Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:28 AM GMT

PDB ID	:	3EOE
Title	:	Crystal Structure of Pyruvate Kinase from toxoplasma gondii, 55.m00007
Authors	:	Wernimont, A.K.; Lew, J.; Kozieradzki, I.; Wasney, G.; Hassani, A.; Vedadi, M.; Cossar, D.; Schapiro, M.; Bochkarev, A.; Arrowsmith, C.H.; Bountra, C.; Weigelt, J.; Edwards, A.M.; Hui, R.; Pizarro, J.; Structural Genomics Consortium (SGC)
Deposited on	:	2008-09-26
Resolution	:	2.31 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:

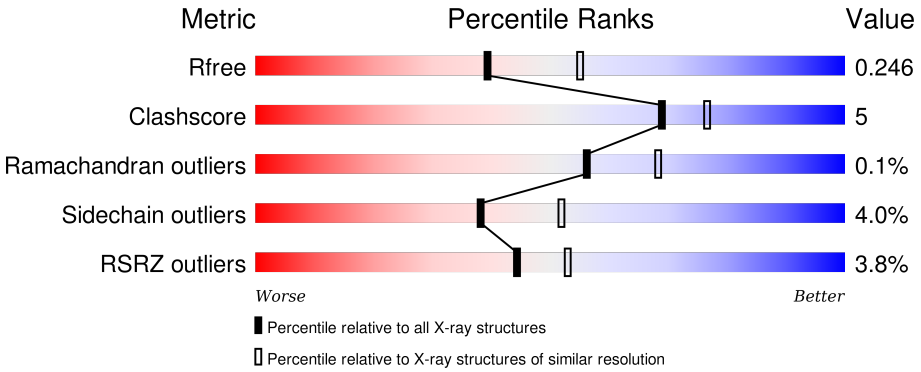
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.31 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	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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	511	5% 79% 14% 8%
1	B	511	3% 84% 10% • 5%
1	C	511	2% 80% 12% • 7%
1	D	511	3% 65% 9% • 25%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	B	512	-	-	X	-
2	GOL	B	513	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14040 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 Pyruvate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	1	0
			3464	2179	603	654	28			
1	B	483	Total	C	N	O	S	0	2	0
			3617	2273	632	684	28			
1	C	475	Total	C	N	O	S	3	1	0
			3510	2201	621	661	27			
1	D	382	Total	C	N	O	S	3	0	0
			2792	1762	485	519	26			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q969A2
A	2	HIS	-	EXPRESSION TAG	UNP Q969A2
A	3	HIS	-	EXPRESSION TAG	UNP Q969A2
A	4	HIS	-	EXPRESSION TAG	UNP Q969A2
A	5	HIS	-	EXPRESSION TAG	UNP Q969A2
A	6	HIS	-	EXPRESSION TAG	UNP Q969A2
A	7	HIS	-	EXPRESSION TAG	UNP Q969A2
A	8	SER	-	EXPRESSION TAG	UNP Q969A2
A	9	SER	-	EXPRESSION TAG	UNP Q969A2
A	10	GLY	-	EXPRESSION TAG	UNP Q969A2
A	11	ARG	-	EXPRESSION TAG	UNP Q969A2
A	12	GLU	-	EXPRESSION TAG	UNP Q969A2
A	13	ASN	-	EXPRESSION TAG	UNP Q969A2
A	14	LEU	-	EXPRESSION TAG	UNP Q969A2
A	15	TYR	-	EXPRESSION TAG	UNP Q969A2
A	16	PHE	-	EXPRESSION TAG	UNP Q969A2
A	17	GLN	-	EXPRESSION TAG	UNP Q969A2
A	18	GLY	-	EXPRESSION TAG	UNP Q969A2
B	1	MET	-	EXPRESSION TAG	UNP Q969A2
B	2	HIS	-	EXPRESSION TAG	UNP Q969A2
B	3	HIS	-	EXPRESSION TAG	UNP Q969A2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	EXPRESSION TAG	UNP Q969A2
B	5	HIS	-	EXPRESSION TAG	UNP Q969A2
B	6	HIS	-	EXPRESSION TAG	UNP Q969A2
B	7	HIS	-	EXPRESSION TAG	UNP Q969A2
B	8	SER	-	EXPRESSION TAG	UNP Q969A2
B	9	SER	-	EXPRESSION TAG	UNP Q969A2
B	10	GLY	-	EXPRESSION TAG	UNP Q969A2
B	11	ARG	-	EXPRESSION TAG	UNP Q969A2
B	12	GLU	-	EXPRESSION TAG	UNP Q969A2
B	13	ASN	-	EXPRESSION TAG	UNP Q969A2
B	14	LEU	-	EXPRESSION TAG	UNP Q969A2
B	15	TYR	-	EXPRESSION TAG	UNP Q969A2
B	16	PHE	-	EXPRESSION TAG	UNP Q969A2
B	17	GLN	-	EXPRESSION TAG	UNP Q969A2
B	18	GLY	-	EXPRESSION TAG	UNP Q969A2
C	1	MET	-	EXPRESSION TAG	UNP Q969A2
C	2	HIS	-	EXPRESSION TAG	UNP Q969A2
C	3	HIS	-	EXPRESSION TAG	UNP Q969A2
C	4	HIS	-	EXPRESSION TAG	UNP Q969A2
C	5	HIS	-	EXPRESSION TAG	UNP Q969A2
C	6	HIS	-	EXPRESSION TAG	UNP Q969A2
C	7	HIS	-	EXPRESSION TAG	UNP Q969A2
C	8	SER	-	EXPRESSION TAG	UNP Q969A2
C	9	SER	-	EXPRESSION TAG	UNP Q969A2
C	10	GLY	-	EXPRESSION TAG	UNP Q969A2
C	11	ARG	-	EXPRESSION TAG	UNP Q969A2
C	12	GLU	-	EXPRESSION TAG	UNP Q969A2
C	13	ASN	-	EXPRESSION TAG	UNP Q969A2
C	14	LEU	-	EXPRESSION TAG	UNP Q969A2
C	15	TYR	-	EXPRESSION TAG	UNP Q969A2
C	16	PHE	-	EXPRESSION TAG	UNP Q969A2
C	17	GLN	-	EXPRESSION TAG	UNP Q969A2
C	18	GLY	-	EXPRESSION TAG	UNP Q969A2
D	1	MET	-	EXPRESSION TAG	UNP Q969A2
D	2	HIS	-	EXPRESSION TAG	UNP Q969A2
D	3	HIS	-	EXPRESSION TAG	UNP Q969A2
D	4	HIS	-	EXPRESSION TAG	UNP Q969A2
D	5	HIS	-	EXPRESSION TAG	UNP Q969A2
D	6	HIS	-	EXPRESSION TAG	UNP Q969A2
D	7	HIS	-	EXPRESSION TAG	UNP Q969A2
D	8	SER	-	EXPRESSION TAG	UNP Q969A2
D	9	SER	-	EXPRESSION TAG	UNP Q969A2

