W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 11, 2016 – 02:14 PM EDT

PDB ID	:	5AFV
Title	:	Pharmacophore-based virtual screening to discover new active compounds for human choline kinase alpha1.
Authors	:	Serran-Aguilera, L.; Nuti, R.; Lopez-Cara, L.C.; Gallo Mezo, M.A.; Macchiarulo, A.; Entrena, A.; Hurtado-Guerrero, R.
Deposited on	:	2015-01-26
Resolution	:	2.25 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

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 2.25 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	Percentile Ranks	Value
Rfree		0.273
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		3.6%
RSRZ outliers		5.4%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
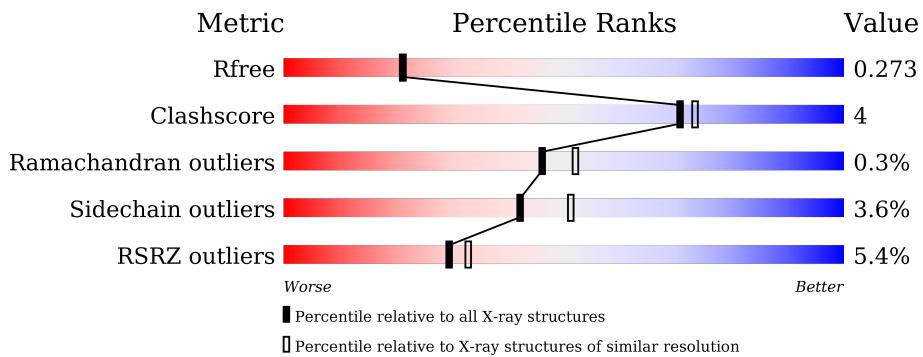
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	378	3% ▮ 83% 10% · 6%
1	B	378	7% ▮ 84% 9% · 6%
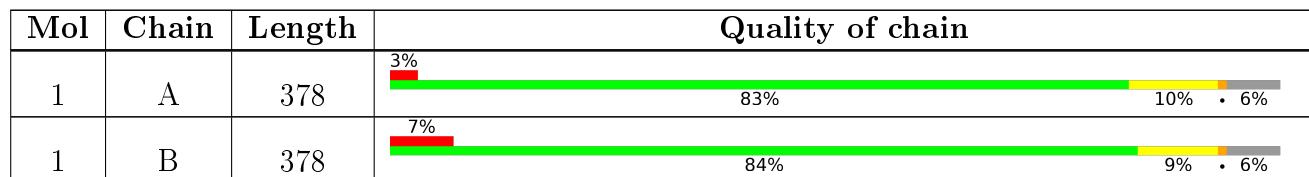
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	1458	-	-	-	X
2	EDO	A	1461	-	-	-	X
3	JH5	A	1463	-	-	-	X
3	JH5	B	1460	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6268 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 CHOLINE KINASE ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total 2966	C 1916	N 499	O 534	S 17	0	3	0
1	B	354	Total 2949	C 1905	N 495	O 533	S 16	0	1	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0
2	A	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total C O 4 2 2			0	0
2	B	1	Total C O 4 2 2			0	0

- Molecule 3 is 1-BENZYL-4-(BENZYLAMINO)-1H-1,2,4-TRIAZOL-4-IUM (three-letter code: JH5) (formula: $C_{16}H_{17}N_4$).
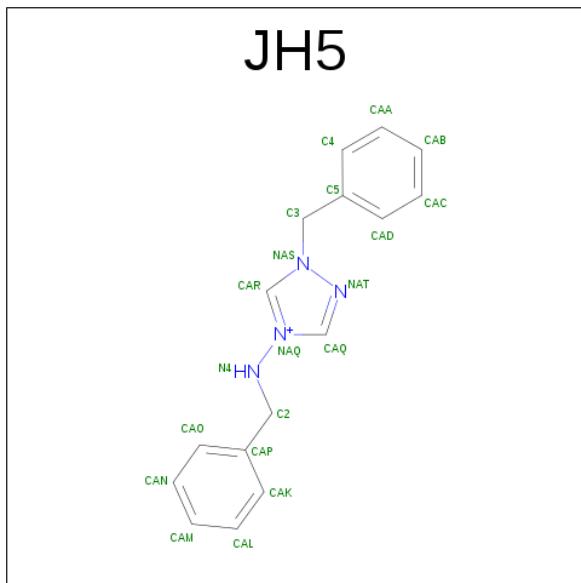
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total C N 20 16 4			0	0
3	B	1	Total C N 20 16 4			0	0
3	B	1	Total C N 20 16 4			0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total O 131 131		0	0
4	B	138	Total O 138 138		0	0

