Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 03:30 pm GMT

PDB ID	:	4A1W
Title	:	Crystal structure of alpha-beta foldamer 4c in complex with Bcl-xL
Authors	:	Boersma, M.D.; Haase, H.S.; Kaufman, K.J.; Horne, W.S.; Lee, E.F.; Clarke, O.B.; Smith, B.J.; Colman, P.M.; Gellman, S.H.; Fairlie, W.D.
Deposited on	:	2011-09-20
Resolution	:	2.50 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

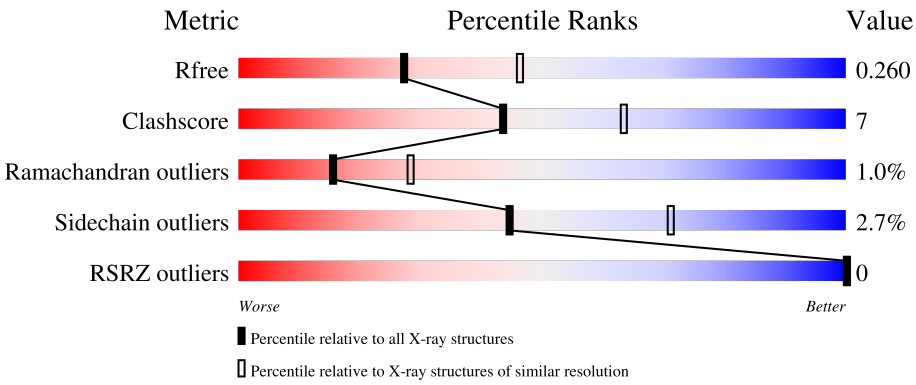
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 of 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	158	79% 9% • 11%
1	B	158	77% 15% 9%
1	C	158	76% 11% • 13%
1	D	158	79% 10% 11%
2	P	19	47% 32% 16% 5%

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Mol	Chain	Length	Quality of chain
2	Q	19	58% 26% 11% 5%
2	R	19	47% 42% 5% 5%
2	S	19	58% 26% 16%

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	HT7	S	207[A]	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5505 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 BCL-2-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	141	1137	727	192	214	4	15	0	0
1	B	144	1166	746	196	219	5	34	1	0
1	C	138	1121	718	189	210	4	28	0	0
1	D	141	1140	729	192	214	5	39	0	0

- Molecule 2 is a protein called ALPHA-BETA-FOLDAMER 2C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	18	170	115	28	27	0	1	1
2	Q	19	166	110	28	28	1	0	1
2	R	18	170	115	28	27	0	1	1
2	S	19	178	121	29	28	1	1	1

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	74	75	75	0	1
3	B	53	53	53	0	0
3	C	41	41	41	0	0
3	D	62	62	62	0	0

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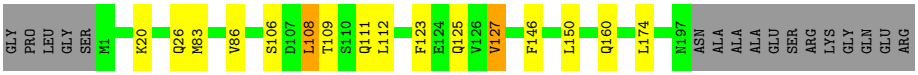
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	P	7	7	7	0	0
			Total	O		
3	Q	10	10	10	0	0
			Total	O		
3	R	1	1	1	0	0
			Total	O		
3	S	8	8	8	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: BCL-2-LIKE PROTEIN 1

Chain A:

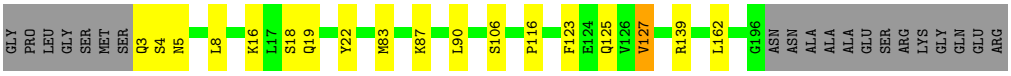


• Molecule 1: BCL-2-LIKE PROTEIN 1

Chain B:

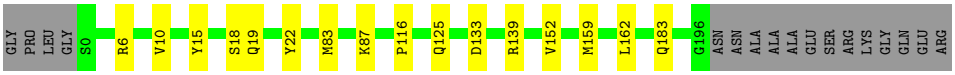
• Molecule 1: BCL-2-LIKE PROTEIN 1

Chain C:



• Molecule 1: BCL-2-LIKE PROTEIN 1

Chain D:

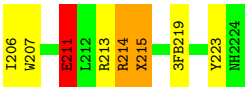


• Molecule 2: ALPHA-BETA-FOLDAMER 2C

Chain P:

