	298	Total O 298 298	0	0
4	D	280	Total O 280 280	0	0

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 errors 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.

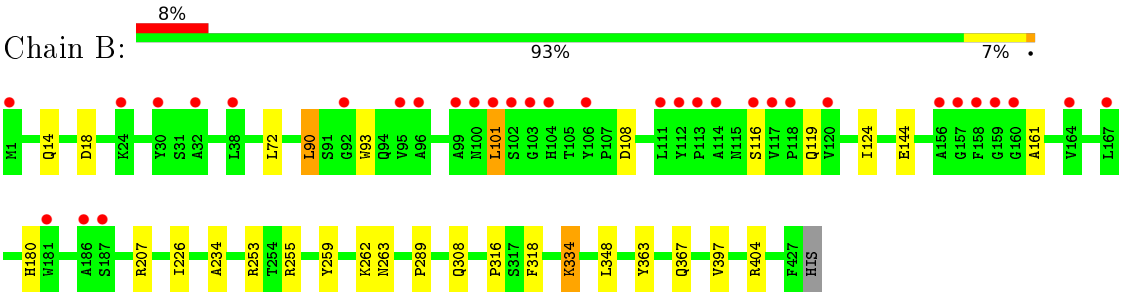
- Molecule 1: Isocitrate lyase 1

Chain A:



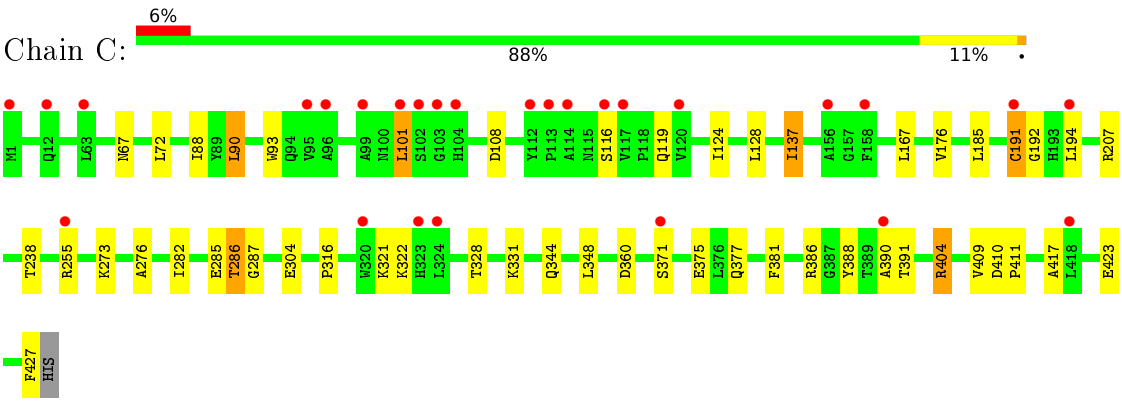
- Molecule 1: Isocitrate lyase 1

Chain B:



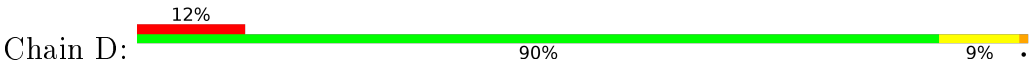
- Molecule 1: Isocitrate lyase 1

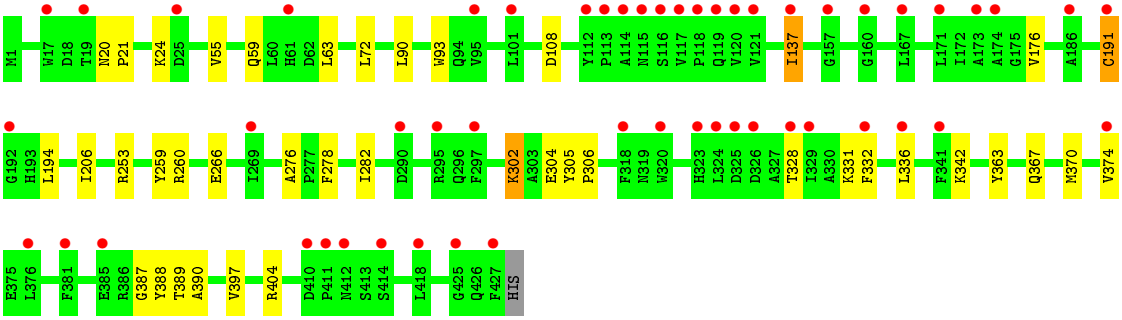
Chain C:



- Molecule 1: Isocitrate lyase 1

Chain D:




M1
W17
D18
T19
N20
P21
K24
D25
V55
Q59
L60
H61
D62
L63
L72
L90
W93
Q94
V95
L101
D108
Y112
P113
A114
N115
S116
V117
P118
Q119
V120
V121
I137
G157
G160
L167
L171
I172
A173
A174
G175
V176
A186
G191
G192
H193
L194
I206
R253
Y259
R260
E266
I269
A276
P277
F278
I282
D290
R295
Q296
F297
K302
A303
E304
Y305
P306
F318
N319
W320
H323
L324
D325
D326
A327
T328
I329
A330
K331
F332
L336
F341
K342
Y363
Q367
M370
V374
E375
L376
F381
E385
R386
G387
Y388
T389
A390
V397
R404
D410
P411
N412
S413
S414
L418
G425
Q426
F427
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	75.09Å 129.24Å 167.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.27 – 1.78 42.31 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.4 (34.27-1.78) 99.3 (42.31-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.203 , 0.246 0.202 , 0.246	Depositor DCC
R_{free} test set	7797 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14521	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: MG, VGX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.40	0/3379	0.54	0/4595
1	B	0.41	0/3379	0.57	0/4595
1	C	0.40	0/3401	0.54	0/4623
1	D	0.38	0/3379	0.53	0/4595
All	All	0.40	0/13538	0.55	0/18408

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	3308	0	3188	19	0
1	B	3308	0	3189	19	0
1	C	3324	0	3215	28	0
1	D	3308	0	3189	24	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	7	0	0	1	0
3	C	7	0	0	0	0
3	D	7	0	0	0	0
4	A	330	0	0	1	0
4	B	332	0	0	4	0
4	C	298	0	0	5	0
4	D	280	0	0	4	0
All	All	14521	0	12781	87	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 3.

