Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:06 PM GMT

PDB ID	:	4BHY
Title	:	Structure of alanine racemase from Aeromonas hydrophila
Authors	:	Otero, L.H.; Carrasco-Lopez, C.; Bernardo-Garcia, N.; Hermoso, J.A.
Deposited on	:	2013-04-09
Resolution	:	3.25 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:

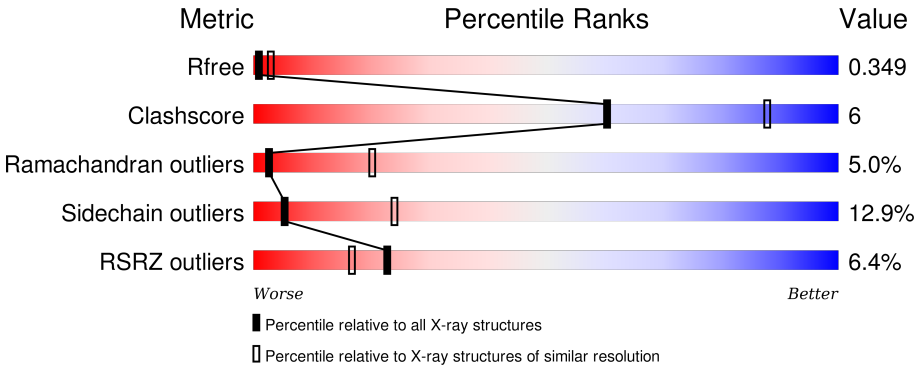
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.25 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

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	6% 67% 18% • 14%
1	B	378	4% 61% 19% • • 15%
1	C	378	5% 61% 19% • • 16%
1	D	378	7% 67% 18% • • 11%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10083 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 ALANINE RACEMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2493	1600	423	457	13			
1	B	320	Total	C	N	O	S	0	0	0
			2473	1582	424	454	13			
1	C	317	Total	C	N	O	S	0	0	0
			2412	1542	411	444	15			
1	D	336	Total	C	N	O	S	0	0	0
			2570	1644	436	476	14			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	EXPRESSION TAG	UNP A0KH11
A	-19	HIS	-	EXPRESSION TAG	UNP A0KH11
A	-18	HIS	-	EXPRESSION TAG	UNP A0KH11
A	-17	HIS	-	EXPRESSION TAG	UNP A0KH11
A	-16	HIS	-	EXPRESSION TAG	UNP A0KH11
A	-15	HIS	-	EXPRESSION TAG	UNP A0KH11
A	-14	HIS	-	EXPRESSION TAG	UNP A0KH11
A	-13	ASP	-	EXPRESSION TAG	UNP A0KH11
A	-12	TYR	-	EXPRESSION TAG	UNP A0KH11
A	-11	ASP	-	EXPRESSION TAG	UNP A0KH11
A	-10	ILE	-	EXPRESSION TAG	UNP A0KH11
A	-9	PRO	-	EXPRESSION TAG	UNP A0KH11
A	-8	THR	-	EXPRESSION TAG	UNP A0KH11
A	-7	THR	-	EXPRESSION TAG	UNP A0KH11
A	-6	GLU	-	EXPRESSION TAG	UNP A0KH11
A	-5	ASN	-	EXPRESSION TAG	UNP A0KH11
A	-4	LEU	-	EXPRESSION TAG	UNP A0KH11
A	-3	TYR	-	EXPRESSION TAG	UNP A0KH11
A	-2	PHE	-	EXPRESSION TAG	UNP A0KH11
A	-1	GLN	-	EXPRESSION TAG	UNP A0KH11
A	0	SER	-	EXPRESSION TAG	UNP A0KH11