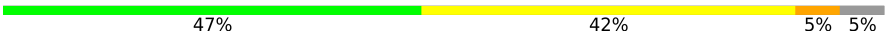
• Molecule 2: ALPHA-BETA-FOLDAMER 2C

Chain Q:



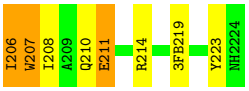
- Molecule 2: ALPHA-BETA-FOLDAMER 2C

Chain R:



- Molecule 2: ALPHA-BETA-FOLDAMER 2C

Chain S:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	80.21Å 106.29Å 100.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.03 – 2.50 64.03 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (64.03-2.50) 99.4 (64.03-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.197 , 0.264 0.195 , 0.260	Depositor DCC
R_{free} test set	1523 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.587	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5505	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.75% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BIL, NH2, 3FB, B3Y, B3E, HT7

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	0.44	0/1165	0.55	0/1578
1	B	0.43	0/1197	0.54	0/1620
1	C	0.44	0/1149	0.54	0/1556
1	D	0.39	0/1168	0.51	0/1581
2	P	0.45	0/95	0.64	0/121
2	Q	0.46	0/102	0.67	0/129
2	R	0.38	0/95	0.75	0/121
2	S	0.42	0/102	0.63	0/129
All	All	0.43	0/5073	0.55	0/6835

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
2	P	0	5
2	Q	0	4
2	R	0	4
2	S	0	5
All	All	0	18

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	211	B3E	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
2	P	214	ARG	Peptide
2	P	219	3FB	Mainchain,Peptide
2	Q	211	B3E	Mainchain
2	Q	214	ARG	Peptide
2	Q	219	3FB	Mainchain,Peptide
2	R	211	B3E	Mainchain
2	R	214	ARG	Peptide
2	R	219	3FB	Mainchain,Peptide
2	S	211	B3E	Mainchain,Peptide
2	S	214	ARG	Peptide
2	S	219	3FB	Mainchain,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	1137	0	1078	11	0
1	B	1166	0	1119	13	0
1	C	1121	0	1066	12	0
1	D	1140	0	1085	11	0
2	P	170	0	152	10	0
2	Q	166	0	146	9	0
2	R	170	0	153	9	0
2	S	178	0	158	9	0
3	A	75	0	0	1	0
3	B	53	0	0	1	0
3	C	41	0	0	0	0
3	D	62	0	0	1	0
3	P	7	0	0	0	0
3	Q	10	0	0	0	0
3	R	1	0	0	0	0
3	S	8	0	0	0	0
All	All	5505	0	4957	67	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 7.