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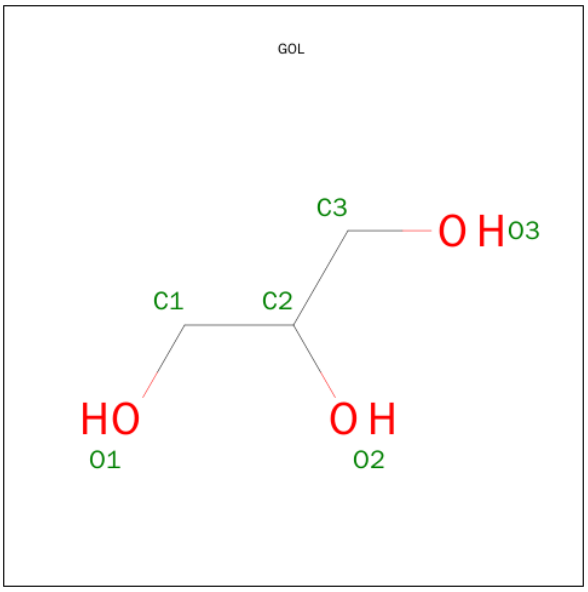
Chain	Residue	Modelled	Actual	Comment	Reference
D	10	GLY	-	EXPRESSION TAG	UNP Q969A2
D	11	ARG	-	EXPRESSION TAG	UNP Q969A2
D	12	GLU	-	EXPRESSION TAG	UNP Q969A2
D	13	ASN	-	EXPRESSION TAG	UNP Q969A2
D	14	LEU	-	EXPRESSION TAG	UNP Q969A2
D	15	TYR	-	EXPRESSION TAG	UNP Q969A2
D	16	PHE	-	EXPRESSION TAG	UNP Q969A2
D	17	GLN	-	EXPRESSION TAG	UNP Q969A2
D	18	GLY	-	EXPRESSION TAG	UNP Q969A2

