Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:44 AM GMT

PDB ID	:	2Y5Y
Title	:	CRYSTAL STRUCTURE OF LACY IN COMPLEX WITH AN AFFINITY INACTIVATOR
Authors	:	Chaptal, V.; Kwon, S.; Sawaya, M.R.; Guan, L.; Kaback, H.R.; Abramson, J.
Deposited on	:	2011-01-19
Resolution	:	3.38 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:

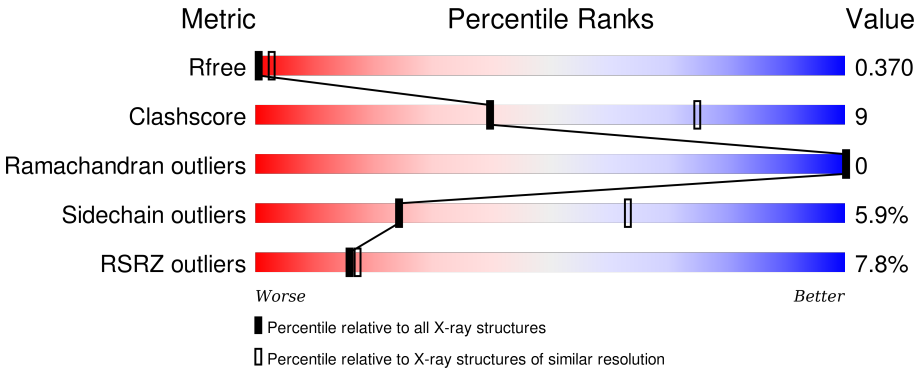
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.38 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	1084 (3.46-3.30)
Clashscore	102246	1158 (3.46-3.30)
Ramachandran outliers	100387	1139 (3.46-3.30)
Sidechain outliers	100360	1138 (3.46-3.30)
RSRZ outliers	91569	1089 (3.46-3.30)

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	423	8% 71% 18% • 9%
1	B	423	7% 73% 19% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6209 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 LACTOSE PERMEASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3065	2086	466	498	15			
1	B	394	Total	C	N	O	S	0	0	0
			3112	2114	475	508	15			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	SER	CYS	ENGINEERED MUTATION	UNP P02920
A	122	CYS	ALA	ENGINEERED MUTATION	UNP P02920
A	148	ALA	CYS	ENGINEERED MUTATION	UNP P02920
A	154	VAL	CYS	ENGINEERED MUTATION	UNP P02920
A	176	MET	CYS	ENGINEERED MUTATION	UNP P02920
A	234	SER	CYS	ENGINEERED MUTATION	UNP P02920
A	333	SER	CYS	ENGINEERED MUTATION	UNP P02920
A	353	ALA	CYS	ENGINEERED MUTATION	UNP P02920
A	355	ALA	CYS	ENGINEERED MUTATION	UNP P02920
A	418	HIS	-	EXPRESSION TAG	UNP P02920
A	419	HIS	-	EXPRESSION TAG	UNP P02920
A	420	HIS	-	EXPRESSION TAG	UNP P02920
A	421	HIS	-	EXPRESSION TAG	UNP P02920
A	422	HIS	-	EXPRESSION TAG	UNP P02920
A	423	HIS	-	EXPRESSION TAG	UNP P02920
B	117	SER	CYS	ENGINEERED MUTATION	UNP P02920
B	122	CYS	ALA	ENGINEERED MUTATION	UNP P02920
B	148	ALA	CYS	ENGINEERED MUTATION	UNP P02920
B	154	VAL	CYS	ENGINEERED MUTATION	UNP P02920
B	176	MET	CYS	ENGINEERED MUTATION	UNP P02920
B	234	SER	CYS	ENGINEERED MUTATION	UNP P02920
B	333	SER	CYS	ENGINEERED MUTATION	UNP P02920
B	353	ALA	CYS	ENGINEERED MUTATION	UNP P02920
B	355	ALA	CYS	ENGINEERED MUTATION	UNP P02920
B	418	HIS	-	EXPRESSION TAG	UNP P02920

