Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:02 am BST

PDB ID	:	5XQ3
Title	:	Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from Penicillium chrysogenum
Authors	:	Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.
Deposited on	:	2017-06-06
Resolution	:	2.85 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

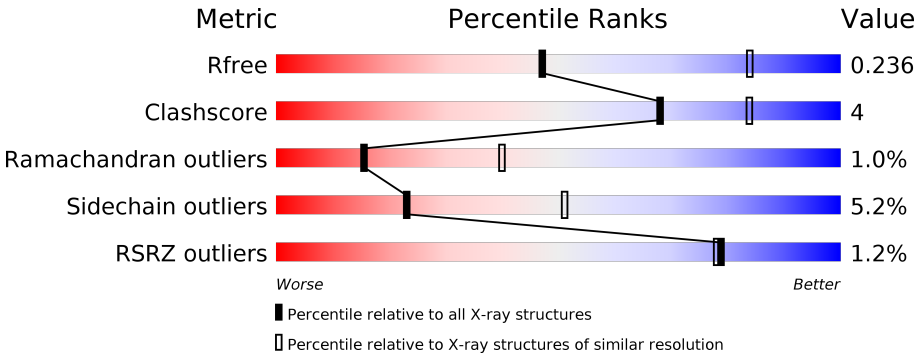
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

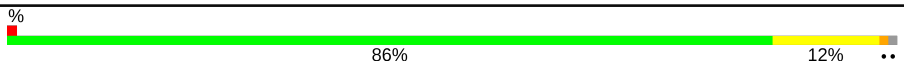
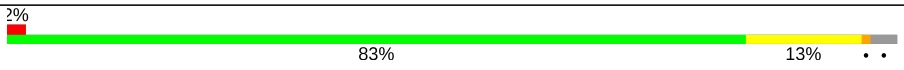
The reported resolution of this entry is 2.85 Å.

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}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 respectively. 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	908	
2	B	906	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14033 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 Pcrglx protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	901	7040	4490	1181	1363	3	3	0	1	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	928	LEU	-	expression tag	UNP A0A0C6EFY4
A	929	GLU	-	expression tag	UNP A0A0C6EFY4

- Molecule 2 is a protein called Pcrglx protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	881	6889	4403	1157	1323	3	3	0	2	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

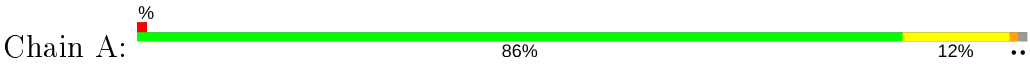
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	61	61	61	0	0
			Total	O		
4	B	41	41	41	0	0

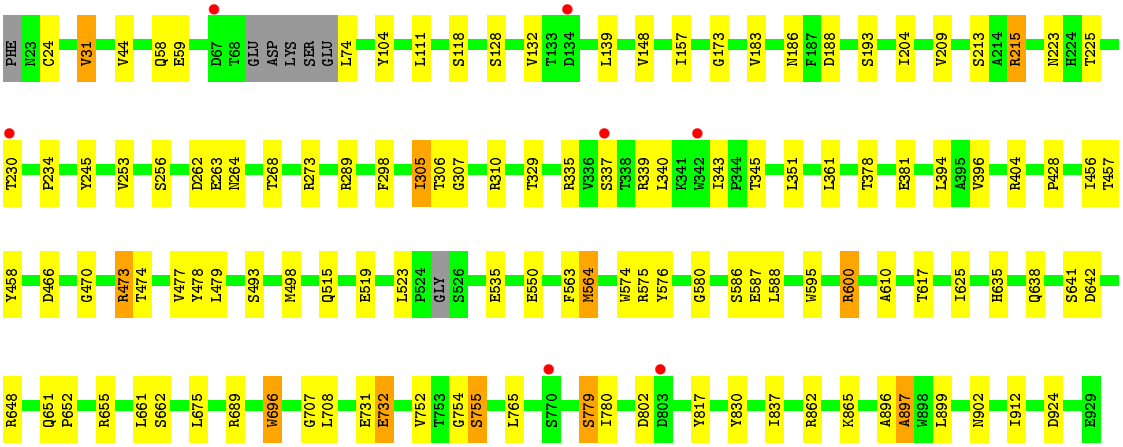
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Pcrglx protein