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 6 3 3	0	0
2	B	1	Total C O 6 3 3	0	0
2	C	1	Total C O 6 3 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	166	Total O 166 166	0	0
3	B	195	Total O 195 195	0	0

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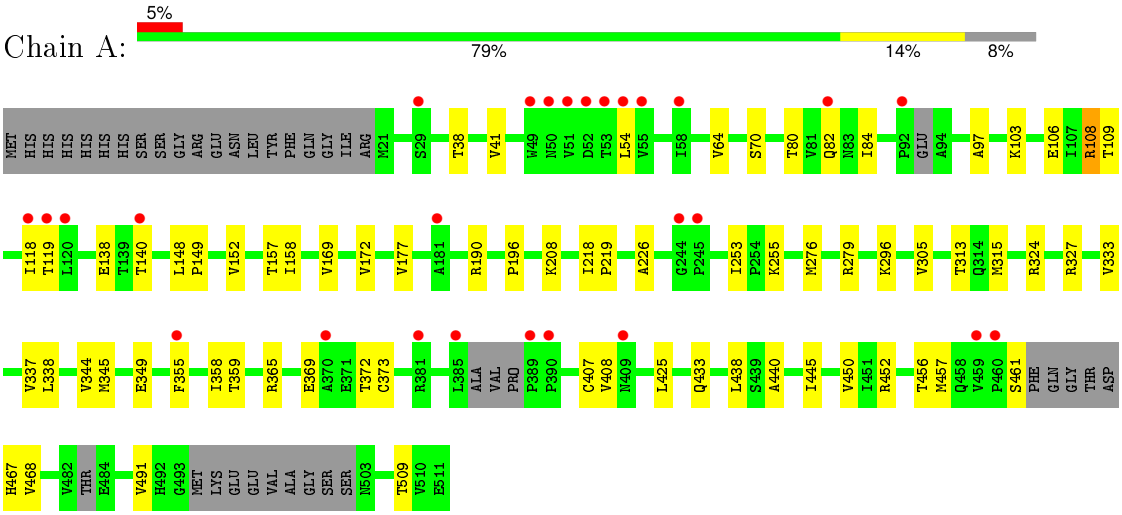
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	190	Total O 190 190	0	0
3	D	88	Total O 88 88	0	0

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.

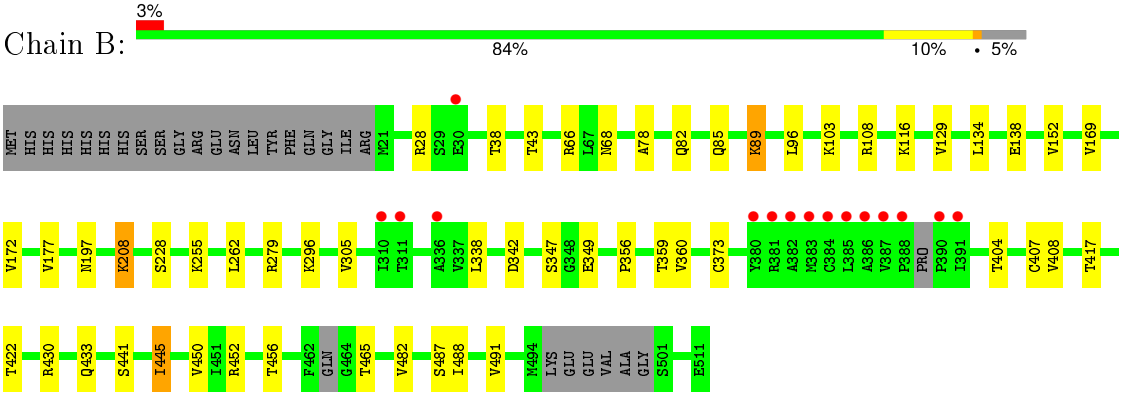
- Molecule 1: Pyruvate kinase

Chain A:



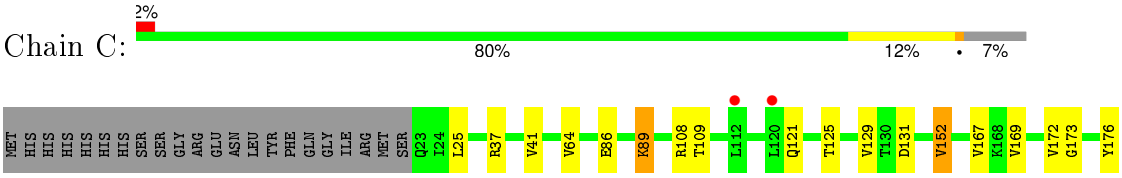
- Molecule 1: Pyruvate kinase

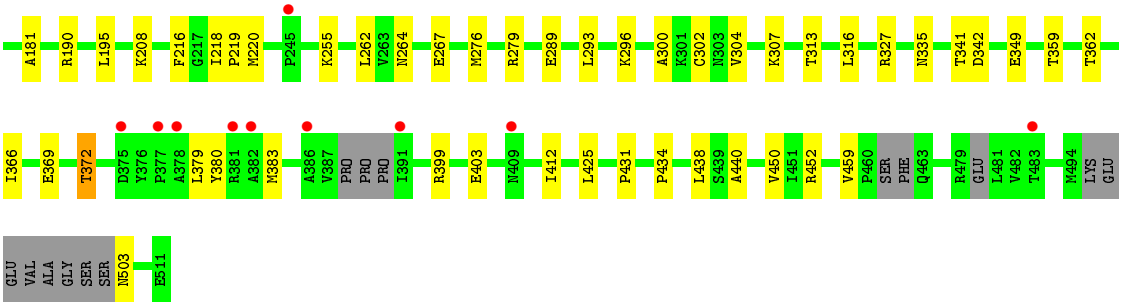
Chain B:



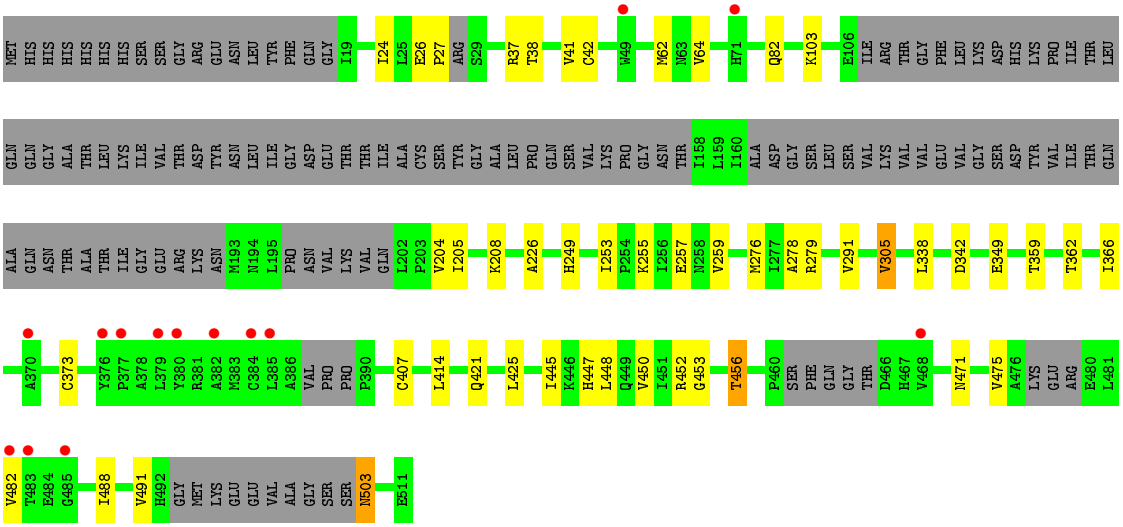
- Molecule 1: Pyruvate kinase

Chain C:





- Molecule 1: Pyruvate kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.04Å 130.68Å 113.85Å 90.00° 117.40° 90.00°	Depositor
Resolution (Å)	42.68 – 2.31 43.56 – 2.31	Depositor EDS
% Data completeness (in resolution range)	90.9 (42.68-2.31) 90.9 (43.56-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.253 0.201 , 0.246	Depositor DCC
R_{free} test set	5071 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.1	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 100883 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14040	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL

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	0.38	0/3514	0.56	0/4776
1	B	0.39	0/3668	0.55	0/4982
1	C	0.39	0/3557	0.57	1/4833 (0.0%)
1	D	0.41	1/2826 (0.0%)	0.54	0/3836
All	All	0.39	1/13565 (0.0%)	0.56	1/18427 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	GLN	CG-CD	9.57	1.73	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	89	LYS	CB-CG-CD	5.27	125.31	111.60

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	3464	0	3431	37	0
1	B	3617	0	3647	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3510	0	3492	31	0
1	D	2792	0	2759	29	0
2	B	12	0	16	9	0
2	C	6	0	8	0	0
3	A	166	0	0	0	0
3	B	195	0	0	2	0
3	C	190	0	0	3	0
3	D	88	0	0	1	0
All	All	14040	0	13353	124	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 5.

