Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:07 PM GMT

PDB ID	:	4BL2
Title	:	Crystal structure of PBP2a clinical mutant E150K from MRSA
Authors	:	Otero, L.H.; Rojas-Altuve, A.; Hermoso, J.A.
Deposited on	:	2013-04-30
Resolution	:	2.72 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:

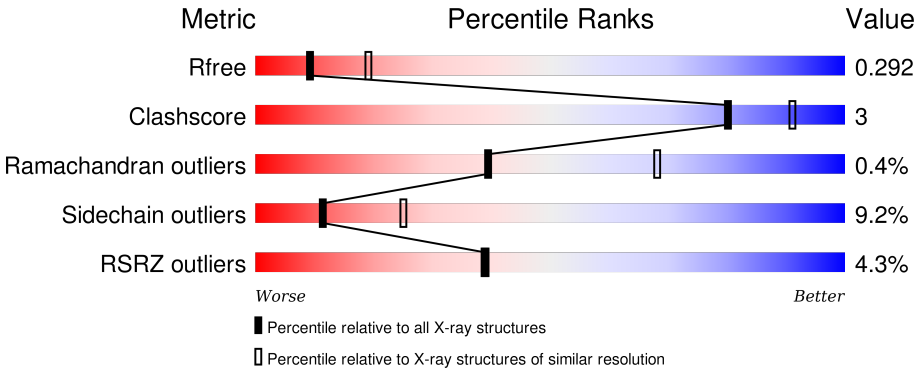
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.72 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	643	3% 83% 14%
1	B	643	6% 85% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10453 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 PENICILLIN BINDING PROTEIN 2 PRIME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			5114	3226	865	1008	15			
1	B	637	Total	C	N	O	S	0	0	0
			5112	3224	864	1009	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	150	LYS	GLU	ENGINEERED MUTATION	UNP Q54113
B	150	LYS	GLU	ENGINEERED MUTATION	UNP Q54113

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Cd	0	0
			3	3		
2	A	4	Total	Cd	0	0
			4	4		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		

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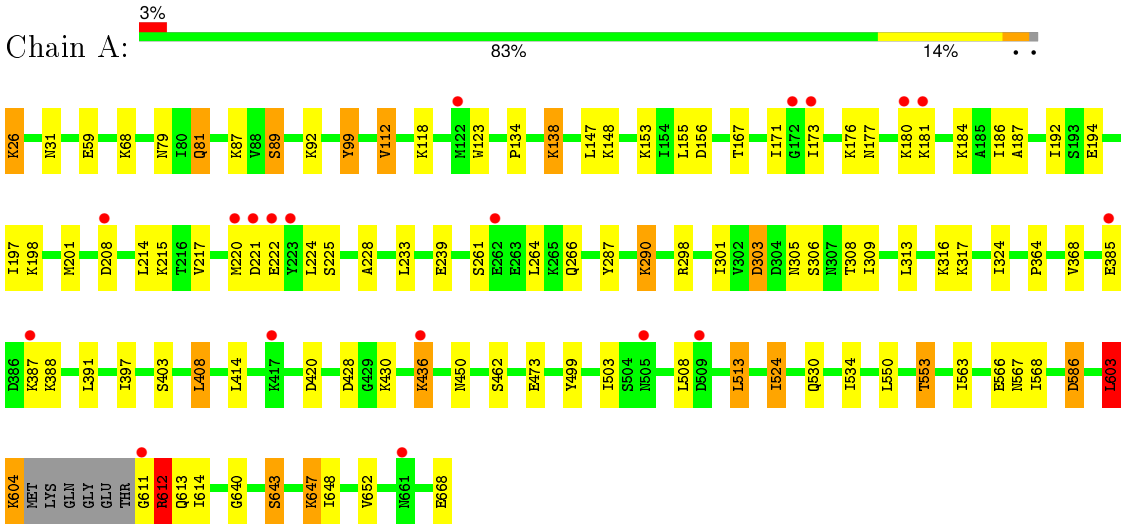
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	120	Total	O	0	0
			120	120		

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.