All (67) 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)
2:S:206:ILE:HG13	2:S:207[A]:HT7:HE1	1.65	0.79
1:C:125:GLN:HG2	2:R:207[A]:HT7:HH2	1.72	0.71
1:B:95:ASP:OD1	1:C:16:LYS:NZ	2.29	0.66
2:R:207[A]:HT7:HA2	2:R:210:GLN:H	1.49	0.61
2:S:207[A]:HT7:HZ3	2:S:208:ILE:N	2.17	0.59
1:C:116:PRO:HA	1:C:162:LEU:HD21	1.85	0.59
2:Q:211:B3E:OF1	2:Q:214:ARG:NH1	2.33	0.58
2:S:207[B]:HT7:HB2	2:S:210:GLN:HG3	1.85	0.57
3:B:2021:HOH:O	2:Q:206:ILE:HG13	2.05	0.57
2:Q:211:B3E:OF1	2:Q:214:ARG:HD3	2.05	0.56
2:S:207[A]:HT7:HZ3	2:S:208:ILE:H	1.71	0.56
1:A:125:GLN:CD	2:P:207[B]:HT7:HH2	2.27	0.55
1:A:109:THR:HA	1:A:112:LEU:HD23	1.88	0.55
1:D:133:ASP:OD1	1:D:139:ARG:NH1	2.31	0.54
2:P:207[B]:HT7:HZ3	2:P:208:ILE:HG12	1.89	0.54
2:S:207[A]:HT7:HB2	2:S:210:GLN:HG3	1.89	0.54
1:D:125:GLN:NE2	2:S:207[A]:HT7:HH2	2.22	0.54
1:D:125:GLN:CD	2:S:207[A]:HT7:HH2	2.28	0.54
2:R:207[B]:HT7:CE1	2:R:207[B]:HT7:HN1	2.21	0.53
1:B:103:ARG:HD3	2:P:222:TYR:CE2	2.45	0.51
2:R:210:GLN:HG2	2:R:213:ARG:HH21	1.74	0.51
2:S:206:ILE:HG13	2:S:207[A]:HT7:CE1	2.39	0.51
1:A:160:GLN:HB3	3:A:2061:HOH:O	2.10	0.50
2:R:207[B]:HT7:HA2	2:R:210:GLN:H	1.57	0.50
2:P:219:3FB:HC2	2:P:219:3FB:CD2	2.43	0.49
1:B:96:GLU:HB3	1:B:100:ARG:NH1	2.26	0.49
1:B:139:ARG:NH2	2:Q:213:ARG:HD3	2.29	0.48
1:C:125:GLN:CG	2:R:207[A]:HT7:HH2	2.41	0.48
1:D:116:PRO:HA	1:D:162:LEU:HD21	1.94	0.48
1:A:123:PHE:O	1:A:127:VAL:HG13	2.14	0.47
1:B:8[A]:LEU:HD11	1:C:90:LEU:HD12	1.96	0.47
1:D:83:MET:SD	1:D:87:LYS:HE3	2.54	0.47
1:C:123:PHE:O	1:C:127:VAL:HG13	2.15	0.47
2:Q:214:ARG:NH1	2:Q:215:BIL:H2E1	2.30	0.47
1:B:175:ASN:OD1	1:C:5:ASN:ND2	2.32	0.47
1:A:108:LEU:HD13	2:P:208:ILE:HD13	1.97	0.46
1:A:108:LEU:HB3	2:P:208:ILE:HD12	1.97	0.46
1:B:129:GLU:OE2	2:Q:213:ARG:NH2	2.49	0.46
1:C:139:ARG:NH2	2:R:213:ARG:HD2	2.30	0.46
2:Q:211:B3E:CE	2:Q:214:ARG:HH11	2.27	0.46
1:D:183:GLN:HG3	3:D:2055:HOH:O	2.16	0.45
1:C:16:LYS:HD3	1:C:16:LYS:HA	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:LYS:HD3	1:B:16:LYS:HA	1.72	0.44
1:C:83:MET:O	1:C:87:LYS:HG3	2.17	0.44
2:S:206:ILE:HG13	2:S:207[B]:HT7:CZ3	2.46	0.44
2:R:210:GLN:HG2	2:R:213:ARG:NH2	2.33	0.43
2:P:207[A]:HT7:HE1	2:P:209:ALA:H	1.83	0.43
1:A:146:PHE:CZ	1:A:150:LEU:HD11	2.53	0.43
1:B:123:PHE:O	1:B:127:VAL:HG13	2.18	0.43
1:A:20:LYS:HG3	1:D:152:VAL:HG11	2.01	0.42
1:A:26:GLN:O	1:A:86:VAL:HG23	2.19	0.42
1:D:6:ARG:O	1:D:10:VAL:HG23	2.19	0.42
1:C:16:LYS:HD3	1:C:19:GLN:OE1	2.19	0.42
2:P:207[B]:HT7:HZ3	2:P:208:ILE:N	2.35	0.42
1:A:108:LEU:HB3	2:P:208:ILE:HG23	2.02	0.42
1:B:137:TRP:HH2	1:B:182:ILE:HG23	1.83	0.42
1:C:18:SER:HA	1:C:22:TYR:O	2.20	0.41
1:D:15:TYR:O	1:D:19:GLN:HG3	2.20	0.41
1:B:174:LEU:HD12	1:B:178:LEU:HB2	2.02	0.41
2:R:207[B]:HT7:HA2	2:R:210:GLN:HB2	1.86	0.41
1:B:18:SER:HA	1:B:22:TYR:O	2.20	0.41
2:Q:211:B3E:CE	2:Q:214:ARG:NH1	2.84	0.40
1:B:179:GLU:HB3	1:B:180:PRO:HD3	2.04	0.40
1:D:116:PRO:HD3	1:D:159:MET:SD	2.61	0.40
2:Q:211:B3E:O	2:Q:215:BIL:H1D2	2.20	0.40
1:A:125:GLN:OE1	2:P:207[B]:HT7:HH2	2.20	0.40
1:D:18:SER:HA	1:D:22:TYR:O	2.22	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	139/158 (88%)	134 (96%)	3 (2%)	2 (1%)	11 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	143/158 (90%)	139 (97%)	2 (1%)	2 (1%)	11	20
1	C	136/158 (86%)	132 (97%)	2 (2%)	2 (2%)	10	18
1	D	139/158 (88%)	137 (99%)	2 (1%)	0	100	100
2	P	12/19 (63%)	12 (100%)	0	0	100	100
2	Q	12/19 (63%)	12 (100%)	0	0	100	100
2	R	12/19 (63%)	11 (92%)	1 (8%)	0	100	100
2	S	12/19 (63%)	12 (100%)	0	0	100	100
All	All	605/708 (86%)	589 (97%)	10 (2%)	6 (1%)	15	28