All (124) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ILE:HG23	1:B:456:THR:HG21	1.35	1.07
1:B:66:ARG:HH12	2:B:512:GOL:H32	1.12	1.05
1:B:43:THR:HG21	2:B:512:GOL:H11	1.49	0.95
1:B:347:SER:HB3	2:B:512:GOL:H31	1.50	0.93
1:B:152:VAL:CG1	1:B:169:VAL:HG21	2.03	0.88
1:D:42:CYS:HB2	1:D:62:MET:HE3	1.57	0.86
1:D:445:ILE:HG23	1:D:456:THR:HG21	1.60	0.83
1:B:152:VAL:HG11	1:B:169:VAL:HG21	1.60	0.83
1:B:66:ARG:NH1	2:B:512:GOL:H32	1.94	0.80
1:B:68:ASN:HD22	2:B:512:GOL:H12	1.48	0.77
1:B:172:VAL:HG12	1:B:177:VAL:HG22	1.65	0.77
1:C:255:LYS:HD2	1:C:276:MET:SD	2.26	0.75
1:B:68:ASN:ND2	2:B:512:GOL:H12	2.04	0.73
1:A:54:LEU:HD21	1:A:84:ILE:HD13	1.69	0.73
1:C:129:VAL:HG12	1:C:131:ASP:H	1.55	0.69
1:B:78:ALA:O	1:B:82:GLN:HG2	1.94	0.68
1:B:28:ARG:NE	1:B:28:ARG:HA	2.10	0.67
1:B:68:ASN:HD22	2:B:512:GOL:C1	2.08	0.66
1:A:315:MET:HE3	1:A:333:VAL:HG22	1.78	0.66
1:B:43:THR:CG2	2:B:512:GOL:H11	2.26	0.65
1:A:152:VAL:CG1	1:A:169:VAL:HG21	2.28	0.63
1:D:42:CYS:HB2	1:D:62:MET:CE	2.29	0.63
1:C:362:THR:O	1:C:366:ILE:HG12	2.00	0.62
1:A:106:GLU:OE2	1:A:108:ARG:NH1	2.32	0.62
1:A:172:VAL:HG12	1:A:177:VAL:HG22	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:SER:O	1:B:445:ILE:HD12	2.00	0.60
1:B:482:VAL:HG11	1:B:488:ILE:HD11	1.84	0.60
1:C:293:LEU:HD12	1:D:373:CYS:SG	2.42	0.59
1:C:300:ALA:O	1:C:304:VAL:HG23	2.03	0.59
1:B:430:ARG:NH1	3:B:708:HOH:O	2.33	0.58
1:B:338:LEU:HD21	1:B:373:CYS:HB2	1.86	0.57
1:B:129:VAL:HG21	1:B:134:LEU:HD13	1.87	0.56
1:A:152:VAL:HG21	1:A:158:ILE:HD11	1.87	0.56
1:B:28:ARG:HE	1:B:28:ARG:HA	1.69	0.56
1:C:296:LYS:HE2	1:D:338:LEU:HD13	1.88	0.55
1:A:152:VAL:HG13	1:A:169:VAL:HG21	1.89	0.55
1:B:66:ARG:HH12	2:B:512:GOL:C3	2.04	0.55
1:B:305:VAL:HG12	1:B:305:VAL:O	2.07	0.55
1:C:37:ARG:NH1	1:C:431:PRO:O	2.37	0.55
1:A:157:THR:O	1:A:196:PRO:HD2	2.07	0.55
1:D:37:ARG:HE	1:D:453:GLY:HA2	1.71	0.55
1:C:503:ASN:N	3:C:574:HOH:O	2.40	0.54
1:A:327:ARG:HD2	3:B:608:HOH:O	2.08	0.53
1:D:204:VAL:HG12	1:D:205:ILE:HD12	1.90	0.53
1:A:152:VAL:HG11	1:A:169:VAL:HG21	1.90	0.52
1:D:342:ASP:HA	1:D:452:ARG:HB2	1.91	0.52
1:A:70:SER:HA	1:A:103:LYS:HG3	1.92	0.52
1:A:103:LYS:HD2	1:A:208:LYS:HE2	1.91	0.52
1:B:349:GLU:HB3	1:B:359:THR:HG21	1.93	0.51
1:C:342:ASP:HA	1:C:452:ARG:HB2	1.93	0.51
1:B:342:ASP:HA	1:B:452:ARG:HB2	1.93	0.50
1:D:362:THR:O	1:D:366:ILE:HG12	2.11	0.50
1:A:38:THR:HA	1:A:452:ARG:HG3	1.92	0.50
1:A:296:LYS:HE2	1:B:338:LEU:CD1	2.43	0.49
1:A:255:LYS:HD2	1:A:276:MET:SD	2.52	0.49
1:A:467:HIS:CG	1:A:468:VAL:H	2.30	0.49
1:C:304:VAL:HA	1:C:383:MET:HE2	1.93	0.49
1:A:109:THR:O	1:A:190:ARG:HA	2.12	0.49
1:C:412:ILE:HG22	1:C:434:PRO:HB2	1.94	0.49
1:C:152:VAL:HG13	1:C:169:VAL:HG21	1.94	0.49
1:D:349:GLU:HB3	1:D:359:THR:HG21	1.95	0.49
1:C:369:GLU:O	1:C:372:THR:HB	2.13	0.49
1:A:338:LEU:HD13	1:B:296:LYS:HE2	1.95	0.49
1:A:296:LYS:HE2	1:B:338:LEU:HD13	1.95	0.48
1:C:173:GLY:HA3	1:C:176:TYR:CE1	2.49	0.48