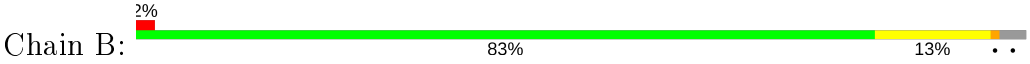
Chain A:

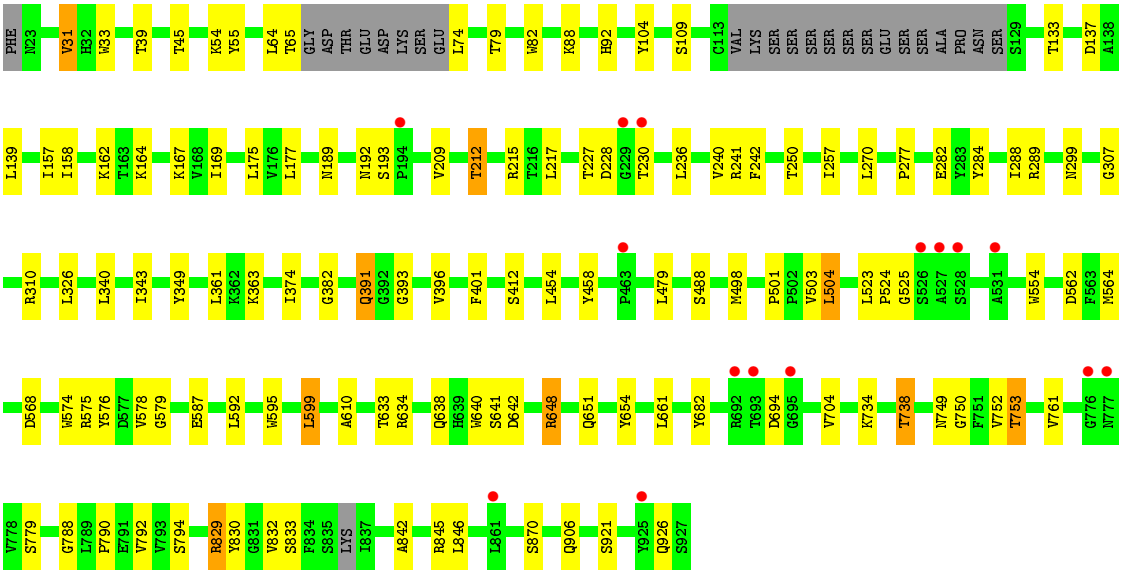




- Molecule 2: Pcrglx protein

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	167.47Å 167.47Å 172.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	120.09 – 2.85 48.80 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (120.09-2.85) 97.9 (48.80-2.85)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.171 , 0.237 0.175 , 0.236	Depositor DCC
R_{free} test set	1956 reflections (3.47%)	wwPDB-VP
Wilson B-factor (Å^2)	62.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 30.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k 0.009 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14033	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: CA

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	0.65	0/7244	0.83	9/9890 (0.1%)
2	B	0.67	0/7094	0.84	4/9688 (0.0%)
All	All	0.66	0/14338	0.83	13/19578 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	600	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	339	ARG	NE-CZ-NH1	6.40	123.50	120.30
2	B	648	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	339	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	404	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	600	ARG	NE-CZ-NH1	5.95	123.27	120.30
2	B	562	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	24	CYS	CA-CB-SG	-5.40	104.28	114.00
2	B	454	LEU	CB-CG-CD2	5.20	119.83	111.00
1	A	696	TRP	N-CA-C	5.09	124.75	111.00
2	B	562	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	473	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	689	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	7040	0	6589	50	0
2	B	6889	0	6418	53	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	61	0	0	1	0
4	B	41	0	0	0	0
All	All	14033	0	13007	101	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 4.