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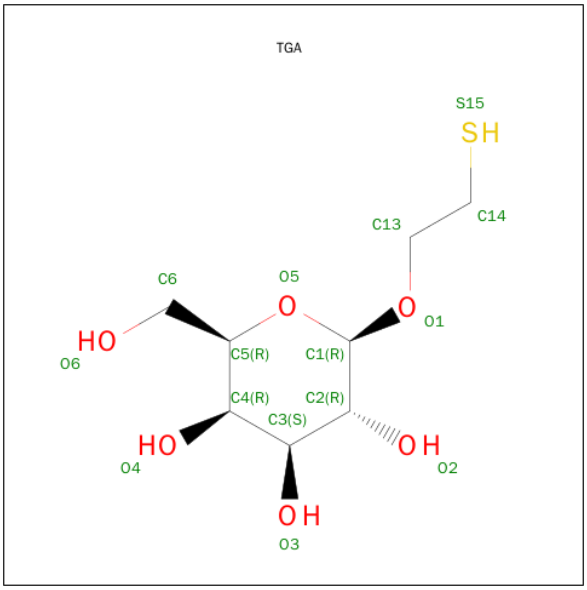
Chain	Residue	Modelled	Actual	Comment	Reference
B	419	HIS	-	EXPRESSION TAG	UNP P02920
B	420	HIS	-	EXPRESSION TAG	UNP P02920
B	421	HIS	-	EXPRESSION TAG	UNP P02920
B	422	HIS	-	EXPRESSION TAG	UNP P02920
B	423	HIS	-	EXPRESSION TAG	UNP P02920

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ba 1 1	0	0
2	A	1	Total Ba 1 1	0	0

- Molecule 3 is METHANETHIOSULFONYL-GALACTOSIDE (three-letter code: TGA) (formula: $C_8H_{16}O_6S$).



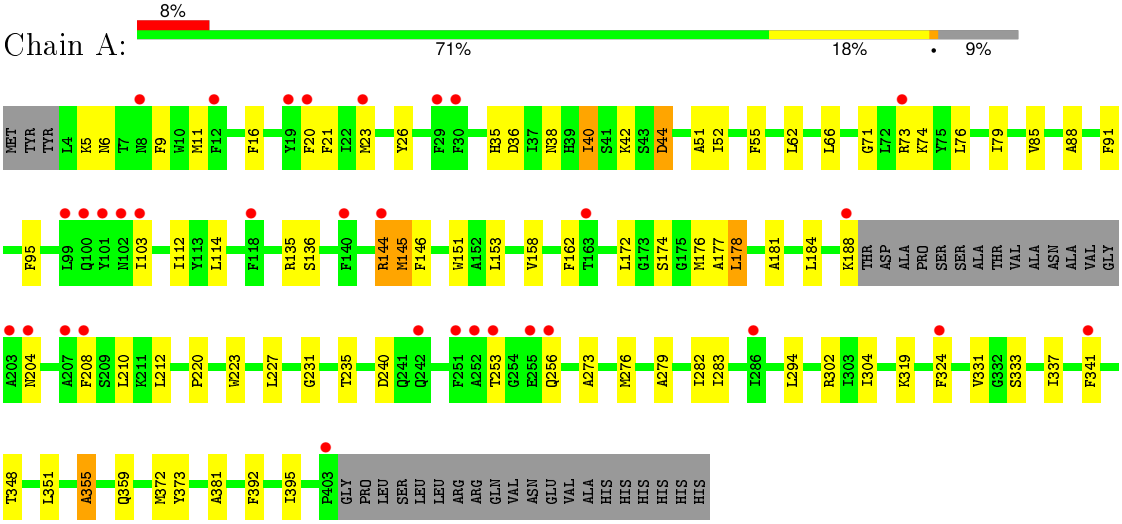
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 15 8 6 1	0	0
3	B	1	Total C O S 15 8 6 1	0	0

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.