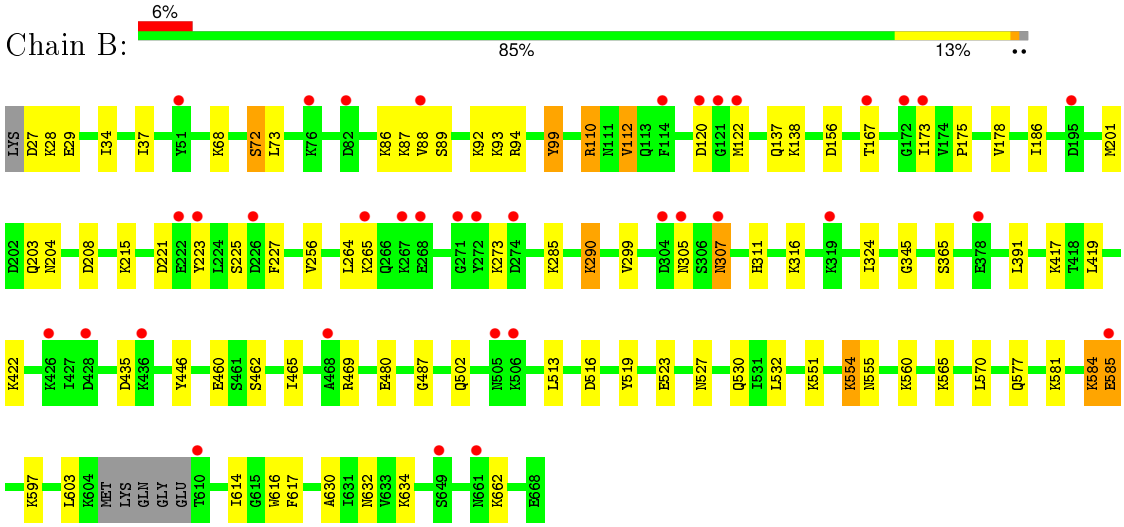
- Molecule 1: PENICILLIN BINDING PROTEIN 2 PRIME

Chain A:



- Molecule 1: PENICILLIN BINDING PROTEIN 2 PRIME

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	81.44Å 101.64Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.89 – 2.72 19.89 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.89-2.72) 99.1 (19.89-2.72)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.71Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.207 , 0.287 0.210 , 0.292	Depositor DCC
R_{free} test set	3004 reflections (7.72%)	DCC
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.883	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 41942 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10453	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: CL, CD

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	0.53	1/5199 (0.0%)	0.78	6/6988 (0.1%)
1	B	0.49	0/5197	0.69	0/6987
All	All	0.51	1/10396 (0.0%)	0.74	6/13975 (0.0%)

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	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	612	ARG	C-N	-13.40	1.03	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	612	ARG	O-C-N	-20.43	90.01	122.70
1	A	612	ARG	C-N-CA	14.24	157.30	121.70
1	A	612	ARG	CA-C-N	12.94	145.66	117.20
1	A	612	ARG	N-CA-C	-9.39	85.66	111.00
1	A	603	LEU	C-N-CA	6.06	136.86	121.70
1	A	26	LYS	C-N-CA	6.02	136.75	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	612	ARG	Mainchain,Peptide