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	EXPRESSION TAG	UNP A0KH11
B	-19	HIS	-	EXPRESSION TAG	UNP A0KH11
B	-18	HIS	-	EXPRESSION TAG	UNP A0KH11
B	-17	HIS	-	EXPRESSION TAG	UNP A0KH11
B	-16	HIS	-	EXPRESSION TAG	UNP A0KH11
B	-15	HIS	-	EXPRESSION TAG	UNP A0KH11
B	-14	HIS	-	EXPRESSION TAG	UNP A0KH11
B	-13	ASP	-	EXPRESSION TAG	UNP A0KH11
B	-12	TYR	-	EXPRESSION TAG	UNP A0KH11
B	-11	ASP	-	EXPRESSION TAG	UNP A0KH11
B	-10	ILE	-	EXPRESSION TAG	UNP A0KH11
B	-9	PRO	-	EXPRESSION TAG	UNP A0KH11
B	-8	THR	-	EXPRESSION TAG	UNP A0KH11
B	-7	THR	-	EXPRESSION TAG	UNP A0KH11
B	-6	GLU	-	EXPRESSION TAG	UNP A0KH11
B	-5	ASN	-	EXPRESSION TAG	UNP A0KH11
B	-4	LEU	-	EXPRESSION TAG	UNP A0KH11
B	-3	TYR	-	EXPRESSION TAG	UNP A0KH11
B	-2	PHE	-	EXPRESSION TAG	UNP A0KH11
B	-1	GLN	-	EXPRESSION TAG	UNP A0KH11
B	0	SER	-	EXPRESSION TAG	UNP A0KH11
C	-20	MET	-	EXPRESSION TAG	UNP A0KH11
C	-19	HIS	-	EXPRESSION TAG	UNP A0KH11
C	-18	HIS	-	EXPRESSION TAG	UNP A0KH11
C	-17	HIS	-	EXPRESSION TAG	UNP A0KH11
C	-16	HIS	-	EXPRESSION TAG	UNP A0KH11
C	-15	HIS	-	EXPRESSION TAG	UNP A0KH11
C	-14	HIS	-	EXPRESSION TAG	UNP A0KH11
C	-13	ASP	-	EXPRESSION TAG	UNP A0KH11
C	-12	TYR	-	EXPRESSION TAG	UNP A0KH11
C	-11	ASP	-	EXPRESSION TAG	UNP A0KH11
C	-10	ILE	-	EXPRESSION TAG	UNP A0KH11
C	-9	PRO	-	EXPRESSION TAG	UNP A0KH11
C	-8	THR	-	EXPRESSION TAG	UNP A0KH11
C	-7	THR	-	EXPRESSION TAG	UNP A0KH11
C	-6	GLU	-	EXPRESSION TAG	UNP A0KH11
C	-5	ASN	-	EXPRESSION TAG	UNP A0KH11
C	-4	LEU	-	EXPRESSION TAG	UNP A0KH11
C	-3	TYR	-	EXPRESSION TAG	UNP A0KH11
C	-2	PHE	-	EXPRESSION TAG	UNP A0KH11
C	-1	GLN	-	EXPRESSION TAG	UNP A0KH11
C	0	SER	-	EXPRESSION TAG	UNP A0KH11

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	EXPRESSION TAG	UNP A0KH11
D	-19	HIS	-	EXPRESSION TAG	UNP A0KH11
D	-18	HIS	-	EXPRESSION TAG	UNP A0KH11
D	-17	HIS	-	EXPRESSION TAG	UNP A0KH11
D	-16	HIS	-	EXPRESSION TAG	UNP A0KH11
D	-15	HIS	-	EXPRESSION TAG	UNP A0KH11
D	-14	HIS	-	EXPRESSION TAG	UNP A0KH11
D	-13	ASP	-	EXPRESSION TAG	UNP A0KH11
D	-12	TYR	-	EXPRESSION TAG	UNP A0KH11
D	-11	ASP	-	EXPRESSION TAG	UNP A0KH11
D	-10	ILE	-	EXPRESSION TAG	UNP A0KH11
D	-9	PRO	-	EXPRESSION TAG	UNP A0KH11
D	-8	THR	-	EXPRESSION TAG	UNP A0KH11
D	-7	THR	-	EXPRESSION TAG	UNP A0KH11
D	-6	GLU	-	EXPRESSION TAG	UNP A0KH11
D	-5	ASN	-	EXPRESSION TAG	UNP A0KH11
D	-4	LEU	-	EXPRESSION TAG	UNP A0KH11
D	-3	TYR	-	EXPRESSION TAG	UNP A0KH11
D	-2	PHE	-	EXPRESSION TAG	UNP A0KH11
D	-1	GLN	-	EXPRESSION TAG	UNP A0KH11
D	0	SER	-	EXPRESSION TAG	UNP A0KH11