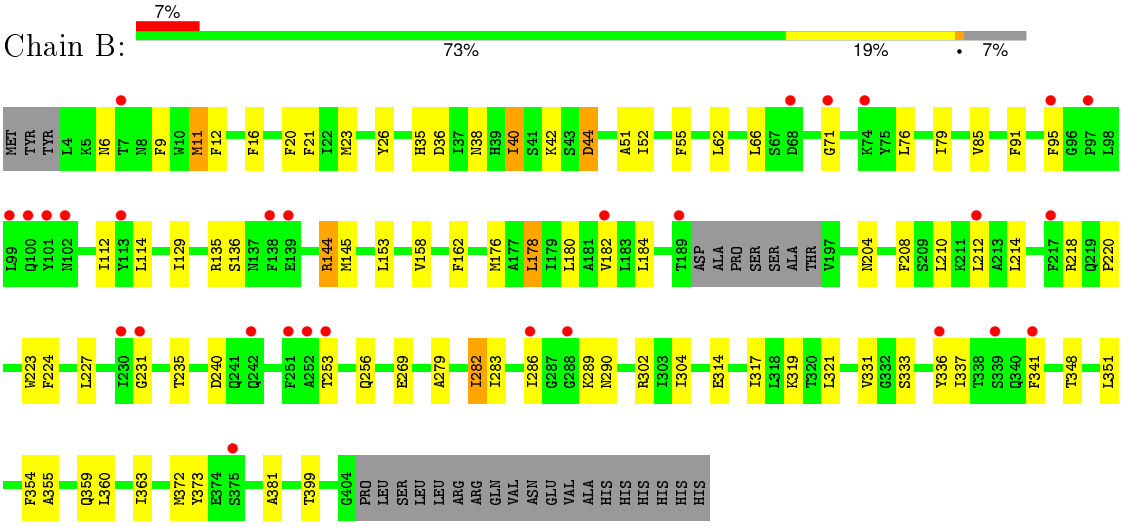
- Molecule 1: LACTOSE PERMEASE

Chain A:



- Molecule 1: LACTOSE PERMEASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	102.56Å 127.84Å 189.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.28 – 3.38 45.12 – 3.38	Depositor EDS
% Data completeness (in resolution range)	(Not available) (28.28-3.38) 98.4 (45.12-3.38)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.286 , 0.303 0.363 , 0.370	Depositor DCC
R_{free} test set	1759 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	105.2	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 73.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 35081 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	6209	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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: TGA, BA

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	0.43	0/3157	0.73	7/4273 (0.2%)
1	B	0.43	0/3204	0.72	5/4338 (0.1%)
All	All	0.43	0/6361	0.72	12/8611 (0.1%)

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

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

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	135	ARG	CB-CA-C	8.80	127.99	110.40
1	A	135	ARG	CB-CA-C	8.18	126.76	110.40
1	B	136	SER	N-CA-CB	-7.85	98.72	110.50
1	A	36	ASP	CB-CA-C	7.69	125.79	110.40
1	A	136	SER	N-CA-CB	-7.32	99.53	110.50
1	B	36	ASP	CB-CA-C	6.64	123.69	110.40
1	A	145	MET	CB-CA-C	6.56	123.53	110.40
1	A	324	PHE	CB-CA-C	6.10	122.60	110.40
1	A	355	ALA	CB-CA-C	5.84	118.87	110.10
1	B	11	MET	CB-CA-C	5.82	122.05	110.40
1	B	354	PHE	CB-CA-C	5.32	121.04	110.40
1	A	103	ILE	N-CA-C	-5.12	97.17	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	B	144	ARG	Sidechain

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	3065	0	3112	52	0
1	B	3112	0	3159	58	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	15	1	0
3	B	15	0	15	3	0
All	All	6209	0	6301	110	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 9.