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	5114	0	5122	44	0
1	B	5112	0	5117	29	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	96	0	0	1	0
4	B	120	0	0	0	0
All	All	10453	0	10239	69	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 (69) 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:A:603:LEU:HA	1:A:604:LYS:HB2	1.60	0.83
1:A:138:LYS:H	1:A:138:LYS:HD2	1.52	0.74
1:A:79:ASN:HB3	1:A:81:GLN:HE22	1.53	0.73
1:B:290:LYS:HB3	1:B:324:ILE:HD11	1.75	0.67
1:A:112:VAL:HG13	1:A:134:PRO:HB3	1.78	0.66
1:B:290:LYS:CB	1:B:324:ILE:HD11	2.29	0.62
1:A:176:LYS:HB2	1:A:176:LYS:HZ2	1.65	0.61
1:B:88:VAL:HG13	1:B:89:SER:H	1.65	0.60
1:B:186:ILE:HA	1:B:227:PHE:HZ	1.66	0.60
1:A:187:ALA:HA	1:A:192:ILE:HG13	1.83	0.60
1:B:290:LYS:HE3	1:B:324:ILE:HG12	1.83	0.59
1:B:110:ARG:NH2	1:B:311:HIS:CE1	2.71	0.58
1:A:436:LYS:HE3	1:A:436:LYS:H	1.69	0.57
1:A:603:LEU:CA	1:A:604:LYS:HB2	2.35	0.56
1:A:290:LYS:HB3	1:A:324:ILE:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ASP:HA	1:A:450:ASN:OD1	2.06	0.55
1:B:465:ILE:O	1:B:469:ARG:HG2	2.07	0.54
1:B:554:LYS:HE2	1:B:555:ASN:H	1.73	0.53
1:A:364:PRO:HG2	1:A:388:LYS:HB3	1.90	0.52
1:A:611:GLY:N	4:A:2082:HOH:O	2.41	0.52
1:A:186:ILE:HD12	1:A:233:LEU:HD11	1.91	0.52
1:A:397:ILE:HA	1:A:499:TYR:CD2	2.45	0.51
1:A:89:SER:HB3	1:A:92:LYS:HB2	1.92	0.51
1:B:89:SER:HB3	1:B:92:LYS:HB2	1.93	0.51
1:A:99:TYR:HD2	1:A:112:VAL:HG11	1.76	0.50
1:A:138:LYS:H	1:A:138:LYS:CD	2.20	0.50
1:B:516:ASP:HA	1:B:519:TYR:CE1	2.46	0.50
1:A:397:ILE:HA	1:A:499:TYR:HD2	1.75	0.50
1:B:614:ILE:HG22	1:B:634:LYS:HA	1.95	0.49
1:A:586:ASP:HB3	1:A:647:LYS:HG2	1.94	0.47
1:B:173:ILE:HG12	1:B:178:VAL:HG21	1.96	0.47
1:B:584:LYS:HG2	1:B:585:GLU:N	2.29	0.47
1:A:414:LEU:HD13	1:A:567:ASN:HB3	1.96	0.47
1:A:153:LYS:HD3	1:A:155:LEU:HD21	1.96	0.47
1:A:305:ASN:HB3	1:B:72:SER:HB2	1.96	0.47
1:A:217:VAL:HG21	1:A:224:LEU:HD13	1.95	0.46
1:A:503:ILE:HA	1:A:524:ILE:HG23	1.96	0.46
1:B:99:TYR:HB2	1:B:112:VAL:HG22	1.97	0.46
1:A:408:LEU:HD22	1:A:534:ILE:HG21	1.99	0.45
1:A:305:ASN:HB3	1:B:72:SER:CB	2.47	0.44
1:A:508:LEU:HD23	1:A:513:LEU:HD13	1.98	0.43
1:A:261:SER:HA	1:A:264:LEU:HD12	2.00	0.43
1:A:303:ASP:HB3	1:A:306:SER:HB2	2.00	0.43
1:A:176:LYS:HG3	1:A:208:ASP:O	2.17	0.43
1:B:581:LYS:O	1:B:584:LYS:HD3	2.18	0.43
1:B:616:TRP:HZ3	1:B:630:ALA:HB1	1.83	0.43
1:A:301:ILE:HG13	1:A:313:LEU:HD11	2.00	0.43
1:A:603:LEU:HB3	1:A:614:ILE:HD11	2.01	0.42
1:A:287:TYR:CZ	1:A:550:LEU:HD11	2.54	0.42
1:A:563:ILE:HG12	1:A:568:ILE:HG13	2.01	0.42
1:B:27:ASP:O	1:B:29:GLU:N	2.53	0.42
1:A:197:ILE:O	1:A:201:MET:HG2	2.20	0.41
1:A:305:ASN:OD1	1:B:68:LYS:HB3	2.20	0.41
1:A:648:ILE:O	1:A:652:VAL:HG23	2.19	0.41
1:B:487:GLY:O	1:B:530:GLN:NE2	2.54	0.41
1:B:305:ASN:C	1:B:307:ASN:H	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:LEU:O	1:A:553:THR:OG1	2.38	0.41
1:B:73:LEU:HD21	1:B:299:VAL:HG11	2.03	0.41
1:A:173:ILE:HD12	1:A:214:LEU:HD11	2.03	0.41
1:A:147:LEU:HD21	1:A:298:ARG:HE	1.86	0.41
1:B:87:LYS:HA	1:B:93:LYS:HG2	2.02	0.41
1:A:640:GLY:O	1:A:643:SER:HB2	2.21	0.41
1:B:345:GLY:HA3	1:B:632:ASN:O	2.21	0.41
1:A:118:LYS:HB3	1:A:123:TRP:CE2	2.55	0.41
1:B:460:GLU:HG3	1:B:577:GLN:HB3	2.03	0.41
1:A:228:ALA:HA	1:A:233:LEU:HB2	2.03	0.40
1:B:597:LYS:O	1:B:617:PHE:HA	2.20	0.40
1:A:68:LYS:HB3	1:B:305:ASN:OD1	2.22	0.40
1:B:34:ILE:HA	1:B:37:ILE:HD12	2.03	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	633/643 (98%)	603 (95%)	28 (4%)	2 (0%)	46	74
1	B	633/643 (98%)	605 (96%)	25 (4%)	3 (0%)	34	62
All	All	1266/1286 (98%)	1208 (95%)	53 (4%)	5 (0%)	39	68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	613	GLN
1	B	307	ASN
1	A	221	ASP
1	B	265	LYS
1	B	28	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	568/573 (99%)	514 (90%)	54 (10%)	11 24
1	B	568/573 (99%)	518 (91%)	50 (9%)	12 28
All	All	1136/1146 (99%)	1032 (91%)	104 (9%)	11 25