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	23	Total O 23 23	0	0
2	B	34	Total O 34 34	0	0
2	C	30	Total O 30 30	0	0
2	D	26	Total O 26 26	0	0
2	B	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0
2	B	2	Total O 2 2	0	0
2	D	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0

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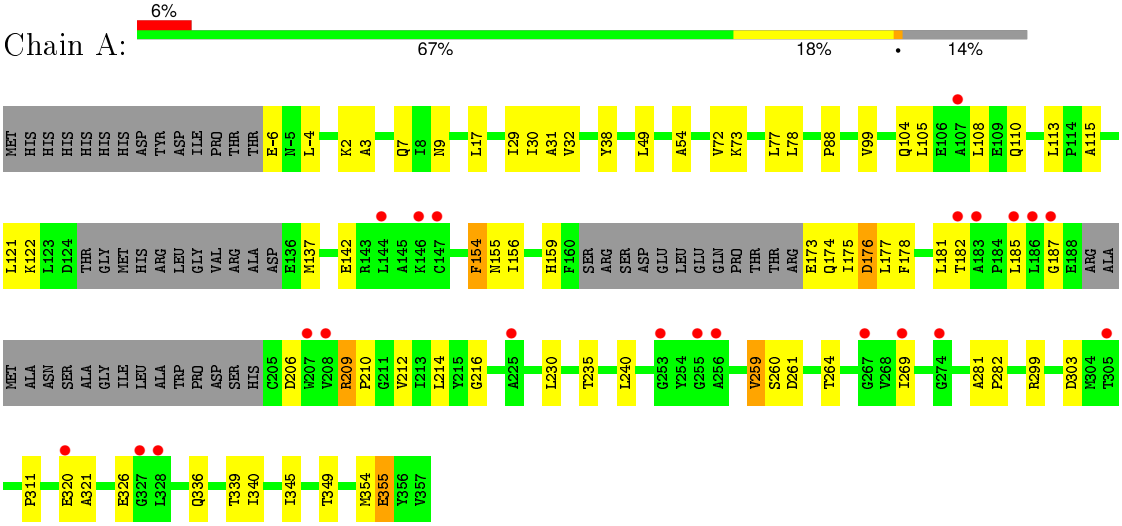
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O 1 1	0	0
2	A	2	Total O 2 2	0	0
2	B	2	Total O 2 2	0	0
2	D	1	Total O 1 1	0	0
2	B	1	Total O 1 1	0	0
2	D	1	Total O 1 1	0	0
2	C	2	Total O 2 2	0	0
2	D	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0
2	B	1	Total O 1 1	0	0
2	A	1	Total O 1 1	0	0

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.

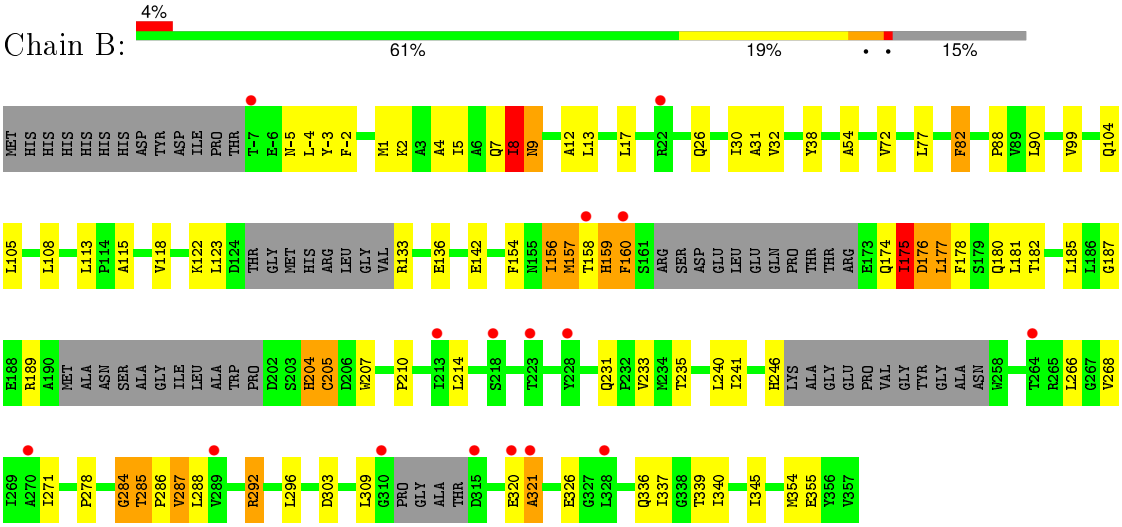
- Molecule 1: ALANINE RACEMASE

Chain A:



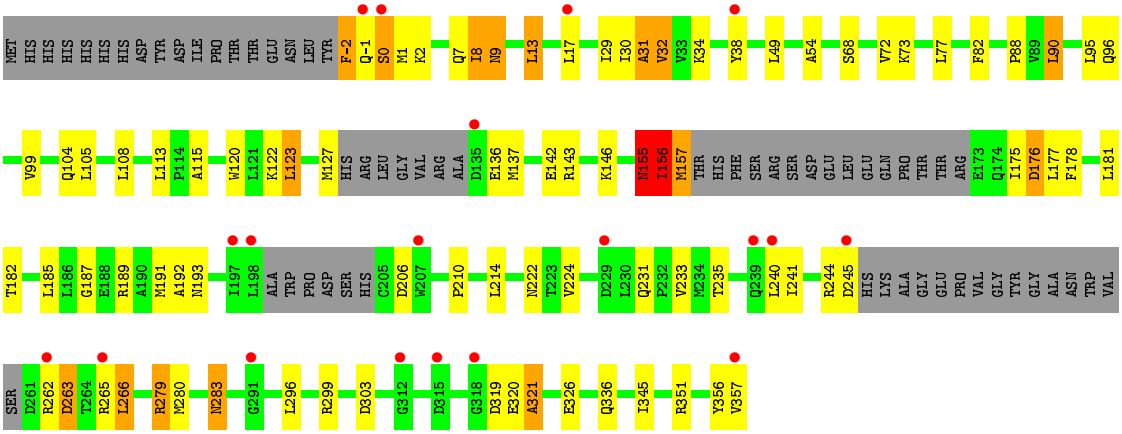
- Molecule 1: ALANINE RACEMASE

Chain B:



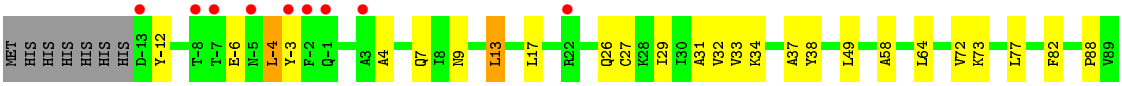
- Molecule 1: ALANINE RACEMASE

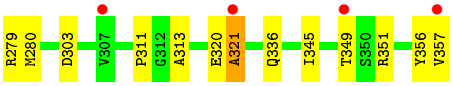
Chain C:



- Molecule 1: ALANINE RACEMASE

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	110.80Å 134.74Å 192.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 3.25 47.99 – 3.25	Depositor EDS
% Data completeness (in resolution range)	92.5 (47.32-3.25) 92.5 (47.99-3.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.256 , 0.292 0.302 , 0.349	Depositor DCC
R_{free} test set	2173 reflections (11.37%)	DCC
Wilson B-factor (Å^2)	95.5	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 131.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 21285 reflections	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	10083	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: KCX

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	0.43	0/2532	0.62	1/3453 (0.0%)
1	B	0.46	0/2508	0.69	6/3415 (0.2%)
1	C	0.45	0/2442	0.69	4/3325 (0.1%)
1	D	0.44	0/2607	0.65	4/3552 (0.1%)
All	All	0.44	0/10089	0.66	15/13745 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	ALA	C-N-CA	7.54	140.54	121.70
1	B	156	ILE	C-N-CA	6.62	138.25	121.70
1	D	154	PHE	C-N-CA	6.30	137.44	121.70
1	B	31	ALA	C-N-CA	6.28	137.41	121.70
1	A	31	ALA	C-N-CA	6.23	137.28	121.70
1	D	31	ALA	C-N-CA	6.20	137.20	121.70
1	D	191	MET	C-N-CA	5.96	136.59	121.70
1	C	155	ASN	C-N-CA	5.87	136.37	121.70
1	B	8	ILE	C-N-CA	5.83	136.27	121.70
1	D	229	ASP	C-N-CA	5.70	135.96	121.70
1	C	8	ILE	C-N-CA	5.61	135.72	121.70
1	B	284	GLY	C-N-CA	5.42	135.26	121.70
1	C	-2	PHE	C-N-CA	5.34	135.04	121.70
1	B	204	HIS	C-N-CA	5.25	134.83	121.70
1	B	175	ILE	C-N-CA	5.24	134.80	121.70

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	2493	0	2521	19	0
1	B	2473	0	2496	31	0
1	C	2412	0	2461	35	0
1	D	2570	0	2593	37	0
2	A	26	0	0	0	0
2	B	42	0	0	0	0
2	C	35	0	0	0	0
2	D	32	0	0	0	0
All	All	10083	0	10071	113	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 6.