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	4	SER
1	A	106	SER
1	C	106	SER
1	A	111	GLN
1	B	102	ARG
1	B	196	GLY

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	118/131 (90%)	114 (97%)	4 (3%)	37	63
1	B	123/131 (94%)	121 (98%)	2 (2%)	62	84
1	C	117/131 (89%)	114 (97%)	3 (3%)	46	72
1	D	119/131 (91%)	119 (100%)	0	100	100
2	P	9/10 (90%)	7 (78%)	2 (22%)	1	1
2	Q	10/10 (100%)	10 (100%)	0	100	100
2	R	9/10 (90%)	7 (78%)	2 (22%)	1	1
2	S	10/10 (100%)	9 (90%)	1 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	515/564 (91%)	501 (97%)	14 (3%)	44 71

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	MET
1	A	108	LEU
1	A	127	VAL
1	A	174	LEU
1	B	121	GLN
1	B	197	ASN
1	C	3	GLN
1	C	8	LEU
1	C	127	VAL
2	P	208	ILE
2	P	210	GLN
2	R	208	ILE
2	R	213	ARG
2	S	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

19 non-standard protein/DNA/RNA residues 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	HT7	S	207[A]	-	15,16,17	0.58	0	14,21,23	1.11	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	BIL	R	215	2	7,8,9	0.56	0	5,9,11	1.30	1 (20%)
2	BIL	P	215	2	7,8,9	0.55	0	5,9,11	1.13	0
2	B3Y	S	223	2	13,13,14	0.38	0	14,16,18	0.94	1 (7%)
2	HT7	P	207[B]	-	15,16,17	0.63	0	14,21,23	1.09	1 (7%)
2	B3E	P	211	2	9,9,10	0.87	0	9,10,12	1.14	0
2	HT7	Q	207	2	15,16,17	0.58	0	14,21,23	1.13	1 (7%)
2	BIL	S	215	2	7,8,9	0.53	0	5,9,11	0.97	0
2	B3E	Q	211	2	9,9,10	1.01	0	9,10,12	1.45	1 (11%)
2	HT7	R	207[B]	-	15,16,17	0.66	0	14,21,23	0.89	0
2	HT7	P	207[A]	-	15,16,17	0.58	0	14,21,23	1.28	2 (14%)
2	B3Y	Q	223	2	13,13,14	0.40	0	14,16,18	1.39	2 (14%)
2	B3E	R	211	2	9,9,10	0.90	0	9,10,12	1.13	0
2	HT7	S	207[B]	-	15,16,17	0.56	0	14,21,23	0.91	0
2	B3E	S	211	2	9,9,10	1.07	1 (11%)	9,10,12	1.15	0
2	HT7	R	207[A]	-	15,16,17	0.59	0	14,21,23	0.96	0
2	B3Y	R	223	2	13,13,14	0.42	0	14,16,18	1.14	1 (7%)
2	BIL	Q	215	2	7,8,9	0.68	0	5,9,11	1.86	2 (40%)
2	B3Y	P	223	2	13,13,14	0.51	0	14,16,18	0.82	1 (7%)