All (87) 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:C:417:ALA:HB1	1:D:194:LEU:HD13	1.75	0.69
1:C:388:TYR:CZ	1:C:390:ALA:HB3	2.33	0.64
1:A:226:ILE:HG12	1:A:281:LEU:HB2	1.78	0.64
1:C:286:THR:HG21	4:C:737:HOH:O	2.00	0.61
1:A:101:LEU:HD22	1:A:116:SER:HA	1.82	0.61
1:A:276:ALA:HA	1:A:282:ILE:HD11	1.83	0.60
1:B:207:ARG:NH1	4:B:606:HOH:O	2.33	0.60
1:D:302:LYS:NZ	4:D:608:HOH:O	2.35	0.59
1:B:253:ARG:HD3	1:B:259:TYR:CZ	2.37	0.59
1:B:404:ARG:NH1	4:B:602:HOH:O	2.24	0.59
1:D:276:ALA:O	4:D:601:HOH:O	2.17	0.58
1:C:328:THR:HA	1:C:331:LYS:HG2	1.87	0.56
1:C:276:ALA:HA	1:C:282:ILE:HD11	1.88	0.55
1:A:101:LEU:HD21	1:A:119:GLN:HG3	1.88	0.55
1:C:93:TRP:CD1	1:C:108:ASP:HB2	2.43	0.54
1:C:101:LEU:HD22	1:C:116:SER:HA	1.89	0.53
1:C:371:SER:O	1:C:375:GLU:HG3	2.08	0.52
1:B:316:PRO:HG2	1:B:348:LEU:HB2	1.91	0.52
1:A:24:LYS:NZ	1:A:307:ASP:OD2	2.40	0.52
1:A:302:LYS:HD3	1:A:306:PRO:O	2.10	0.52
1:B:101:LEU:HD22	1:B:116:SER:HA	1.92	0.52
4:B:605:HOH:O	1:C:404[B]:ARG:NH2	2.42	0.51
1:D:276:ALA:HA	1:D:282:ILE:HD11	1.94	0.50
1:D:93:TRP:CD1	1:D:108:ASP:HB2	2.47	0.49
1:C:207[B]:ARG:NH1	4:C:614:HOH:O	2.46	0.49
1:C:191:CYS:HB3	1:C:194:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:HD22	1:C:124:ILE:HD12	1.93	0.48
1:B:289:PRO:HD3	1:B:318:PHE:CG	2.49	0.48
1:A:67:ASN:HA	1:A:344:GLN:O	2.13	0.48
1:A:302:LYS:NZ	1:A:340:GLY:HA3	2.29	0.48
1:B:308:GLN:NE2	4:B:601:HOH:O	2.14	0.47
1:C:286:THR:HG22	1:C:287:GLY:H	1.80	0.47
1:B:90:LEU:HD22	1:B:124:ILE:HD12	1.97	0.47
1:B:363:TYR:O	1:B:367:GLN:HG2	2.16	0.46
1:A:70:GLY:HA2	1:A:89:TYR:O	2.16	0.46
1:B:101:LEU:HD21	1:B:119:GLN:HG3	1.98	0.46
1:C:137:ILE:HD12	1:C:137:ILE:HA	1.66	0.46
1:D:137:ILE:HD11	1:D:404:ARG:HG2	1.98	0.46
1:A:302:LYS:HA	1:A:305:TYR:O	2.16	0.45
1:C:316:PRO:HG2	1:C:348:LEU:HB2	1.98	0.45
1:B:234:ALA:O	1:B:263:ASN:HB3	2.16	0.45
1:D:328:THR:HA	1:D:331:LYS:HG2	1.99	0.45
1:A:93:TRP:CD1	1:A:108:ASP:HB2	2.52	0.45
1:B:348:LEU:HD11	3:B:502:VGX:O07	2.17	0.45
1:C:192:GLY:HA3	1:C:285:GLU:HG2	1.99	0.45
1:D:388:TYR:CZ	1:D:390:ALA:HB3	2.51	0.45
1:D:363:TYR:O	1:D:367:GLN:HG2	2.17	0.44
1:D:59:GLN:O	1:D:63:LEU:HB2	2.17	0.44
1:D:260:ARG:HD3	4:D:828:HOH:O	2.16	0.44
1:B:334:LYS:H	1:B:334:LYS:HG2	1.54	0.44
1:D:370:MET:O	1:D:374:VAL:HG23	2.18	0.44
1:D:55:VAL:O	1:D:59:GLN:HG3	2.18	0.44
1:D:59:GLN:HA	1:D:63:LEU:HD23	2.00	0.44
1:B:180:HIS:HB3	1:B:226:ILE:HB	2.00	0.44
1:A:245:ASP:OD1	4:A:601:HOH:O	2.21	0.43
1:A:302:LYS:HZ3	1:A:340:GLY:HA3	1.83	0.43
1:A:316:PRO:HG2	1:A:348:LEU:HB2	2.00	0.43
1:C:360:ASP:C	4:C:620:HOH:O	2.56	0.43
1:C:119:GLN:NE2	4:C:608:HOH:O	2.38	0.43
1:C:377:GLN:HG2	1:C:381:PHE:CE2	2.54	0.43
1:B:93:TRP:CD1	1:B:108:ASP:HB2	2.54	0.42
1:C:386:ARG:HD2	1:D:363:TYR:CE2	2.53	0.42
1:B:207:ARG:HG2	1:C:409:VAL:HG12	2.00	0.42
1:D:108:ASP:HB3	1:D:191:CYS:HB3	2.01	0.42
1:A:295:ARG:CZ	1:A:339:MET:HE2	2.49	0.42
1:C:423:GLU:O	1:C:427:PHE:HB2	2.19	0.42
1:D:20:ASN:HA	1:D:21:PRO:HD2	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:SER:OG	1:A:11:GLU:HG2	2.19	0.42
1:A:55:VAL:O	1:A:59:GLN:HG3	2.19	0.42
1:C:67:ASN:HA	1:C:344:GLN:O	2.19	0.42
1:C:410:ASP:HA	1:C:411:PRO:HD2	1.87	0.42
1:C:273:LYS:HE2	1:C:304:GLU:HG3	2.02	0.42
1:D:206:ILE:HD12	1:D:278:PHE:CD2	2.54	0.42
1:D:266:GLU:HB2	4:D:757:HOH:O	2.20	0.42
1:A:348:LEU:HD11	3:A:503:VGX:O07	2.20	0.41
1:D:387:GLY:O	1:D:389:THR:HG23	2.20	0.41
1:D:253:ARG:HD3	1:D:259:TYR:CE2	2.55	0.41
1:D:342:LYS:HA	1:D:342:LYS:HD2	1.91	0.41
1:B:14:GLN:HG3	1:B:18:ASP:OD2	2.21	0.41
1:B:262:LYS:HB2	1:B:262:LYS:HE3	1.87	0.41
1:B:161:ALA:HB2	1:B:207:ARG:HD2	2.03	0.41
1:C:276:ALA:O	4:C:601:HOH:O	2.22	0.41
1:A:410:ASP:HA	1:A:411:PRO:HD2	1.87	0.40
1:C:185:LEU:HD13	1:C:238:THR:HG21	2.03	0.40
1:D:305:TYR:HA	1:D:306:PRO:HD2	1.85	0.40
1:D:332:PHE:CE2	1:D:336:LEU:HD11	2.56	0.40
1:C:88:ILE:CD1	1:C:128:LEU:HD11	2.52	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	425/428 (99%)	417 (98%)	8 (2%)	0	100	100
1	B	425/428 (99%)	418 (98%)	7 (2%)	0	100	100
1	C	427/428 (100%)	415 (97%)	12 (3%)	0	100	100
1	D	425/428 (99%)	414 (97%)	10 (2%)	1 (0%)	52	34
All	All	1702/1712 (99%)	1664 (98%)	37 (2%)	1 (0%)	56	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	24	LYS