3 Residue-property plots ⓘ

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: CHOLINE KINASE ALPHA

- Molecule 1: CHOLINE KINASE ALPHA
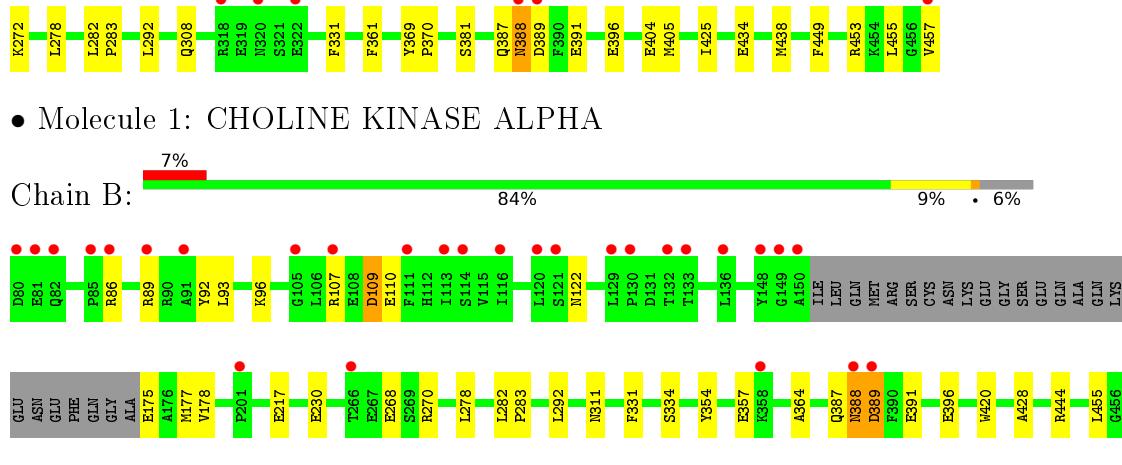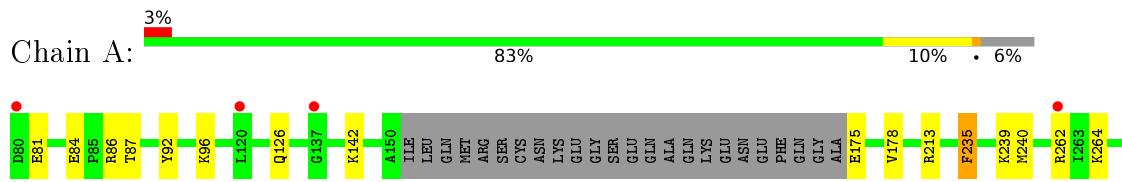
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	56.13Å 120.18Å 132.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	132.39 – 2.25 19.87 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (132.39-2.25) 99.7 (19.87-2.25)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.224 , 0.267 0.227 , 0.273	Depositor DCC
R_{free} test set	1236 reflections (2.95%)	DCC
Wilson B-factor (Å^2)	37.4	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 37.7	EDS
L-test for twinning[2]	$< |L| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6268	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: JH5, EDO