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LYS
1	A	31	ASN
1	A	59	GLU
1	A	81	GLN
1	A	87	LYS
1	A	89	SER
1	A	99	TYR
1	A	112	VAL
1	A	138	LYS
1	A	148	LYS
1	A	156	ASP
1	A	167	THR
1	A	171	ILE
1	A	177	ASN
1	A	180	LYS
1	A	181	LYS
1	A	184	LYS
1	A	194	GLU
1	A	198	LYS
1	A	215	LYS
1	A	220	MET
1	A	222	GLU
1	A	225	SER
1	A	239	GLU
1	A	266	GLN
1	A	290	LYS
1	A	303	ASP

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Mol	Chain	Res	Type
1	A	308	THR
1	A	309	ILE
1	A	316	LYS
1	A	317	LYS
1	A	368	VAL
1	A	385	GLU
1	A	387	LYS
1	A	391	LEU
1	A	403	SER
1	A	408	LEU
1	A	420	ASP
1	A	430	LYS
1	A	436	LYS
1	A	462	SER
1	A	473	GLU
1	A	513	LEU
1	A	524	ILE
1	A	530	GLN
1	A	553	THR
1	A	566	GLU
1	A	586	ASP
1	A	603	LEU
1	A	604	LYS
1	A	612	ARG
1	A	643	SER
1	A	647	LYS
1	A	668	GLU
1	B	72	SER
1	B	86	LYS
1	B	94	ARG
1	B	99	TYR
1	B	110	ARG
1	B	112	VAL
1	B	120	ASP
1	B	122	MET
1	B	137	GLN
1	B	138	LYS
1	B	156	ASP
1	B	167	THR
1	B	175	PRO
1	B	201	MET
1	B	203	GLN