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	337/339 (99%)	329 (98%)	8 (2%)	57	38
1	B	337/339 (99%)	330 (98%)	7 (2%)	61	44
1	C	339/339 (100%)	325 (96%)	14 (4%)	37	17
1	D	337/339 (99%)	329 (98%)	8 (2%)	57	38
All	All	1350/1356 (100%)	1313 (97%)	37 (3%)	52	34

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	33	GLU
1	A	90	LEU
1	A	101	LEU
1	A	144	GLU
1	A	176	VAL
1	A	213	ARG
1	A	391	THR
1	B	72	LEU
1	B	90	LEU
1	B	101	LEU
1	B	144	GLU
1	B	255	ARG
1	B	334	LYS
1	B	397	VAL
1	C	72	LEU
1	C	90	LEU
1	C	101	LEU
1	C	137	ILE

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Mol	Chain	Res	Type
1	C	167	LEU
1	C	176	VAL
1	C	191	CYS
1	C	255	ARG
1	C	286	THR
1	C	321	LYS
1	C	322	LYS
1	C	391	THR
1	C	404[A]	ARG
1	C	404[B]	ARG
1	D	72	LEU
1	D	90	LEU
1	D	137	ILE
1	D	176	VAL
1	D	191	CYS
1	D	302	LYS
1	D	304	GLU
1	D	397	VAL

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

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

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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	VGX	A	503	1	3,6,7	0.42	0	3,7,8	3.91	1 (33%)
3	VGX	B	502	1	3,6,7	0.57	0	3,7,8	3.04	1 (33%)
3	VGX	C	502	1	3,6,7	0.43	0	3,7,8	0.61	0
3	VGX	D	502	1	3,6,7	0.42	0	3,7,8	0.61	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
3	VGX	A	503	1	-	0/2/6/7	0/0/0/0
3	VGX	B	502	1	-	0/2/6/7	0/0/0/0
3	VGX	C	502	1	-	0/2/6/7	0/0/0/0
3	VGX	D	502	1	-	0/2/6/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	VGX	C01-C02-C03	-6.76	103.34	113.82
3	B	502	VGX	C01-C02-C03	-4.99	106.08	113.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	VGX	1	0
3	B	502	VGX	1	0

