Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:34 AM GMT

PDB ID	:	3PBB
Title	:	Crystal structure of human secretory glutaminyl cyclase in complex with PBD150
Authors	:	Huang, K.F.; Liaw, S.S.; Huang, W.L.; Chia, C.Y.; Lo, Y.C.; Chen, Y.L.; Wang, A.H.J.
Deposited on	:	2010-10-20
Resolution	:	1.95 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:

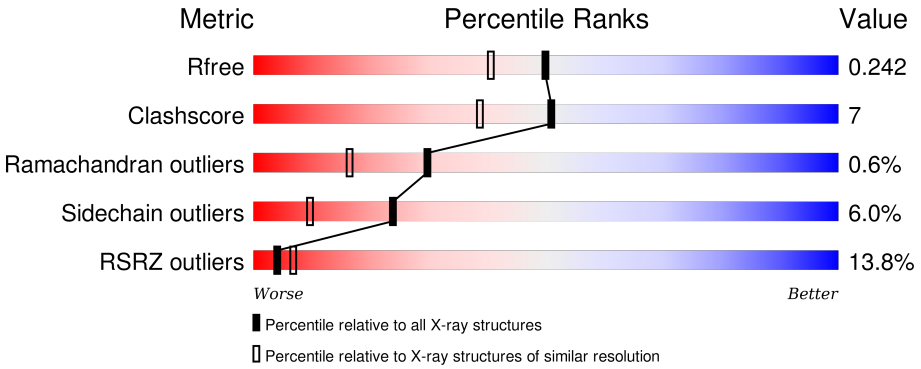
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	329	14% 84% 12%
1	B	329	13% 79% 15%

2 Entry composition

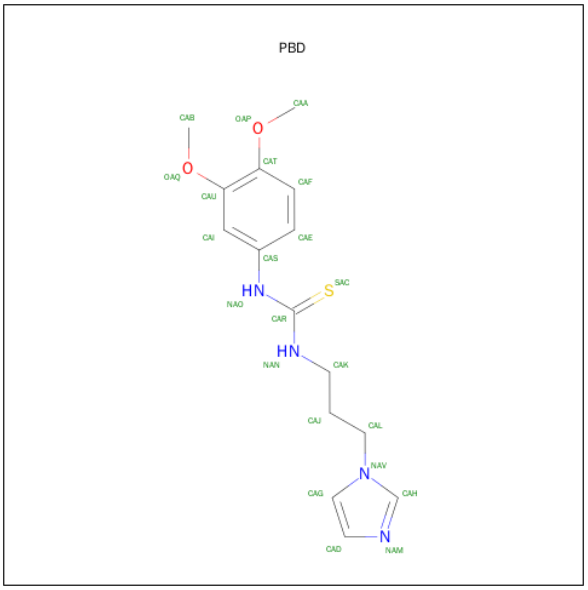
There are 4 unique types of molecules in this entry. The entry contains 5550 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutaminyl-peptide cyclotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			
1	B	323	Total	C	N	O	S	5	0	0
			2610	1673	450	478	9			

- Molecule 2 is 1-(3,4-DIMETHOXYPHENYL)-3-[3-(1H-IMIDAZOL-1-YL)PROPYL]THIO UREA (three-letter code: PBD) (formula: $C_{15}H_{20}N_4O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			22	15	4	2	1		
2	B	1	Total	C	N	O	S	0	0
			22	15	4	2	1		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0

- Molecule 4 is water.

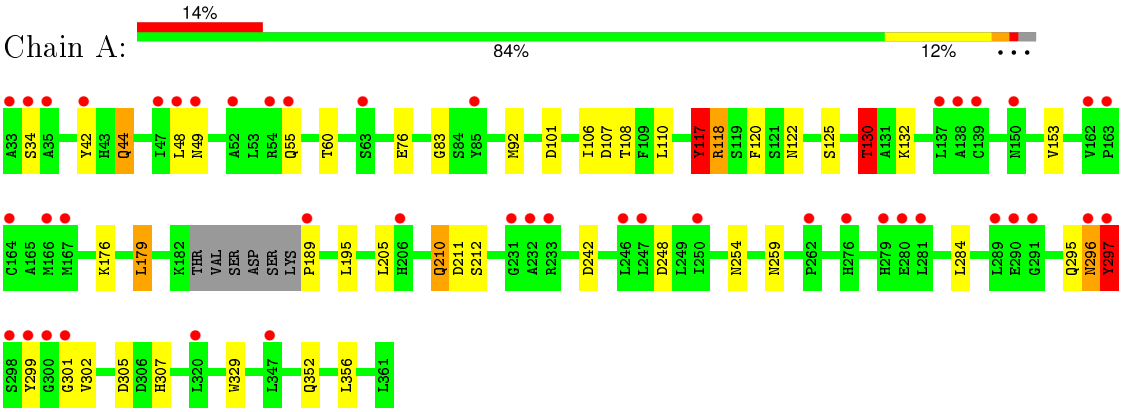
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	142	Total O 142 142	0	0
4	B	142	Total O 142 142	0	0

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.