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	0.68	0/3045	0.79	0/4100
1	B	0.65	0/3025	0.76	1/4074 (0.0%)
All	All	0.66	0/6070	0.77	1/8174 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	444	ARG	NE-CZ-NH1	5.58	123.09	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2966	0	2935	27	0
1	B	2949	0	2911	22	0
2	A	20	0	30	3	0
2	B	4	0	6	1	0
3	A	20	0	17	4	0
3	B	40	0	34	6	0
4	A	131	0	0	3	4
4	B	138	0	0	3	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6268	0	5933	52	4

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 (52) 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:425:ILE:HA	1:A:438[B]:MET:HE1	1.33	1.10
1:A:438[B]:MET:HE2	1:A:438[B]:MET:HA	1.39	1.03
1:A:438[B]:MET:CE	1:A:438[B]:MET:HA	1.98	0.94
1:A:178:VAL:HG22	1:B:178:VAL:HG22	1.56	0.88
3:A:1463:JH5:HAR	3:A:1463:JH5:C4	2.06	0.85
1:A:126:GLN:OE1	1:A:142:LYS:HD3	1.81	0.79
1:A:308:GLN:HE22	3:A:1463:JH5:HAL	1.56	0.70
3:B:1460:JH5:CAR	3:B:1460:JH5:C4	2.61	0.68
1:A:235:PHE:HZ	1:A:331:PHE:CE1	2.15	0.65
1:A:438[B]:MET:CE	1:A:438[B]:MET:CA	2.76	0.63
1:A:84[B]:GLU:HG3	1:A:87:THR:OG1	1.99	0.62
1:B:107:ARG:N	1:B:110:GLU:OE1	2.33	0.62
1:B:331:PHE:HB3	1:B:334:SER:OG	2.00	0.60
1:A:453:ARG:NH1	4:A:2126:HOH:O	2.35	0.60
1:A:235:PHE:CZ	1:A:331:PHE:CE1	2.90	0.58
1:B:92:TYR:OH	1:B:107:ARG:HA	2.04	0.58
3:A:1463:JH5:C4	3:A:1463:JH5:CAR	2.76	0.56
1:B:109:ASP:HB3	4:B:2007:HOH:O	2.04	0.56
1:B:311:ASN:OD1	3:B:1459:JH5:N4	2.38	0.56
1:B:270:ARG:NH1	1:B:428:ALA:O	2.39	0.55
1:B:292:LEU:HD22	1:B:457:VAL:HG11	1.91	0.51
1:A:449:PHE:O	1:A:453:ARG:HG3	2.10	0.51
1:B:389:ASP:N	1:B:389:ASP:OD1	2.41	0.51
1:B:364:ALA:HB1	2:B:1458:EDO:H12	1.94	0.49
1:A:86:ARG:NH1	4:A:2005:HOH:O	2.45	0.49
1:A:292:LEU:HD22	1:A:457:VAL:HG11	1.93	0.49
1:B:89:ARG:O	1:B:93:LEU:HG	2.13	0.49
3:B:1459:JH5:CAR	3:B:1459:JH5:C4	2.89	0.49
1:B:331:PHE:HB3	1:B:334:SER:HG	1.78	0.49
1:A:175:GLU:N	4:A:2029:HOH:O	2.46	0.48
1:B:107:ARG:CA	1:B:110:GLU:OE1	2.62	0.48
1:A:387:GLN:O	1:A:388:ASN:HB2	2.13	0.47
1:A:361:PHE:CE2	1:A:434:GLU:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLN:HE22	3:A:1463:JH5:CAL	2.27	0.46
1:A:391:GLU:H	1:A:391:GLU:CD	2.19	0.45
1:A:404:GLU:HA	2:A:1462:EDO:H11	1.99	0.45
1:B:387:GLN:O	1:B:388:ASN:HB2	2.16	0.45
1:A:84[B]:GLU:CG	1:A:87:THR:OG1	2.63	0.45
1:B:420:TRP:CZ3	3:B:1460:JH5:H31C	2.53	0.44
1:A:92:TYR:OH	1:A:96:LYS:NZ	2.50	0.44
1:A:282:LEU:N	1:A:283:PRO:CD	2.81	0.43
1:A:240:MET:HA	2:A:1459:EDO:H11	2.01	0.43
1:B:282:LEU:N	1:B:283:PRO:CD	2.81	0.42
1:B:107:ARG:CB	1:B:110:GLU:OE1	2.67	0.42
1:B:354:TYR:OH	3:B:1460:JH5:HAQ	2.18	0.42
1:B:217:GLU:CD	1:B:217:GLU:H	2.24	0.41
1:A:369:TYR:CG	1:A:370:PRO:HD2	2.56	0.41
1:B:175:GLU:N	4:B:2011:HOH:O	2.54	0.41
1:B:177:MET:HE1	4:B:2026:HOH:O	2.21	0.41
1:B:122:ASN:HD22	3:B:1459:JH5:H32C	1.85	0.40
1:A:405:MET:N	2:A:1461:EDO:H21	2.36	0.40
1:A:126:GLN:HE21	1:A:126:GLN:HB3	1.68	0.40