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	427/428 (99%)	0.56	38 (8%) 12 11	16, 29, 43, 52	4 (0%)
1	B	427/428 (99%)	0.47	33 (7%) 16 15	15, 29, 42, 52	8 (1%)
1	C	427/428 (99%)	0.50	27 (6%) 23 22	17, 30, 47, 56	5 (1%)
1	D	427/428 (99%)	0.80	52 (12%) 5 5	18, 34, 51, 61	3 (0%)
All	All	1708/1712 (99%)	0.58	150 (8%) 12 11	15, 31, 47, 61	20 (1%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	101	LEU	6.3
1	D	101	LEU	5.3
1	C	101	LEU	4.8
1	A	101	LEU	4.7
1	D	117	VAL	4.7
1	B	1	MET	4.3
1	B	158	PHE	4.3
1	A	171	LEU	4.1
1	A	120	VAL	4.1
1	D	114	ALA	4.0
1	D	121	VAL	3.9
1	D	414	SER	3.9
1	B	112	TYR	3.8
1	B	111	LEU	3.8
1	D	112	TYR	3.7
1	A	176	VAL	3.7
1	D	425	GLY	3.7
1	B	113	PRO	3.6
1	D	171	LEU	3.6
1	D	118	PRO	3.5
1	A	124	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	103	GLY	3.5
1	C	194	LEU	3.5
1	A	170	ALA	3.5
1	B	102	SER	3.5
1	C	323	HIS	3.5
1	A	172	ILE	3.4
1	B	99	ALA	3.4
1	A	167	LEU	3.4
1	D	318	PHE	3.4
1	A	121	VAL	3.3
1	D	381	PHE	3.3
1	D	412	ASN	3.3
1	D	323	HIS	3.3
1	D	95	VAL	3.2
1	D	115	ASN	3.2
1	A	117	VAL	3.2
1	C	324	LEU	3.2
1	D	328	THR	3.2
1	B	167	LEU	3.2
1	D	297	PHE	3.2
1	C	102	SER	3.2
1	B	156	ALA	3.1
1	B	106	TYR	3.1
1	B	103	GLY	3.1
1	C	1	MET	3.0
1	B	95	VAL	3.0
1	B	120	VAL	3.0
1	D	116	SER	3.0
1	B	96	ALA	2.9
1	B	117	VAL	2.9
1	D	418	LEU	2.9
1	B	160	GLY	2.9
1	A	95	VAL	2.8
1	B	159	GLY	2.8
1	A	150	ILE	2.8
1	B	157	GLY	2.8
1	C	120	VAL	2.8
1	A	328	THR	2.8
1	B	114	ALA	2.8
1	A	30	TYR	2.8
1	D	173	ALA	2.8
1	A	174	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	113	PRO	2.7
1	D	113	PRO	2.7
1	D	295	ARG	2.7
1	D	336	LEU	2.7
1	D	120	VAL	2.7
1	A	113	PRO	2.7
1	D	186	ALA	2.6
1	D	320	TRP	2.6
1	B	100	ASN	2.6
1	D	427	PHE	2.6
1	D	324	LEU	2.6
1	C	95	VAL	2.6
1	A	114	ALA	2.6
1	D	19	THR	2.6
1	B	164	VAL	2.6
1	B	116	SER	2.6
1	A	118	PRO	2.6
1	B	181	TRP	2.5
1	A	332	PHE	2.5
1	C	116	SER	2.5
1	A	10	ALA	2.5
1	C	191	CYS	2.5
1	B	92	GLY	2.5
1	A	303	ALA	2.5
1	C	96	ALA	2.5
1	D	341	PHE	2.5
1	A	181	TRP	2.5
1	A	72	LEU	2.4
1	D	167	LEU	2.4
1	D	174	ALA	2.4
1	C	320	TRP	2.4
1	D	269	ILE	2.4
1	A	115	ASN	2.4
1	B	32	ALA	2.4
1	D	376	LEU	2.4
1	A	116	SER	2.4
1	A	324	LEU	2.3
1	A	123	ARG	2.3
1	D	332	PHE	2.3
1	B	187	SER	2.3
1	D	192	GLY	2.3
1	D	329	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	71	ALA	2.3
1	C	156	ALA	2.3
1	C	112	TYR	2.3
1	C	255	ARG	2.3
1	A	338	ALA	2.3
1	D	326	ASP	2.3
1	A	301	VAL	2.2
1	D	25	ASP	2.2
1	D	290	ASP	2.2
1	A	102	SER	2.2
1	D	137	ILE	2.2
1	D	61	HIS	2.2
1	D	119	GLN	2.2
1	A	175	GLY	2.2
1	C	99	ALA	2.2
1	C	371	SER	2.2
1	A	164	VAL	2.2
1	C	117	VAL	2.2
1	A	168	GLN	2.2
1	C	12	GLN	2.2
1	C	63	LEU	2.2
1	D	411	PRO	2.2
1	D	157	GLY	2.2
1	D	160	GLY	2.2
1	D	410	ASP	2.2
1	C	114	ALA	2.2
1	B	118	PRO	2.1
1	D	374	VAL	2.1
1	A	88	ILE	2.1
1	D	17	TRP	2.1
1	A	103	GLY	2.1
1	B	38	LEU	2.1
1	B	186	ALA	2.1
1	D	191	CYS	2.1
1	C	158	PHE	2.1
1	A	291	LEU	2.1
1	C	418	LEU	2.1
1	D	385	GLU	2.1
1	B	24	LYS	2.0
1	B	30	TYR	2.0
1	D	325	ASP	2.0
1	C	104	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	390	ALA	2.0
1	B	104	HIS	2.0
1	A	112	TYR	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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	VGX	C	502	7/8	0.94	0.18	3.19	22,31,31,33	2
3	VGX	A	503	7/8	0.96	0.12	0.75	23,26,28,29	3
3	VGX	B	502	7/8	0.98	0.11	0.24	24,24,27,27	2
3	VGX	D	502	7/8	0.85	0.13	-0.09	25,32,35,39	1
2	MG	A	501	1/1	0.84	0.11	-0.88	40,40,40,40	0
2	MG	A	502	1/1	0.90	0.05	-1.87	37,37,37,37	0
2	MG	C	501	1/1	0.82	0.09	-2.39	43,43,43,43	0
2	MG	B	501	1/1	0.87	0.09	-2.52	35,35,35,35	0
2	MG	D	501	1/1	0.77	0.08	-4.64	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.