All (101) 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:586:SER:OG	1:A:617:THR:HG21	1.73	0.88
1:A:564:MSE:HE1	1:A:576:TYR:HB3	1.58	0.83
1:A:754:GLY:O	1:A:755:SER:OG	1.98	0.81
1:A:74:LEU:HA	4:A:1122:HOH:O	1.86	0.74
1:A:564:MSE:HE3	1:A:574:TRP:HB2	1.72	0.71
2:B:340:LEU:HD23	2:B:343:ILE:HD12	1.75	0.68
1:A:515:GLN:NE2	1:A:519:GLU:OE2	2.26	0.68
1:A:580:GLY:O	1:A:635:HIS:HD2	1.78	0.66
1:A:588:LEU:HD12	1:A:902:ASN:HB3	1.78	0.65
2:B:382:GLY:O	2:B:498:MSE:HE1	1.98	0.64
2:B:564:MSE:HE1	2:B:576:TYR:HB3	1.82	0.61
2:B:842:ALA:O	2:B:845:ARG:HD3	2.02	0.60
1:A:456:ILE:HG23	1:A:457:THR:HG23	1.83	0.60
1:A:754:GLY:HA2	1:A:779:SER:HB3	1.86	0.58
2:B:554:TRP:HE1	2:B:564:MSE:HE2	1.69	0.58
2:B:750:GLY:O	2:B:753:THR:HG23	2.03	0.57
2:B:282[B]:GLU:HG2	2:B:284:TYR:CZ	2.39	0.57
2:B:212:THR:HG22	2:B:215:ARG:O	2.05	0.57
2:B:158:ILE:HD11	2:B:242:PHE:CE2	2.41	0.56
2:B:363:LYS:HB2	2:B:374:ILE:HD11	1.89	0.55
1:A:752:VAL:HG13	1:A:780:ILE:HD11	1.88	0.55
2:B:595:TRP:CE2	2:B:610:ALA:HB1	2.42	0.55
1:A:587:GLU:OE2	1:A:648:ARG:NH1	2.40	0.54
1:A:595:TRP:CE2	1:A:610:ALA:HB1	2.43	0.53
2:B:564:MSE:HE3	2:B:574:TRP:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:734:LYS:O	2:B:738:THR:OG1	2.26	0.53
1:A:817:TYR:O	1:A:862:ARG:NH2	2.37	0.52
2:B:575:ARG:HB3	2:B:578:VAL:HG22	1.90	0.52
1:A:708:LEU:HG	1:A:755:SER:HA	1.92	0.52
2:B:31:VAL:HG13	2:B:504:LEU:HG	1.91	0.52
2:B:578:VAL:O	2:B:578:VAL:HG23	2.10	0.52
2:B:752:VAL:HG21	2:B:830:TYR:CZ	2.44	0.52
2:B:788:GLY:O	2:B:792:VAL:HG23	2.10	0.52
2:B:458:TYR:O	2:B:634:ARG:NH2	2.42	0.51
2:B:749:ASN:HB2	2:B:753:THR:HG22	1.92	0.51
1:A:707:GLY:HA2	1:A:755:SER:HB3	1.93	0.51
2:B:288:ILE:HD13	2:B:349:TYR:CE1	2.46	0.51
1:A:307:GLY:O	2:B:578:VAL:HG21	2.11	0.50
1:A:139:LEU:HD21	1:A:209:VAL:HG22	1.94	0.50
1:A:652:PRO:HG3	1:A:675:LEU:HD13	1.94	0.50
2:B:568:ASP:HB2	2:B:575:ARG:HG2	1.95	0.49
2:B:633:THR:HG21	2:B:640:TRP:HA	1.95	0.49
1:A:478:TYR:CD1	1:A:498:MSE:HG3	2.48	0.49
2:B:169:ILE:HD13	2:B:393:GLY:O	2.13	0.48
1:A:253:VAL:HB	1:A:477:VAL:HB	1.95	0.48
1:A:754:GLY:HA2	1:A:779:SER:CB	2.43	0.48
2:B:829:ARG:HD2	2:B:830:TYR:CE2	2.48	0.48
1:A:173:GLY:HA2	1:A:273:ARG:O	2.14	0.48
2:B:227:THR:OG1	2:B:228:ASP:N	2.45	0.48
2:B:33:TRP:CE3	2:B:504:LEU:HD13	2.49	0.48