All (110) 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:55:PHE:HB2	1:B:112:ILE:HG21	1.41	1.02
1:A:55:PHE:HB2	1:A:112:ILE:HG21	1.41	0.99
1:A:55:PHE:CD2	1:A:112:ILE:HG22	2.10	0.87
1:B:55:PHE:CD2	1:B:112:ILE:HG22	2.12	0.85
1:B:253:THR:OG1	1:B:256:GLN:HG2	1.77	0.84
1:A:253:THR:OG1	1:A:256:GLN:HG2	1.77	0.84
1:A:55:PHE:CB	1:A:112:ILE:HG21	2.16	0.74
1:B:55:PHE:CB	1:B:112:ILE:HG21	2.16	0.74
1:B:11:MET:O	1:B:184:LEU:HD22	1.89	0.73
1:B:66:LEU:HD23	1:B:71:GLY:HA3	1.70	0.72
1:B:231:GLY:O	1:B:235:THR:OG1	2.06	0.72
1:A:66:LEU:HD23	1:A:71:GLY:HA3	1.71	0.72
1:B:55:PHE:HB2	1:B:112:ILE:CG2	2.19	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PHE:HB2	1:A:112:ILE:CG2	2.19	0.69
1:A:55:PHE:CB	1:A:112:ILE:CG2	2.70	0.69
1:A:231:GLY:O	1:A:235:THR:OG1	2.06	0.69
1:A:55:PHE:CG	1:A:112:ILE:HG22	2.27	0.68
1:B:55:PHE:CB	1:B:112:ILE:CG2	2.71	0.68
1:A:51:ALA:CB	1:A:112:ILE:HD13	2.24	0.68
1:B:51:ALA:CB	1:B:112:ILE:HD13	2.23	0.68
1:A:355:ALA:O	1:A:359:GLN:HG2	1.95	0.67
1:B:55:PHE:CG	1:B:112:ILE:HG22	2.29	0.66
1:B:51:ALA:HB1	1:B:112:ILE:HD13	1.79	0.64
1:A:172:LEU:O	1:A:176:MET:HG2	1.99	0.63
1:B:224:PHE:HB3	1:B:399:THR:HB	1.80	0.63
1:B:224:PHE:CG	1:B:399:THR:O	2.52	0.63
1:A:55:PHE:CG	1:A:112:ILE:CG2	2.82	0.62
1:B:224:PHE:CD2	1:B:399:THR:O	2.52	0.62
1:A:51:ALA:HB1	1:A:112:ILE:HD13	1.80	0.62
1:B:178:LEU:O	1:B:182:VAL:HG22	2.00	0.62
1:B:55:PHE:CG	1:B:112:ILE:CG2	2.83	0.61
1:B:282:ILE:HG22	1:B:286:ILE:HD11	1.82	0.61
1:B:52:ILE:HA	1:B:112:ILE:HG12	1.82	0.60
1:A:52:ILE:HA	1:A:112:ILE:HG12	1.83	0.60
1:A:74:LYS:HE3	1:A:188:LYS:HD3	1.84	0.60
1:A:208:PHE:HB2	1:A:348:THR:HG23	1.83	0.59
1:B:355:ALA:O	1:B:359:GLN:HG2	2.04	0.58
1:B:208:PHE:HB2	1:B:348:THR:HG23	1.85	0.57
1:B:20:PHE:HA	1:B:23:MET:HB3	1.86	0.57
1:A:151:TRP:CG	3:A:701:TGA:H61C	2.40	0.57
1:A:20:PHE:HA	1:A:23:MET:HB3	1.86	0.57
1:A:114:LEU:O	1:A:114:LEU:HD23	2.05	0.56
1:A:35:HIS:HD2	1:A:42:LYS:HE3	1.71	0.56
1:B:35:HIS:HD2	1:B:42:LYS:HE3	1.71	0.56
1:B:302:ARG:HH21	1:B:319:LYS:HA	1.69	0.56
1:A:11:MET:O	1:A:184:LEU:HD22	2.07	0.55
1:A:144:ARG:HH11	1:A:145:MET:HE1	1.74	0.53
1:A:21:PHE:CE1	1:A:176:MET:HG3	2.45	0.52
1:A:392:PHE:HA	1:A:395:ILE:HG22	1.93	0.51
1:A:181:ALA:HA	1:A:184:LEU:HD12	1.93	0.51
1:A:279:ALA:O	1:A:283:ILE:HG12	2.11	0.51
1:B:40:ILE:HG23	1:B:44:ASP:HB2	1.93	0.50
1:B:279:ALA:O	1:B:283:ILE:HG12	2.11	0.50
1:A:40:ILE:HG23	1:A:44:ASP:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ASN:HB2	1:B:9:PHE:HB3	1.94	0.49
1:B:283:ILE:HG13	1:B:331:VAL:HG13	1.94	0.49
1:B:114:LEU:O	1:B:114:LEU:HD23	2.12	0.49
1:A:88:ALA:H	1:A:174:SER:HB3	1.78	0.48