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	HT7	S	207[A]	-	-	3/6/7/8	0/2/2/2
2	BIL	R	215	2	-	1/9/9/10	-
2	BIL	P	215	2	-	1/9/9/10	-
2	B3Y	S	223	2	-	3/7/7/8	0/1/1/1
2	HT7	P	207[B]	-	-	5/6/7/8	0/2/2/2
2	B3E	P	211	2	-	4/8/8/9	-
2	HT7	Q	207	2	-	1/6/7/8	0/2/2/2
2	BIL	S	215	2	-	1/9/9/10	-
2	B3E	Q	211	2	-	5/8/8/9	-
2	HT7	R	207[B]	-	-	2/6/7/8	0/2/2/2
2	HT7	P	207[A]	-	-	5/6/7/8	0/2/2/2
2	B3Y	Q	223	2	-	0/7/7/8	0/1/1/1
2	B3E	R	211	2	-	2/8/8/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HT7	S	207[B]	-	-	3/6/7/8	0/2/2/2
2	B3E	S	211	2	-	3/8/8/9	-
2	HT7	R	207[A]	-	-	2/6/7/8	0/2/2/2
2	B3Y	R	223	2	-	3/7/7/8	0/1/1/1
2	BIL	Q	215	2	-	7/9/9/10	-
2	B3Y	P	223	2	-	3/7/7/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	211	B3E	CB-C	2.00	1.55	1.49

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Q	223	B3Y	CA-CB-C	-3.76	106.73	112.25
2	R	223	B3Y	CA-CB-C	-2.95	107.92	112.25
2	Q	207	HT7	CB-CA-C	2.62	116.10	112.25
2	S	223	B3Y	CB-CA-CG	-2.38	107.37	110.81
2	Q	215	BIL	CB-CA-C	-2.31	108.60	113.39
2	Q	215	BIL	CA-CB-CG	2.22	118.45	113.19
2	Q	211	B3E	CD-CG-CA	2.21	117.39	112.74
2	S	207[A]	HT7	O-C-CA	-2.13	119.22	125.43
2	S	207[A]	HT7	CA-CB-CG	2.11	113.87	110.81
2	P	207[A]	HT7	CT2-CH2-CZ2	-2.10	117.05	120.08
2	P	207[A]	HT7	CB-CA-C	2.08	115.31	112.25
2	Q	223	B3Y	CB-CA-CG	-2.07	107.81	110.81
2	P	223	B3Y	CA-CB-C	-2.07	109.20	112.25
2	P	207[B]	HT7	CA-CB-CG	2.06	113.80	110.81
2	R	215	BIL	CB-CA-C	-2.05	109.13	113.39

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	207[A]	HT7	N-CB-CG-CD
2	P	207[A]	HT7	C-CA-CB-CG
2	P	207[B]	HT7	CA-CB-CG-CD
2	P	207[B]	HT7	C-CA-CB-CG
2	P	211	B3E	CB-CA-CG-CD

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Mol	Chain	Res	Type	Atoms
2	Q	207	HT7	O-C-CA-CB
2	Q	211	B3E	CB-CA-CG-CD
2	R	207[A]	HT7	C-CA-CB-N
2	R	207[A]	HT7	C-CA-CB-CG
2	R	207[B]	HT7	C-CA-CB-N
2	R	207[B]	HT7	C-CA-CB-CG
2	S	207[A]	HT7	CA-CB-CG-CD
2	S	207[A]	HT7	C-CA-CB-CG
2	S	207[B]	HT7	CA-CB-CG-CD
2	S	207[B]	HT7	C-CA-CB-CG
2	S	223	B3Y	CG-CA-CB-C
2	P	215	BIL	C-CA-CB-N
2	Q	215	BIL	CA-CB-CG-CD2
2	Q	215	BIL	CA-CB-CG-CD1
2	Q	215	BIL	N-CB-CG-CD2
2	Q	215	BIL	N-CB-CG-CD1
2	Q	215	BIL	CE1-CD1-CG-CD2
2	Q	215	BIL	CE1-CD1-CG-CB
2	P	223	B3Y	N-CA-CG-CD
2	R	223	B3Y	N-CA-CG-CD
2	S	207[A]	HT7	N-CB-CG-CD
2	S	207[B]	HT7	N-CB-CG-CD
2	P	207[B]	HT7	O-C-CA-CB
2	P	207[A]	HT7	C-CA-CB-N
2	P	207[B]	HT7	C-CA-CB-N
2	P	207[B]	HT7	N-CB-CG-CD
2	P	207[A]	HT7	CA-CB-CG-CD
2	P	223	B3Y	CB-CA-CG-CD
2	R	223	B3Y	CB-CA-CG-CD
2	P	211	B3E	N-CA-CG-CD
2	Q	211	B3E	N-CA-CG-CD
2	R	215	BIL	C-CA-CB-N
2	P	207[A]	HT7	O-C-CA-CB
2	P	211	B3E	O-C-CB-CA
2	Q	211	B3E	O-C-CB-CA
2	R	211	B3E	O-C-CB-CA
2	R	223	B3Y	O-C-CB-CA
2	S	211	B3E	O-C-CB-CA
2	Q	215	BIL	O-C-CA-CB
2	S	215	BIL	O-C-CA-CB
2	Q	211	B3E	CG-CD-CE-OF1
2	S	223	B3Y	N-CA-CB-C