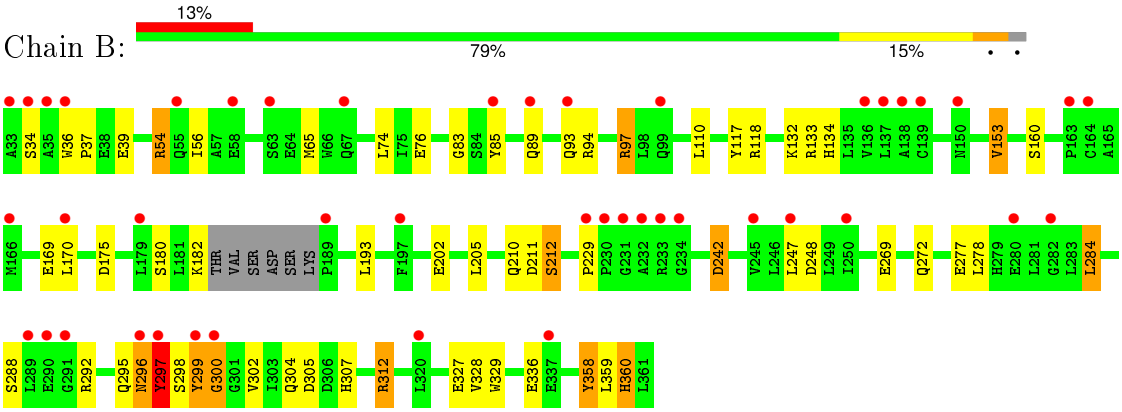
- Molecule 1: Glutaminyl-peptide cyclotransferase

Chain A:



- Molecule 1: Glutaminyl-peptide cyclotransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	155.75Å 155.75Å 80.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.95 29.43 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.00-1.95) 98.7 (29.43-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.181 , 0.239 0.204 , 0.242	Depositor DCC
R_{free} test set	2679 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.635	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 57.0	EDS
Estimated twinning fraction	0.018 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 53123 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5550	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: PBD, ZN

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	0.98	3/2687 (0.1%)	0.91	6/3656 (0.2%)
1	B	1.00	5/2687 (0.2%)	0.89	2/3656 (0.1%)
All	All	0.99	8/5374 (0.1%)	0.90	8/7312 (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

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	ARG	CG-CD	7.21	1.70	1.51
1	A	117	TYR	CD2-CE2	6.99	1.49	1.39
1	B	358	TYR	CD1-CE1	6.84	1.49	1.39
1	B	202	GLU	CB-CG	6.21	1.64	1.52
1	A	117	TYR	CZ-OH	6.14	1.48	1.37
1	A	329	TRP	CB-CG	5.36	1.59	1.50
1	B	329	TRP	CB-CG	5.12	1.59	1.50
1	B	328	VAL	CB-CG1	5.02	1.63	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	101	ASP	CB-CG-OD1	6.35	124.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	THR	O-C-N	-6.12	112.91	122.70
1	A	101	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	118	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	175	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	297	TYR	CA-CB-CG	5.17	123.22	113.40
1	B	247	LEU	CB-CG-CD1	-5.16	102.23	111.00
1	A	48	LEU	CA-CB-CG	5.13	127.09	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	THR	Mainchain
1	B	297	TYR	Peptide

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	2610	0	2529	30	1
1	B	2610	0	2529	41	1
2	A	22	0	20	0	0
2	B	22	0	20	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	142	0	0	8	1
4	B	142	0	0	6	1
All	All	5550	0	5098	71	2

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 7.