1:A:337:VAL:O	1:A:452:ARG:NH2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:349:GLU:HB3	1:C:359:THR:HG21	1.94	0.48
1:A:365:ARG:O	1:A:369:GLU:HG2	2.14	0.48
1:A:349:GLU:HB3	1:A:359:THR:HG21	1.96	0.48
1:A:338:LEU:HD21	1:A:373:CYS:HB2	1.96	0.47
1:C:293:LEU:HD23	1:D:24:ILE:HG23	1.95	0.47
1:A:41:VAL:HB	1:A:345:MET:HG3	1.96	0.47
1:C:380:TYR:CZ	1:C:403:GLU:HG3	2.50	0.47
1:C:289:GLU:HB3	1:D:366:ILE:HD13	1.96	0.47
1:C:440:ALA:HA	1:C:459:VAL:O	2.14	0.47
1:C:327:ARG:HG3	1:D:291:VAL:HB	1.97	0.47
1:A:80:THR:O	1:A:84:ILE:HG12	2.15	0.46
1:B:85:GLN:O	1:B:89:LYS:HG2	2.16	0.46
1:A:355:PHE:HB3	1:A:358:ILE:HB	1.96	0.46
1:A:315:MET:HE2	1:A:344:VAL:HB	1.97	0.46
1:A:438:LEU:HD23	1:A:457:MET:HB3	1.98	0.46
1:D:503:ASN:N	1:D:503:ASN:OD1	2.49	0.45
1:A:440:ALA:HB2	1:A:461:SER:HB3	1.97	0.45
1:C:167:VAL:HG12	1:C:181:ALA:HA	1.99	0.45
1:B:404:THR:O	1:B:408:VAL:HG22	2.17	0.45
1:D:38:THR:HA	1:D:452:ARG:HG3	1.99	0.45
1:C:86:GLU:HG2	3:C:566:HOH:O	2.17	0.45
1:B:169:VAL:HG13	1:B:177:VAL:HG13	1.98	0.44
1:D:226:ALA:HA	1:D:253:ILE:O	2.17	0.44
1:B:38:THR:HA	1:B:452:ARG:HG3	1.99	0.44
1:D:255:LYS:HG2	1:D:276:MET:HB3	2.00	0.43
1:A:118:ILE:HB	1:A:138:GLU:HG3	2.01	0.43
1:C:264:ASN:O	1:C:267:GLU:HG2	2.18	0.43
1:D:421:GLN:O	1:D:425:LEU:HB2	2.17	0.43
1:A:64:VAL:HG22	1:A:97:ALA:HB3	2.01	0.43
1:A:369:GLU:O	1:A:372:THR:HB	2.18	0.43
1:A:226:ALA:HA	1:A:253:ILE:O	2.18	0.43
1:B:356:PRO:O	1:B:360:VAL:HG23	2.19	0.43
1:A:324:ARG:HE	1:A:324:ARG:HB3	1.70	0.43
1:D:338:LEU:HD21	1:D:373:CYS:HB2	1.99	0.42
1:D:482:VAL:HG11	1:D:488:ILE:HD11	2.01	0.42
1:C:302:CYS:HB3	1:C:307:LYS:O	2.19	0.42
1:B:305:VAL:CG1	1:B:305:VAL:O	2.66	0.42
1:D:103:LYS:HD2	1:D:208:LYS:HE3	2.01	0.42
1:C:216:PHE:O	1:C:220:MET:HB2	2.19	0.42
1:B:228:SER:HA	1:B:255:LYS:HD3	2.01	0.42
1:A:218:ILE:HB	1:A:219:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:HG23	1:A:456:THR:HG21	2.02	0.42
1:C:293:LEU:CD1	1:D:373:CYS:SG	3.08	0.42
1:B:103:LYS:HD3	1:B:208:LYS:HE2	2.02	0.42
1:C:335:ASN:HB3	3:C:663:HOH:O	2.18	0.42
1:C:218:ILE:HB	1:C:219:PRO:HD3	2.01	0.41
1:D:26:GLU:HA	1:D:27:PRO:HD3	1.87	0.41
1:D:249:HIS:O	1:D:447:HIS:NE2	2.51	0.41
1:D:257:GLU:HG2	1:D:278:ALA:HB3	2.02	0.41
1:D:305:VAL:HG22	3:D:594:HOH:O	2.19	0.41
1:A:148:LEU:HB3	1:A:149:PRO:HD3	2.03	0.41
1:C:109:THR:O	1:C:190:ARG:HA	2.20	0.41
1:C:41:VAL:HG22	1:C:64:VAL:HB	2.02	0.40
1:C:25:LEU:HD21	1:D:259:VAL:HG13	2.04	0.40
1:B:116:LYS:HD2	1:B:116:LYS:HA	1.88	0.40
1:D:471:ASN:O	1:D:475:VAL:HG23	2.21	0.40
1:D:41:VAL:HG22	1:D:64:VAL:HB	2.04	0.40
1:B:417:THR:HB	1:B:422:THR:HB	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	461/511 (90%)	449 (97%)	11 (2%)	1 (0%)	52 64
1	B	477/511 (93%)	471 (99%)	6 (1%)	0	100 100
1	C	466/511 (91%)	454 (97%)	11 (2%)	1 (0%)	52 64
1	D	364/511 (71%)	357 (98%)	7 (2%)	0	100 100
All	All	1768/2044 (86%)	1731 (98%)	35 (2%)	2 (0%)	56 68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	THR
1	C	313	THR