All (113) 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:204:HIS:HA	1:B:205:CYS:HB2	1.29	1.13
1:D:229:ASP:HA	1:D:230:LEU:HB2	1.39	1.01
1:B:8:ILE:HA	1:B:9:ASN:HB2	1.60	0.84
1:D:245:ASP:H	1:D:246:HIS:HA	1.43	0.83
1:C:155:ASN:HA	1:C:156:ILE:HG22	1.61	0.83
1:C:31:ALA:HA	1:C:32:VAL:HG22	1.67	0.76
1:D:191:MET:HA	1:D:192:ALA:CB	2.18	0.73
1:C:191:MET:HB3	1:C:192:ALA:HB2	1.69	0.73
1:A:339:THR:HG22	1:D:279:ARG:HE	1.54	0.72
1:B:204:HIS:CA	1:B:205:CYS:HB2	2.15	0.69
1:D:229:ASP:CA	1:D:230:LEU:HB2	2.20	0.69
1:D:191:MET:HA	1:D:192:ALA:HB3	1.76	0.66
1:B:122:KCX:HB3	1:B:157:MET:HB3	1.79	0.65
1:D:121:LEU:HB3	1:D:156:ILE:HG22	1.80	0.64
1:D:356:TYR:H	1:D:357:VAL:HA	1.64	0.63
1:B:156:ILE:HA	1:B:157:MET:HB2	1.83	0.60
1:D:34:LYS:HG3	1:D:58:ALA:HB2	1.83	0.59
1:C:88:PRO:HB2	1:D:72:VAL:HG11	1.83	0.59
1:B:284:GLY:HA2	1:B:285:THR:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:LEU:HD22	1:D:233:VAL:HG11	1.85	0.58
1:A:259:VAL:HG13	1:A:260:SER:H	1.69	0.58
1:C:263:ASP:HB2	1:C:266:LEU:HD13	1.85	0.58
1:C:157:MET:H	1:C:189:ARG:HA	1.70	0.57
1:C:72:VAL:HG11	1:D:88:PRO:HB2	1.86	0.57
1:B:175:ILE:HA	1:B:176:ASP:HB2	1.86	0.56
1:A:264:THR:HA	1:A:311:PRO:HG3	1.87	0.55
1:B:82:PHE:HB2	1:C:241:ILE:HG23	1.88	0.55
1:B:292:ARG:HH22	1:B:309:LEU:HB2	1.72	0.54
1:C:96:GLN:HB3	1:C:120:TRP:HE1	1.73	0.54
1:C:-2:PHE:HB2	1:C:0:SER:H	1.73	0.54
1:D:191:MET:HG3	1:D:192:ALA:HB3	1.90	0.54
1:D:259:VAL:HG22	1:D:260:SER:H	1.74	0.53
1:B:156:ILE:O	1:B:189:ARG:HA	2.09	0.53
1:B:38:TYR:HB3	1:B:345:ILE:HD12	1.92	0.52
1:A:88:PRO:HB2	1:B:72:VAL:HG11	1.92	0.52
1:B:235:THR:HG22	1:B:326:GLU:H	1.75	0.51
1:A:99:VAL:HG13	1:A:104:GLN:HG3	1.91	0.51
1:A:235:THR:HG22	1:A:326:GLU:H	1.74	0.51
1:C:38:TYR:HB3	1:C:345:ILE:HD12	1.92	0.51
1:D:38:TYR:HB3	1:D:345:ILE:HD12	1.91	0.51
1:C:13:LEU:HB3	1:C:233:VAL:HG11	1.93	0.51
1:A:17:LEU:HD13	1:A:49:LEU:HD22	1.93	0.51
1:D:7:GLN:HB3	1:D:235:THR:HG23	1.91	0.51
1:D:182:THR:HA	1:D:185:LEU:HD12	1.91	0.51
1:C:99:VAL:HG13	1:C:104:GLN:HG3	1.92	0.51