All (71) 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:312:ARG:HD3	4:B:616:HOH:O	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:GLN:HG2	2:B:381:PBD:SAC	2.17	0.84
1:B:76:GLU:HG3	1:B:153:VAL:HG13	1.60	0.83
1:B:54:ARG:HD2	4:B:603:HOH:O	1.80	0.82
1:A:210:GLN:HG2	4:A:428:HOH:O	1.80	0.81
1:A:302:VAL:HB	4:A:542:HOH:O	1.83	0.79
1:B:292:ARG:NH2	1:B:296:ASN:HD21	1.82	0.77
1:B:292:ARG:NH2	1:B:296:ASN:ND2	2.34	0.75
1:B:292:ARG:HH21	1:B:296:ASN:ND2	1.89	0.69
1:B:34:SER:O	1:B:37:PRO:HD2	1.93	0.68
1:B:134:HIS:ND1	4:B:635:HOH:O	2.30	0.63
1:A:60:THR:HB	1:A:352:GLN:OE1	1.99	0.61
1:B:304:GLN:CG	2:B:381:PBD:SAC	2.88	0.61
1:B:292:ARG:HH22	1:B:296:ASN:HD21	1.49	0.61
1:B:118:ARG:NH1	4:B:669:HOH:O	2.32	0.61
1:A:254:ASN:ND2	4:A:664:HOH:O	2.34	0.60
1:B:85:TYR:CE2	1:B:89:GLN:OE1	2.55	0.59
1:B:132:LYS:HG2	1:B:229:PRO:HG3	1.85	0.59
1:B:296:ASN:H	1:B:296:ASN:ND2	1.99	0.59
1:A:295:GLN:C	1:A:297:TYR:H	2.06	0.58
1:B:359:LEU:O	1:B:360:HIS:HB2	2.04	0.58
1:A:42:TYR:O	1:A:44:GLN:NE2	2.39	0.55
1:B:296:ASN:N	1:B:296:ASN:ND2	2.56	0.53
1:A:305:ASP:HB3	1:A:307:HIS:HD2	1.73	0.52
1:B:307:HIS:CD2	1:B:307:HIS:H	2.28	0.51
1:B:305:ASP:HB3	1:B:307:HIS:HD2	1.76	0.51
1:A:307:HIS:H	1:A:307:HIS:CD2	2.29	0.50
1:B:170:LEU:HD23	1:B:170:LEU:C	2.32	0.50
1:A:302:VAL:CA	4:A:542:HOH:O	2.60	0.49
1:B:65:MET:HG3	1:B:169:GLU:HB2	1.94	0.49
1:A:107:ASP:HB3	1:A:122:ASN:HB2	1.94	0.49
1:B:295:GLN:HB3	1:B:297:TYR:HD2	1.78	0.49
1:A:49:ASN:HB2	4:A:644:HOH:O	2.12	0.49
1:B:305:ASP:HB3	1:B:307:HIS:CD2	2.48	0.48
1:A:299:TYR:CD1	1:A:301:GLY:O	2.66	0.48
1:B:296:ASN:N	1:B:296:ASN:HD22	2.10	0.48
1:A:305:ASP:HB3	1:A:307:HIS:CD2	2.49	0.47
1:A:189:PRO:N	4:A:627:HOH:O	2.47	0.47
1:A:92:MET:CE	1:A:106:ILE:HD11	2.44	0.47
1:B:76:GLU:HG3	1:B:153:VAL:CG1	2.38	0.46
1:B:242:ASP:OD2	1:B:358:TYR:OH	2.30	0.46
1:A:125:SER:HB3	1:A:195:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:NZ	4:A:553:HOH:O	2.47	0.46
1:B:97:ARG:HD2	4:B:537:HOH:O	2.15	0.46
1:A:248:ASP:OD2	1:A:305:ASP:OD2	2.34	0.45
1:B:299:TYR:O	1:B:300:GLY:C	2.55	0.45
1:A:92:MET:SD	1:A:106:ILE:HD11	2.56	0.44
1:A:176:LYS:O	1:A:179:LEU:HB2	2.17	0.44
1:A:299:TYR:HD1	1:A:301:GLY:O	2.00	0.44
1:B:182:LYS:NZ	4:B:591:HOH:O	2.51	0.44
1:B:36:TRP:CG	1:B:37:PRO:HD3	2.53	0.43
1:B:278:LEU:HB3	1:B:284:LEU:HD13	2.01	0.43
1:B:94:ARG:HA	1:B:94:ARG:HD2	1.84	0.43
1:B:269:GLU:HA	1:B:272:GLN:HE21	1.84	0.42
1:A:76:GLU:O	1:A:83:GLY:HA3	2.19	0.42
1:A:356:LEU:HA	1:A:356:LEU:HD23	1.91	0.42
1:A:295:GLN:C	1:A:297:TYR:N	2.72	0.42
1:A:205:LEU:HD23	1:A:205:LEU:HA	1.67	0.42
1:A:179:LEU:HA	1:A:179:LEU:HD12	1.76	0.41
1:A:211:ASP:O	1:A:212:SER:HB3	2.20	0.41
1:B:211:ASP:O	1:B:212:SER:HB3	2.21	0.41
1:B:304:GLN:HG2	1:B:304:GLN:H	1.52	0.41
1:A:108:THR:HA	1:A:120:PHE:O	2.20	0.41
1:B:76:GLU:O	1:B:83:GLY:HA3	2.21	0.41
1:B:248:ASP:OD2	1:B:305:ASP:OD2	2.39	0.41
1:B:74:LEU:HD13	1:B:336:GLU:HB2	2.03	0.41
1:A:302:VAL:C	4:A:542:HOH:O	2.60	0.40
1:A:118:ARG:HH11	1:A:118:ARG:HD2	1.65	0.40
1:B:56:ILE:N	1:B:56:ILE:HD13	2.36	0.40
1:B:39:GLU:OE1	1:B:133:ARG:NH1	2.51	0.40
1:B:193:LEU:HB2	1:B:359:LEU:HD11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:ARG:NH1	4:A:500:HOH:O[9_454]	1.86	0.34
1:A:117:TYR:OH	4:B:475:HOH:O[5_565]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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	319/329 (97%)	298 (93%)	20 (6%)	1 (0%)	46 35
1	B	319/329 (97%)	300 (94%)	16 (5%)	3 (1%)	21 9
All	All	638/658 (97%)	598 (94%)	36 (6%)	4 (1%)	30 16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	300	GLY
1	A	296	ASN
1	B	212	SER
1	B	360	HIS