2:B:288:ILE:HD13	2:B:349:TYR:CD1	2.49	0.48
2:B:790:PRO:HG3	2:B:846:LEU:HD21	1.96	0.48
1:A:310:ARG:HG3	1:A:335:ARG:HG2	1.96	0.47
2:B:288:ILE:CD1	2:B:349:TYR:CE1	2.97	0.47
2:B:845:ARG:NH1	2:B:906:GLN:OE1	2.47	0.47
1:A:396:VAL:HG23	1:A:479:LEU:HD23	1.96	0.47
2:B:217:LEU:HD11	2:B:241:ARG:HB3	1.96	0.47
1:A:752:VAL:HG21	1:A:830:TYR:CZ	2.50	0.47
1:A:225:THR:HG22	1:A:234:PRO:HB3	1.97	0.46
1:A:351:LEU:HD12	1:A:361:LEU:HD13	1.98	0.46
1:A:59:GLU:HA	1:A:111:LEU:HD22	1.98	0.46
2:B:177:LEU:HD22	2:B:236:LEU:HD23	1.98	0.46
1:A:661:LEU:O	1:A:662:SER:CB	2.64	0.45
2:B:638:GLN:HB2	2:B:641:SER:HB3	1.97	0.45
2:B:45:THR:HA	2:B:92:HIS:O	2.16	0.45
2:B:299:ASN:OD1	2:B:488:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:TYR:CD1	2:B:326:LEU:HD12	2.51	0.45
1:A:157:ILE:HA	1:A:204:ILE:HD11	1.97	0.45
2:B:592:LEU:HD13	2:B:654:TYR:CD1	2.51	0.45
1:A:340:LEU:HD23	1:A:343:ILE:HD12	1.98	0.45
1:A:575:ARG:HD3	2:B:307:GLY:O	2.17	0.45
2:B:64:LEU:HD22	2:B:74:LEU:HD13	1.99	0.44
1:A:754:GLY:O	1:A:755:SER:CB	2.65	0.44
1:A:268:THR:O	1:A:428:PRO:HA	2.18	0.44
2:B:382:GLY:HA3	2:B:401:PHE:CG	2.53	0.44
2:B:64:LEU:HD11	2:B:104:TYR:HB3	1.98	0.44
2:B:82:TRP:CE2	2:B:88:LYS:HG3	2.53	0.44
1:A:535:GLU:OE1	1:A:600:ARG:NH2	2.51	0.43
1:A:564:MSE:HE3	1:A:574:TRP:CB	2.45	0.43
2:B:501:PRO:O	2:B:503:VAL:HG23	2.19	0.43
1:A:752:VAL:HG21	1:A:830:TYR:CE2	2.54	0.42
1:A:896:ALA:CB	1:A:899:LEU:HG	2.49	0.42
2:B:162:LYS:HA	2:B:167:LYS:O	2.19	0.42
1:A:289:ARG:HA	1:A:298:PHE:O	2.20	0.42
1:A:305:ILE:HD13	1:A:305:ILE:HA	1.77	0.42
2:B:54:LYS:HG2	2:B:55:TYR:CE2	2.55	0.41
2:B:599:LEU:CD1	2:B:661:LEU:HD11	2.50	0.41
1:A:600:ARG:HD3	1:A:912:ILE:HG23	2.02	0.41
2:B:396:VAL:HG12	2:B:479:LEU:HD23	2.01	0.41
2:B:139:LEU:HD21	2:B:209:VAL:CG2	2.51	0.41
2:B:391[B]:GLN:OE1	2:B:391[B]:GLN:HA	2.20	0.41
1:A:638:GLN:HB2	1:A:641:SER:HB3	2.02	0.41
1:A:31:VAL:HG12	1:A:104:TYR:HB2	2.03	0.41
1:A:731:GLU:O	1:A:732:GLU:CB	2.69	0.41
2:B:682:TYR:HB3	2:B:704:VAL:HG11	2.02	0.41
1:A:473:ARG:HG3	1:A:474:THR:N	2.36	0.40
1:A:896:ALA:O	1:A:897:ALA:CB	2.69	0.40
1:A:470:GLY:HA2	1:A:625:ILE:HG12	2.03	0.40
1:A:215:ARG:HB3	1:A:245:TYR:CD2	2.56	0.40
1:A:262:ASP:O	1:A:264:ASN:N	2.55	0.40
2:B:829:ARG:HD2	2:B:830:TYR:CD2	2.56	0.40