All (4) 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)
4:A:2075:HOH:O	4:A:2100:HOH:O[4_445]	1.79	0.41
4:A:2129:HOH:O	4:B:2018:HOH:O[2_555]	1.93	0.27
4:A:2067:HOH:O	4:B:2121:HOH:O[3_544]	1.99	0.21
4:A:2119:HOH:O	4:B:2118:HOH:O[3_544]	2.18	0.02

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	353/378 (93%)	341 (97%)	11 (3%)	1 (0%)	46	52
1	B	351/378 (93%)	338 (96%)	12 (3%)	1 (0%)	46	52
All	All	704/756 (93%)	679 (96%)	23 (3%)	2 (0%)	46	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	B	388	ASN

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	321/338 (95%)	309 (96%)	12 (4%)	41	50
1	B	319/338 (94%)	308 (97%)	11 (3%)	44	54
All	All	640/676 (95%)	617 (96%)	23 (4%)	42	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	GLU
1	A	213	ARG
1	A	235	PHE
1	A	239	LYS
1	A	262	ARG
1	A	264	LYS
1	A	272	LYS
1	A	278	LEU
1	A	381	SER
1	A	389	ASP
1	A	396	GLU
1	A	455	LEU
1	B	86	ARG
1	B	96	LYS

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Mol	Chain	Res	Type
1	B	109	ASP
1	B	230	GLU
1	B	268	GLU
1	B	278	LEU
1	B	357	GLU
1	B	389	ASP
1	B	391	GLU
1	B	396	GLU
1	B	455	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	320	ASN
1	B	122	ASN

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 ⓘ

9 ligands 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	EDO	A	1458	-	3,3,3	0.57	0	2,2,2	0.48	0
2	EDO	A	1459	-	3,3,3	0.40	0	2,2,2	0.85	0
2	EDO	A	1460	-	3,3,3	0.40	0	2,2,2	0.48	0
2	EDO	A	1461	-	3,3,3	0.39	0	2,2,2	0.33	0
2	EDO	A	1462	-	3,3,3	0.59	0	2,2,2	0.41	0
3	JH5	A	1463	-	18,22,22	2.81	2 (11%)	18,28,28	2.01	3 (16%)
2	EDO	B	1458	-	3,3,3	0.61	0	2,2,2	0.29	0
3	JH5	B	1459	-	18,22,22	2.06	3 (16%)	18,28,28	0.97	1 (5%)
3	JH5	B	1460	-	18,22,22	3.20	4 (22%)	18,28,28	2.74	1 (5%)