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	284/290 (98%)	270 (95%)	14 (5%)	31 15
1	B	284/290 (98%)	264 (93%)	20 (7%)	19 6
All	All	568/580 (98%)	534 (94%)	34 (6%)	24 10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	44	GLN

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Mol	Chain	Res	Type
1	A	55	GLN
1	A	110	LEU
1	A	117	TYR
1	A	130	THR
1	A	153	VAL
1	A	179	LEU
1	A	210	GLN
1	A	242	ASP
1	A	259	ASN
1	A	284	LEU
1	A	296	ASN
1	A	297	TYR
1	B	54	ARG
1	B	93	GLN
1	B	97	ARG
1	B	110	LEU
1	B	117	TYR
1	B	153	VAL
1	B	160	SER
1	B	180	SER
1	B	205	LEU
1	B	210	GLN
1	B	242	ASP
1	B	277	GLU
1	B	284	LEU
1	B	288	SER
1	B	296	ASN
1	B	297	TYR
1	B	298	SER
1	B	299	TYR
1	B	302	VAL
1	B	327	GLU

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	44	GLN
1	A	89	GLN
1	A	210	GLN
1	A	259	ASN
1	A	296	ASN
1	A	307	HIS

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Mol	Chain	Res	Type
1	B	89	GLN
1	B	93	GLN
1	B	99	GLN
1	B	279	HIS
1	B	296	ASN
1	B	307	HIS

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 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	$\#\|Z\| > 2$
2	PBD	A	380	3	22,23,23	1.64	4 (18%)	27,29,29	1.82	10 (37%)
2	PBD	B	381	3	22,23,23	1.72	4 (18%)	27,29,29	1.48	5 (18%)

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	PBD	A	380	3	-	0/15/15/15	0/2/2/2
2	PBD	B	381	3	-	0/15/15/15	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	380	PBD	CAS-NAO	-4.90	1.32	1.41
2	B	381	PBD	CAS-NAO	-3.34	1.35	1.41
2	B	381	PBD	CAJ-CAL	2.03	1.59	1.51
2	A	380	PBD	CAR-NAN	2.03	1.37	1.33
2	A	380	PBD	OAQ-CAB	2.44	1.50	1.42
2	A	380	PBD	CAR-SAC	3.24	1.75	1.68
2	B	381	PBD	OAQ-CAU	3.55	1.42	1.37
2	B	381	PBD	CAR-SAC	3.64	1.76	1.68