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Mol	Chain	Res	Type	Atoms
2	Q	211	B3E	CG-CD-CE-OF2
2	P	211	B3E	CE-CD-CG-CA
2	S	211	B3E	CG-CD-CE-OF1
2	R	211	B3E	CG-CD-CE-OF1
2	P	223	B3Y	O-C-CB-CA
2	S	223	B3Y	O-C-CB-CA
2	S	211	B3E	CG-CD-CE-OF2

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	S	207[A]	HT7	7	0
2	P	207[B]	HT7	4	0
2	Q	211	B3E	5	0
2	R	207[B]	HT7	3	0
2	P	207[A]	HT7	1	0
2	S	207[B]	HT7	2	0
2	R	207[A]	HT7	3	0
2	Q	215	BIL	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	141/158 (89%)	-0.20	0	100	100	27, 35, 70, 78	5 (3%)
1	B	144/158 (91%)	-0.22	0	100	100	24, 35, 54, 64	9 (6%)
1	C	138/158 (87%)	-0.19	0	100	100	26, 35, 58, 72	8 (5%)
1	D	141/158 (89%)	-0.19	0	100	100	26, 38, 55, 77	10 (7%)
2	P	12/19 (63%)	-0.10	0	100	100	30, 37, 56, 58	0
2	Q	13/19 (68%)	-0.14	0	100	100	31, 34, 42, 47	0
2	R	12/19 (63%)	-0.25	0	100	100	37, 42, 51, 55	0
2	S	13/19 (68%)	-0.15	0	100	100	36, 41, 50, 51	1 (7%)
All	All	614/708 (86%)	-0.20	0	100	100	24, 36, 58, 78	33 (5%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95th 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
2	HT7	R	207[A]	15/16	0.85	0.26	44,50,53,53	12
2	HT7	R	207[B]	15/16	0.85	0.26	43,50,53,53	12
2	HT7	P	207[A]	15/16	0.88	0.19	46,51,56,56	12
2	HT7	P	207[B]	15/16	0.88	0.19	45,51,56,56	12
2	HT7	S	207[A]	15/16	0.89	0.26	41,44,46,49	12
2	HT7	S	207[B]	15/16	0.89	0.26	41,44,49,49	12
2	B3E	P	211	10/11	0.93	0.20	38,45,60,64	0
2	B3E	R	211	10/11	0.93	0.20	40,47,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HT7	Q	207	15/16	0.94	0.20	39,51,65,66	0
2	B3Y	R	223	13/14	0.94	0.17	38,44,48,53	0
2	BIL	R	215	9/10	0.94	0.19	37,41,42,48	0
2	BIL	Q	215	9/10	0.95	0.19	30,33,36,36	0
2	B3E	S	211	10/11	0.95	0.15	29,37,45,45	0
2	BIL	P	215	9/10	0.96	0.18	32,38,42,44	0
2	B3Y	P	223	13/14	0.96	0.12	31,35,39,39	0
2	B3Y	S	223	13/14	0.96	0.16	34,43,48,54	0
2	B3Y	Q	223	13/14	0.97	0.14	32,34,43,43	0
2	B3E	Q	211	10/11	0.97	0.17	21,32,36,36	0
2	BIL	S	215	9/10	0.97	0.15	28,37,40,42	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.