There are no symmetry-related clashes.

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	896/908 (99%)	832 (93%)	58 (6%)	6 (1%)	22	50
2	B	875/906 (97%)	810 (93%)	53 (6%)	12 (1%)	11	31
All	All	1771/1814 (98%)	1642 (93%)	111 (6%)	18 (1%)	15	40

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLU
1	A	732	GLU
1	A	755	SER
2	B	193	SER
1	A	897	ALA
2	B	137	ASP
2	B	525	GLY
2	B	833	SER
1	A	466	ASP
1	A	651	GLN
2	B	277	PRO
2	B	694	ASP
2	B	579	GLY
2	B	651	GLN
2	B	870	SER
2	B	926	GLN
2	B	524	PRO
2	B	832	VAL

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	722/744 (97%)	683 (95%)	39 (5%)	22	49
2	B	697/742 (94%)	661 (95%)	36 (5%)	23	51
All	All	1419/1486 (96%)	1344 (95%)	75 (5%)	23	50

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	44	VAL
1	A	58	GLN
1	A	118	SER
1	A	128	SER
1	A	132	VAL
1	A	148	VAL
1	A	183	VAL
1	A	186	ASN
1	A	188	ASP
1	A	193	SER
1	A	213	SER
1	A	215	ARG
1	A	223	ASN
1	A	230	THR
1	A	256	SER
1	A	305	ILE
1	A	306	THR
1	A	329	THR
1	A	337	SER
1	A	345	THR
1	A	378	THR
1	A	381	GLU
1	A	394	LEU
1	A	458	TYR
1	A	493	SER
1	A	523	LEU
1	A	550	GLU
1	A	563	PHE
1	A	564	MSE
1	A	642	ASP
1	A	655	ARG
1	A	696	TRP

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Mol	Chain	Res	Type
1	A	765	LEU
1	A	779	SER
1	A	802	ASP
1	A	837	ILE
1	A	865	LYS
1	A	924	ASP
2	B	31	VAL
2	B	39	THR
2	B	65	THR
2	B	79	THR
2	B	109	SER
2	B	133	THR
2	B	157	ILE
2	B	164	LYS
2	B	175	LEU
2	B	189	ASN
2	B	192	ASN
2	B	212	THR
2	B	230	THR
2	B	240	VAL
2	B	250	THR
2	B	257	ILE
2	B	270	LEU
2	B	289	ARG
2	B	310	ARG
2	B	361	LEU
2	B	391[A]	GLN
2	B	391[B]	GLN
2	B	412	SER
2	B	504	LEU
2	B	523	LEU
2	B	587	GLU
2	B	599	LEU
2	B	642	ASP
2	B	648	ARG
2	B	738	THR
2	B	753	THR
2	B	761	VAL
2	B	779	SER
2	B	794	SER
2	B	829	ARG
2	B	921	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	324	GLN
1	A	635	HIS
2	B	178	GLN
2	B	653	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 2 ligands modelled in this entry, 2 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	898/908 (98%)	-0.23	7 (0%)	86	85	41, 59, 86, 108	0
2	B	878/906 (96%)	-0.13	15 (1%)	70	68	39, 61, 87, 119	0
All	All	1776/1814 (97%)	-0.18	22 (1%)	79	78	39, 60, 87, 119	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	693	THR	3.7
2	B	527	ALA	3.3
1	A	67	ASP	3.3
2	B	925	TYR	3.0
2	B	526	SER	3.0
2	B	692	ARG	3.0
2	B	695	GLY	2.9
1	A	342	TRP	2.9
2	B	230	THR	2.8
1	A	337	SER	2.3
2	B	229	GLY	2.3
2	B	528	SER	2.2
2	B	776	GLY	2.2
2	B	861	LEU	2.2
2	B	531	ALA	2.2
2	B	463	PRO	2.1
1	A	770	SER	2.1
1	A	230	THR	2.1
1	A	134	ASP	2.1
1	A	803	ASP	2.1
2	B	777	ASN	2.0
2	B	194	PRO	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. 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	B-factors(Å^2)	Q<0.9
3	CA	B	1001	1/1	0.96	0.20	37,37,37,37	0
3	CA	A	1001	1/1	0.99	0.22	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.