1:B:85:VAL:HG13	1:B:178:LEU:HD12	1.96	0.48
1:B:66:LEU:HD22	1:B:76:LEU:HD22	1.94	0.48
1:A:66:LEU:HD22	1:A:76:LEU:HD22	1.95	0.48
1:B:372:MET:HB3	1:B:381:ALA:HB2	1.96	0.48
1:A:112:ILE:O	1:A:112:ILE:CG2	2.62	0.48
1:A:283:ILE:HG13	1:A:331:VAL:HG13	1.95	0.48
1:A:372:MET:HB3	1:A:381:ALA:HB2	1.96	0.47
1:A:85:VAL:HG13	1:A:178:LEU:HD12	1.96	0.47
1:B:51:ALA:HB3	1:B:112:ILE:CD1	2.44	0.47
1:B:55:PHE:CB	1:B:112:ILE:HG22	2.44	0.47
1:A:55:PHE:CB	1:A:112:ILE:HG22	2.43	0.47
1:B:144:ARG:HD3	1:B:145:MET:HE2	1.97	0.47
1:A:51:ALA:HB3	1:A:112:ILE:CD1	2.45	0.46
1:A:273:ALA:HA	1:A:276:MET:HG2	1.97	0.46
1:B:112:ILE:O	1:B:112:ILE:CG2	2.62	0.46
1:A:220:PRO:HA	1:A:223:TRP:HD1	1.81	0.46
1:B:158:VAL:O	1:B:162:PHE:HB2	2.16	0.46
1:B:220:PRO:HA	1:B:223:TRP:HD1	1.80	0.45
1:A:66:LEU:HD22	1:A:76:LEU:HD13	1.99	0.45
1:A:158:VAL:O	1:A:162:PHE:HB2	2.17	0.45
1:B:51:ALA:CB	1:B:112:ILE:CD1	2.93	0.44
1:B:21:PHE:CE1	1:B:176:MET:HG3	2.52	0.44
1:A:51:ALA:CB	1:A:112:ILE:CD1	2.94	0.44
1:A:337:ILE:HA	1:A:341:PHE:HD2	1.83	0.44
1:B:337:ILE:HA	1:B:341:PHE:HD2	1.83	0.44
1:B:286:ILE:HG22	1:B:290:ASN:HB2	2.00	0.44
1:B:42:LYS:HB3	1:B:373:TYR:HB2	1.99	0.44
1:A:333:SER:O	1:A:337:ILE:HG12	2.18	0.43
1:B:253:THR:H	1:B:256:GLN:HB2	1.83	0.43
1:B:333:SER:O	1:B:337:ILE:HG12	2.19	0.43
1:A:302:ARG:HH21	1:A:319:LYS:HA	1.84	0.43
1:A:253:THR:H	1:A:256:GLN:HB2	1.83	0.43
1:A:6:ASN:HB2	1:A:9:PHE:HB3	2.00	0.43
1:B:66:LEU:HD22	1:B:76:LEU:HD13	2.01	0.43
1:A:42:LYS:HB3	1:A:373:TYR:HB2	2.00	0.43
1:B:20:PHE:HZ	3:B:801:TGA:H142	1.84	0.43
1:B:269:GLU:OE1	3:B:801:TGA:H4	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ARG:O	1:A:74:LYS:HG2	2.19	0.42
1:B:176:MET:SD	1:B:180:LEU:CD1	3.07	0.42
1:B:214:LEU:HD23	1:B:218:ARG:HH21	1.84	0.42
1:A:91:PHE:HA	1:A:95:PHE:HB3	2.02	0.42
1:B:91:PHE:HA	1:B:95:PHE:HB3	2.02	0.42
1:A:76:LEU:HA	1:A:79:ILE:HD12	2.02	0.41
1:A:66:LEU:CD2	1:A:71:GLY:HA3	2.47	0.41
1:B:20:PHE:CZ	3:B:801:TGA:H142	2.55	0.41
1:B:282:ILE:O	1:B:286:ILE:HG13	2.21	0.41
1:B:76:LEU:HA	1:B:79:ILE:HD12	2.02	0.41
1:B:289:LYS:HG2	1:B:336:TYR:HE1	1.85	0.41
1:B:66:LEU:CD2	1:B:71:GLY:HA3	2.46	0.40
1:A:177:ALA:O	1:A:181:ALA:HB3	2.21	0.40
1:B:12:PHE:CD1	1:B:129:ILE:HG12	2.55	0.40
1:B:360:LEU:HA	1:B:363:ILE:HD12	2.02	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	382/423 (90%)	359 (94%)	23 (6%)	0	100	100
1	B	390/423 (92%)	365 (94%)	25 (6%)	0	100	100
All	All	772/846 (91%)	724 (94%)	48 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	320/350 (91%)	301 (94%)	19 (6%)	24	63
1	B	324/350 (93%)	305 (94%)	19 (6%)	24	63
All	All	644/700 (92%)	606 (94%)	38 (6%)	24	63