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	EDO	A	1458	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1459	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1460	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1461	-	-	0/1/1/1	0/0/0/0
2	EDO	A	1462	-	-	0/1/1/1	0/0/0/0
3	JH5	A	1463	-	-	0/7/9/9	0/3/3/3
2	EDO	B	1458	-	-	0/1/1/1	0/0/0/0
3	JH5	B	1459	-	-	0/7/9/9	0/3/3/3
3	JH5	B	1460	-	-	0/7/9/9	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1460	JH5	NAT-NAS	-11.13	1.19	1.35
3	A	1463	JH5	NAT-NAS	-9.28	1.22	1.35
3	A	1463	JH5	C3-C5	-6.39	1.36	1.51
3	B	1460	JH5	C3-C5	-5.69	1.37	1.51
3	B	1459	JH5	NAT-NAS	-5.34	1.27	1.35
3	B	1459	JH5	C3-C5	-4.43	1.40	1.51
3	B	1459	JH5	C2-CAP	-4.36	1.41	1.51
3	B	1460	JH5	C2-CAP	-3.33	1.43	1.51
3	B	1460	JH5	C3-NAS	2.84	1.52	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1460	JH5	C5-C3-NAS	-11.31	95.54	112.17
3	A	1463	JH5	C5-C3-NAS	-6.22	103.03	112.17
3	A	1463	JH5	C2-CAP-CAO	-2.22	116.10	120.91
3	B	1459	JH5	C3-C5-C4	2.21	124.81	120.41
3	A	1463	JH5	C2-CAP-CAK	3.69	128.91	120.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1459	EDO	1	0
2	A	1461	EDO	1	0
2	A	1462	EDO	1	0
3	A	1463	JH5	4	0
2	B	1458	EDO	1	0
3	B	1459	JH5	3	0
3	B	1460	JH5	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 (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(Å²)	Q<0.9
1	A	354/378 (93%)	-0.03	10 (2%)	56	61	22, 38, 64, 79	2 (0%)
1	B	354/378 (93%)	0.28	28 (7%)	15	17	20, 41, 89, 105	2 (0%)
All	All	708/756 (93%)	0.12	38 (5%)	29	33	20, 39, 82, 105	4 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	81	GLU	6.2
1	B	120	LEU	6.0
1	B	121	SER	5.3
1	B	136	LEU	5.2
1	B	129	LEU	5.1
1	B	388	ASN	5.1
1	B	82	GLN	4.8
1	B	80	ASP	4.2
1	B	113	ILE	4.2
1	B	132	THR	4.0
1	B	105	GLY	3.9
1	B	111	PHE	3.9
1	B	149	GLY	3.9
1	B	130	PRO	3.6
1	B	107	ARG	3.6
1	B	89	ARG	3.5
1	B	116	ILE	3.5
1	A	388	ASN	3.4
1	B	266	THR	3.4
1	A	137	GLY	3.4
1	A	389	ASP	3.2
1	A	322	GLU	3.2
1	B	148	TYR	2.9
1	B	133	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	86	ARG	2.8
1	A	80	ASP	2.7
1	B	150	ALA	2.6
1	B	85	PRO	2.6
1	B	201	PRO	2.5
1	A	318	ARG	2.4
1	A	320	ASN	2.4
1	B	389	ASP	2.4
1	B	114	SER	2.3
1	A	457	VAL	2.2
1	A	262	ARG	2.1
1	B	358	LYS	2.1
1	A	120	LEU	2.0
1	B	91	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, 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	LLDF	B-factors($Å^2$)	Q<0.9
3	JH5	A	1463	20/20	0.73	0.31	5.55	63,82,94,95	0
2	EDO	A	1458	4/4	0.67	0.21	3.97	58,59,59,60	0
3	JH5	B	1460	20/20	0.79	0.23	3.00	65,76,92,93	0
2	EDO	A	1461	4/4	0.92	0.17	2.84	42,44,45,46	0
2	EDO	B	1458	4/4	0.89	0.16	1.72	41,49,50,54	0
3	JH5	B	1459	20/20	0.77	0.24	0.94	81,94,100,105	0
2	EDO	A	1462	4/4	0.86	0.15	0.31	50,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
2	EDO	A	1459	4/4	0.92	0.13	-0.21	43,44,46,47	0
2	EDO	A	1460	4/4	0.80	0.41	-	61,62,63,67	0

6.5 Other polymers (i)

There are no such residues in this entry.