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	380	PBD	CAB-OAQ-CAU	-3.53	112.19	117.54
2	A	380	PBD	CAJ-CAK-NAN	-2.79	104.03	112.19
2	A	380	PBD	CAA-OAP-CAT	-2.55	113.67	117.54
2	B	381	PBD	CAS-NAO-CAR	-2.55	121.22	128.60
2	A	380	PBD	OAP-CAT-CAU	-2.35	112.05	115.40
2	A	380	PBD	CAJ-CAL-NAV	-2.31	105.14	111.66
2	B	381	PBD	SAC-CAR-NAO	-2.20	117.53	124.22
2	B	381	PBD	CAB-OAQ-CAU	-2.20	114.21	117.54
2	A	380	PBD	SAC-CAR-NAO	-2.18	117.59	124.22
2	A	380	PBD	CAL-CAJ-CAK	-2.06	106.12	113.93
2	B	381	PBD	NAO-CAR-NAN	2.22	119.77	114.34
2	A	380	PBD	NAO-CAR-NAN	2.81	121.23	114.34
2	A	380	PBD	CAF-CAT-CAU	2.90	123.66	119.74
2	A	380	PBD	CAG-NAV-CAH	4.04	112.12	108.20
2	B	381	PBD	CAG-NAV-CAH	4.60	112.66	108.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	381	PBD	2	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	322/329 (97%)	0.68	45 (13%)	4	6	22, 38, 63, 77	0
1	B	322/329 (97%)	0.67	44 (13%)	4	7	23, 38, 56, 78	0
All	All	644/658 (97%)	0.68	89 (13%)	4	7	22, 38, 62, 78	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ALA	10.9
1	B	299	TYR	8.6
1	B	297	TYR	7.9
1	A	297	TYR	6.1
1	A	33	ALA	5.9
1	A	233	ARG	5.6
1	A	48	LEU	5.3
1	B	233	ARG	5.3
1	A	289	LEU	5.2
1	B	300	GLY	5.1
1	A	300	GLY	4.7
1	B	232	ALA	4.6
1	A	290	GLU	4.3
1	A	138	ALA	4.3
1	A	299	TYR	3.7
1	A	34	SER	3.6
1	A	139	CYS	3.5
1	A	296	ASN	3.5
1	B	290	GLU	3.4
1	A	55	GLN	3.3
1	B	35	ALA	3.3
1	A	231	GLY	3.3
1	B	85	TYR	3.3
1	A	189	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	150	ASN	3.3
1	A	280	GLU	3.3
1	A	262	PRO	3.2
1	B	247	LEU	3.2
1	B	189	PRO	3.0
1	B	250	ILE	3.0
1	A	301	GLY	3.0
1	B	245	VAL	3.0
1	B	280	GLU	2.9
1	A	276	HIS	2.9
1	A	246	LEU	2.9
1	B	139	CYS	2.9
1	B	179	LEU	2.8
1	A	247	LEU	2.8
1	A	320	LEU	2.8
1	B	170	LEU	2.8
1	A	232	ALA	2.7
1	A	291	GLY	2.7
1	B	137	LEU	2.7
1	A	85	TYR	2.7
1	A	250	ILE	2.7
1	B	89	GLN	2.7
1	A	281	LEU	2.7
1	B	55	GLN	2.6
1	B	163	PRO	2.6
1	B	296	ASN	2.6
1	B	289	LEU	2.6
1	B	230	PRO	2.5
1	B	231	GLY	2.5
1	B	67	GLN	2.5
1	B	36	TRP	2.5
1	A	54	ARG	2.5
1	B	138	ALA	2.5
1	A	52	ALA	2.4
1	A	167	MET	2.4
1	A	279	HIS	2.3
1	B	337	GLU	2.3
1	A	42	TYR	2.3
1	B	291	GLY	2.3
1	A	137	LEU	2.3
1	A	206	HIS	2.3
1	B	34	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	47	ILE	2.2
1	A	49	ASN	2.2
1	A	298	SER	2.2
1	B	150	ASN	2.2
1	B	197	PHE	2.2
1	A	162	VAL	2.2
1	B	63	SER	2.2
1	B	166	MET	2.2
1	B	58	GLU	2.1
1	B	93	GLN	2.1
1	A	164	CYS	2.1
1	B	164	CYS	2.1
1	A	347	LEU	2.1
1	B	136	VAL	2.1
1	B	99	GLN	2.1
1	B	320	LEU	2.1
1	A	166	MET	2.1
1	A	163	PRO	2.1
1	B	229	PRO	2.1
1	B	282	GLY	2.1
1	A	63	SER	2.0
1	B	234	GLY	2.0
1	A	35	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	PBD	B	381	22/22	0.97	0.08	-0.93	19,28,35,35	0
3	ZN	B	392	1/1	0.99	0.09	-1.13	26,26,26,26	0
3	ZN	A	391	1/1	1.00	0.10	-1.17	25,25,25,25	0
2	PBD	A	380	22/22	0.96	0.08	-1.35	19,30,35,38	0

6.5 Other polymers (i)

There are no such residues in this entry.