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	355/428 (83%)	342 (96%)	13 (4%)	41	55
1	B	385/428 (90%)	370 (96%)	15 (4%)	39	53
1	C	362/428 (85%)	344 (95%)	18 (5%)	30	41
1	D	283/428 (66%)	274 (97%)	9 (3%)	46	62
All	All	1385/1712 (81%)	1330 (96%)	55 (4%)	38	52

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	108	ARG
1	A	119	THR
1	A	140	THR
1	A	279	ARG
1	A	305	VAL
1	A	407	CYS
1	A	408	VAL
1	A	425	LEU
1	A	433	GLN
1	A	450	VAL
1	A	491	VAL
1	A	509	THR
1	B	89	LYS
1	B	96	LEU
1	B	108	ARG
1	B	138	GLU
1	B	197	ASN
1	B	208	LYS
1	B	262	LEU

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Mol	Chain	Res	Type
1	B	279	ARG
1	B	407	CYS
1	B	433	GLN
1	B	445	ILE
1	B	450	VAL
1	B	465	THR
1	B	487	SER
1	B	491	VAL
1	C	89	LYS
1	C	108	ARG
1	C	121	GLN
1	C	125	THR
1	C	152	VAL
1	C	172	VAL
1	C	195	LEU
1	C	208	LYS
1	C	262	LEU
1	C	279	ARG
1	C	316	LEU
1	C	341	THR
1	C	372	THR
1	C	379	LEU
1	C	399	ARG
1	C	425	LEU
1	C	438	LEU
1	C	450	VAL
1	D	279	ARG
1	D	305	VAL
1	D	407	CYS
1	D	414	LEU
1	D	448	LEU
1	D	450	VAL
1	D	456	THR
1	D	491	VAL
1	D	503	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	215	ASN
1	A	449	GLN