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Mol	Chain	Res	Type
1	B	204	ASN
1	B	208	ASP
1	B	215	LYS
1	B	221	ASP
1	B	223	TYR
1	B	225	SER
1	B	256	VAL
1	B	264	LEU
1	B	273	LYS
1	B	285	LYS
1	B	290	LYS
1	B	316	LYS
1	B	365	SER
1	B	391	LEU
1	B	417	LYS
1	B	419	LEU
1	B	422	LYS
1	B	435	ASP
1	B	446	TYR
1	B	462	SER
1	B	480	GLU
1	B	502	GLN
1	B	513	LEU
1	B	523	GLU
1	B	527	ASN
1	B	532	LEU
1	B	551	LYS
1	B	554	LYS
1	B	560	LYS
1	B	565	LYS
1	B	570	LEU
1	B	584	LYS
1	B	585	GLU
1	B	603	LEU
1	B	662	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	232	HIS
1	A	292	GLN
1	A	457	GLN

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Mol	Chain	Res	Type
1	A	593	ASN
1	B	57	ASN
1	B	107	ASN
1	B	311	HIS
1	B	325	GLN
1	B	393	ASN
1	B	507	ASN
1	B	580	ASN
1	B	613	GLN

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 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	637/643 (99%)	0.20	19 (2%)	54	54	22, 50, 85, 120	0
1	B	637/643 (99%)	0.22	36 (5%)	27	26	25, 49, 86, 117	0
All	All	1274/1286 (99%)	0.21	55 (4%)	39	39	22, 50, 85, 120	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	TYR	5.0
1	A	173	ILE	4.8
1	B	610	THR	4.5
1	B	267	LYS	4.3
1	B	195	ASP	4.1
1	B	222	GLU	3.9
1	B	305	ASN	3.8
1	A	181	LYS	3.7
1	A	505	ASN	3.6
1	A	222	GLU	3.5
1	B	265	LYS	3.5
1	B	274	ASP	3.5
1	A	385	GLU	3.1
1	B	88	VAL	3.0
1	B	268	GLU	3.0
1	A	509	ASP	3.0
1	A	611	GLY	2.9
1	B	223	TYR	2.9
1	B	173	ILE	2.9
1	B	120	ASP	2.8
1	A	172	GLY	2.8
1	B	505	ASN	2.8
1	B	121	GLY	2.8
1	B	51	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	122	MET	2.7
1	A	387	LYS	2.7
1	A	208	ASP	2.6
1	B	304	ASP	2.5
1	B	114	PHE	2.5
1	B	307	ASN	2.5
1	B	585	GLU	2.5
1	B	272	TYR	2.5
1	B	378	GLU	2.5
1	A	262	GLU	2.4
1	B	82	ASP	2.4
1	A	661	ASN	2.4
1	B	506	LYS	2.4
1	B	426	LYS	2.3
1	B	428	ASP	2.3
1	A	417	LYS	2.3
1	A	122	MET	2.2
1	B	271	GLY	2.2
1	A	220	MET	2.2
1	B	172	GLY	2.2
1	B	76	LYS	2.2
1	A	180	LYS	2.2
1	B	436	LYS	2.2
1	B	226	ASP	2.1
1	B	661	ASN	2.0
1	A	221	ASP	2.0
1	B	468	ALA	2.0
1	A	436	LYS	2.0
1	B	167	THR	2.0
1	B	649	SER	2.0
1	B	319	LYS	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	CD	B	1002	1/1	0.99	0.10	-1.02	45,45,45,45	0
2	CD	A	1001	1/1	0.99	0.10	-1.44	46,46,46,46	0
2	CD	A	1003	1/1	0.99	0.12	-1.51	47,47,47,47	0
3	CL	B	1009	1/1	0.99	0.11	-1.74	34,34,34,34	0
2	CD	A	1005	1/1	0.99	0.10	-1.99	48,48,48,48	0
3	CL	A	1010	1/1	1.00	0.08	-2.68	43,43,43,43	0
3	CL	B	1012	1/1	0.99	0.10	-3.40	51,51,51,51	0
3	CL	A	1011	1/1	1.00	0.05	-3.88	40,40,40,40	0
2	CD	A	1004	1/1	0.95	0.09	-	117,117,117,117	0
2	CD	B	1006	1/1	0.96	0.05	-	131,131,131,131	0
2	CD	B	1007	1/1	0.98	0.09	-	75,75,75,75	0

6.5 Other polymers (i)

There are no such residues in this entry.