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	16	PHE
1	A	26	TYR
1	A	38	ASN
1	A	40	ILE
1	A	44	ASP
1	A	62	LEU
1	A	146	PHE
1	A	153	LEU
1	A	178	LEU
1	A	204	ASN
1	A	210	LEU
1	A	212	LEU
1	A	227	LEU
1	A	240	ASP
1	A	282	ILE
1	A	294	LEU
1	A	304	ILE
1	A	351	LEU
1	B	16	PHE
1	B	26	TYR
1	B	38	ASN
1	B	40	ILE
1	B	44	ASP
1	B	62	LEU
1	B	153	LEU
1	B	178	LEU
1	B	204	ASN
1	B	210	LEU
1	B	212	LEU
1	B	227	LEU

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Mol	Chain	Res	Type
1	B	240	ASP
1	B	282	ILE
1	B	304	ILE
1	B	314	GLU
1	B	317	ILE
1	B	321	LEU
1	B	351	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	137	ASN
1	A	241	GLN
1	A	290	ASN
1	A	379	GLN
1	B	8	ASN
1	B	35	HIS
1	B	137	ASN
1	B	241	GLN
1	B	272	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)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	TGA	A	701	1	15,15,15	0.90	1 (6%)	20,20,20	1.10	2 (10%)
3	TGA	B	801	1	15,15,15	0.76	0	20,20,20	1.22	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TGA	A	701	1	-	0/6/26/26	0/1/1/1
3	TGA	B	801	1	-	0/6/26/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	TGA	O1-C1	2.59	1.44	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	801	TGA	C13-O1-C1	-2.87	108.93	113.94
3	B	801	TGA	C1-O5-C5	-2.07	109.73	113.75
3	B	801	TGA	O1-C1-C2	2.11	110.70	108.04
3	A	701	TGA	O5-C5-C6	2.46	112.58	106.36
3	A	701	TGA	O5-C1-C2	2.58	115.57	110.28
3	B	801	TGA	O5-C5-C6	3.27	114.61	106.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	TGA	1	0
3	B	801	TGA	3	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	386/423 (91%)	0.21	32 (8%)	14	15	113, 158, 207, 251	0
1	B	394/423 (93%)	0.32	29 (7%)	17	19	104, 160, 214, 264	0
All	All	780/846 (92%)	0.27	61 (7%)	16	17	104, 159, 212, 264	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	GLN	5.3
1	B	341	PHE	4.8
1	A	102	ASN	4.4
1	A	252	ALA	4.3
1	B	252	ALA	4.2
1	A	101	TYR	4.1
1	A	188	LYS	4.1
1	B	100	GLN	4.0
1	A	29	PHE	3.9
1	A	208	PHE	3.7
1	B	286	ILE	3.5
1	A	99	LEU	3.4
1	A	204	ASN	3.4
1	B	138	PHE	3.4
1	B	101	TYR	3.4
1	A	253	THR	3.4
1	A	286	ILE	3.3
1	B	99	LEU	3.3
1	A	19	TYR	3.2
1	A	12	PHE	3.2
1	A	163	THR	3.1
1	B	102	ASN	3.0
1	A	251	PHE	2.9
1	A	255	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	341	PHE	2.9
1	B	7	THR	2.8
1	B	189	THR	2.8
1	B	113	TYR	2.8
1	A	140	PHE	2.8
1	B	71	GLY	2.7
1	B	182	VAL	2.7
1	B	95	PHE	2.7
1	B	97	PRO	2.6
1	B	230	ILE	2.6
1	A	203	ALA	2.6
1	B	336	TYR	2.5
1	A	242	GLN	2.5
1	A	103	ILE	2.5
1	B	212	LEU	2.4
1	B	375	SER	2.4
1	B	68	ASP	2.4
1	B	253	THR	2.4
1	A	30	PHE	2.4
1	A	207	ALA	2.3
1	B	251	PHE	2.3
1	A	8	ASN	2.3
1	A	256	GLN	2.2
1	A	73	ARG	2.2
1	A	403	PRO	2.2
1	B	231	GLY	2.2
1	A	324	PHE	2.2
1	B	242	GLN	2.2
1	B	74	LYS	2.1
1	B	139	GLU	2.1
1	B	339	SER	2.1
1	A	23	MET	2.1
1	B	217	PHE	2.0
1	A	118	PHE	2.0
1	A	20	PHE	2.0
1	A	144	ARG	2.0
1	B	288	GLY	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	TGA	B	801	15/15	0.86	0.27	0.85	37,157,237,244	0
3	TGA	A	701	15/15	0.84	0.28	-0.07	121,167,242,253	0
2	BA	B	501	1/1	0.93	0.32	-	205,205,205,205	0
2	BA	A	501	1/1	0.76	0.32	-	232,232,232,232	0

6.5 Other polymers (i)

There are no such residues in this entry.