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Mol	Chain	Res	Type
1	B	121	GLN
1	B	211	HIS
1	B	215	ASN
1	B	492	HIS
1	C	36	HIS
1	C	82	GLN
1	C	121	GLN
1	C	197	ASN
1	C	335	ASN
1	C	449	GLN
1	D	36	HIS
1	D	215	ASN
1	D	503	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

3 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	GOL	B	512	-	5,5,5	0.31	0	5,5,5	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	B	513	-	5,5,5	0.33	0	5,5,5	0.36	0
2	GOL	C	512	-	5,5,5	0.32	0	5,5,5	0.21	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	GOL	B	512	-	-	0/4/4/4	0/0/0/0
2	GOL	B	513	-	-	0/4/4/4	0/0/0/0
2	GOL	C	512	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	512	GOL	9	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, 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	472/511 (92%)	0.26	27 (5%)	27	36	30, 35, 41, 47	12 (2%)
1	B	483/511 (94%)	0.15	15 (3%)	52	61	30, 35, 39, 44	9 (1%)
1	C	475/511 (92%)	0.07	12 (2%)	61	69	30, 35, 40, 42	13 (2%)
1	D	382/511 (74%)	0.15	14 (3%)	45	54	30, 35, 41, 53	15 (3%)
All	All	1812/2044 (88%)	0.16	68 (3%)	44	53	30, 35, 40, 53	49 (2%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	385	LEU	7.8
1	A	49	TRP	5.0
1	D	377	PRO	4.6
1	D	380	TYR	4.1
1	D	382	ALA	4.0
1	C	409	ASN	4.0
1	A	390	PRO	3.9
1	A	50	ASN	3.9
1	D	385	LEU	3.8
1	B	390	PRO	3.8
1	B	391	ILE	3.8
1	A	245	PRO	3.6
1	A	389	PRO	3.5
1	D	376	TYR	3.5
1	A	55	VAL	3.4
1	D	485	GLY	3.4
1	C	377	PRO	3.4
1	C	391	ILE	3.3
1	A	53	THR	3.2
1	D	483	THR	3.2
1	D	49	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	370	ALA	2.9
1	B	380	TYR	2.9
1	B	386	ALA	2.8
1	A	140	THR	2.8
1	A	385	LEU	2.8
1	A	51	VAL	2.7
1	C	112	LEU	2.7
1	A	82	GLN	2.7
1	B	382	ALA	2.6
1	A	92	PRO	2.6
1	B	381	ARG	2.6
1	B	388	PRO	2.5
1	A	181	ALA	2.5
1	A	459	VAL	2.5
1	A	460	PRO	2.5
1	B	383	MET	2.5
1	D	379	LEU	2.5
1	D	71	HIS	2.4
1	D	384	CYS	2.4
1	B	310	ILE	2.4
1	A	409	ASN	2.4
1	C	245	PRO	2.4
1	D	482	VAL	2.4
1	C	386	ALA	2.4
1	A	381	ARG	2.4
1	B	384	CYS	2.3
1	A	118	ILE	2.2
1	A	29	SER	2.2
1	C	483	THR	2.2
1	C	378	ALA	2.2
1	D	370	ALA	2.2
1	B	336	ALA	2.2
1	A	120	LEU	2.2
1	C	382	ALA	2.2
1	A	58	ILE	2.1
1	C	375	ASP	2.1
1	A	54	LEU	2.1
1	D	468	VAL	2.1
1	A	52	ASP	2.1
1	A	355	PHE	2.1
1	A	119	THR	2.1
1	A	244	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	387	VAL	2.1
1	B	311	THR	2.0
1	C	120	LEU	2.0
1	B	30	GLU	2.0
1	C	381	ARG	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
2	GOL	B	513	6/6	0.89	0.26	2.67	66,67,67,67	0
2	GOL	B	512	6/6	0.85	0.19	0.33	40,41,43,43	0
2	GOL	C	512	6/6	0.73	0.33	-	80,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.