1:C:235:THR:HG22	1:C:326:GLU:H	1.76	0.51
1:D:252:VAL:HG21	1:D:259:VAL:HG12	1.93	0.51
1:B:182:THR:HA	1:B:185:LEU:HD12	1.91	0.51
1:C:182:THR:HA	1:C:185:LEU:HD12	1.93	0.50
1:A:182:THR:HA	1:A:185:LEU:HD12	1.92	0.50
1:D:17:LEU:HD13	1:D:49:LEU:HD22	1.94	0.50
1:C:320:GLU:HG2	1:C:321:ALA:H	1.76	0.50
1:B:99:VAL:HG13	1:B:104:GLN:HG3	1.92	0.50
1:D:238:THR:HB	1:D:271:ILE:HD12	1.93	0.49
1:A:72:VAL:HG11	1:B:88:PRO:HB2	1.95	0.49
1:A:216:GLY:HA2	1:A:230:LEU:HD12	1.94	0.49
1:C:17:LEU:HD13	1:C:49:LEU:HD22	1.94	0.49
1:B:175:ILE:HG21	1:B:178:PHE:HB2	1.95	0.48
1:A:38:TYR:HB3	1:A:345:ILE:HD12	1.95	0.48
1:B:287:VAL:HG21	1:B:296:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:GLU:HG2	1:D:321:ALA:H	1.77	0.48
1:C:240:LEU:HD13	1:C:319:ASP:HB2	1.95	0.48
1:B:5:ILE:HD11	1:B:355:GLU:HB2	1.95	0.48
1:C:175:ILE:HB	1:C:176:ASP:HA	1.96	0.48
1:A:78:LEU:HD11	1:A:209:ARG:HH12	1.79	0.47
1:A:7:GLN:HA	1:A:355:GLU:HB3	1.97	0.46
1:B:278:PRO:HG2	1:B:337:ILE:HD13	1.97	0.46
1:D:210:PRO:HG2	1:D:214:LEU:HD13	1.98	0.46
1:B:210:PRO:HG2	1:B:214:LEU:HD13	1.97	0.46
1:B:241:ILE:HG13	1:B:268:VAL:HG13	1.97	0.46
1:D:175:ILE:HB	1:D:176:ASP:HA	1.97	0.46
1:A:210:PRO:HG2	1:A:214:LEU:HD13	1.97	0.46
1:B:320:GLU:HG3	1:B:321:ALA:H	1.80	0.46
1:C:210:PRO:HG2	1:C:214:LEU:HD13	1.98	0.45
1:C:68:SER:HA	1:D:64:LEU:HB3	1.98	0.45
1:C:356:TYR:H	1:C:357:VAL:HA	1.82	0.45
1:D:244:ARG:HA	1:D:245:ASP:HA	1.79	0.45
1:B:122:KCX:HG2	1:B:157:MET:O	2.17	0.45
1:D:154:PHE:HA	1:D:155:ASN:HB2	1.97	0.45
1:D:-4:LEU:HD13	1:D:-4:LEU:H	1.82	0.45
1:A:122:KCX:HA	1:A:178:PHE:CZ	2.52	0.45
1:B:8:ILE:CA	1:B:9:ASN:HB2	2.39	0.44
1:C:122:KCX:HA	1:C:178:PHE:CZ	2.53	0.44
1:B:339:THR:HA	1:C:279:ARG:HH21	1.83	0.43
1:C:191:MET:HB3	1:C:192:ALA:CB	2.45	0.43
1:B:246:HIS:HB3	1:B:266:LEU:HD13	1.98	0.43
1:C:122:KCX:HD3	1:C:123:LEU:N	2.33	0.43
1:C:283:ASN:HA	1:C:296:LEU:O	2.18	0.43
1:B:204:HIS:HA	1:B:205:CYS:CB	2.20	0.43
1:D:27:CYS:HB3	1:D:208:VAL:HG22	2.01	0.43
1:C:17:LEU:HD12	1:C:214:LEU:HD11	2.01	0.42
1:C:-2:PHE:HA	1:C:-1:GLN:HB2	2.00	0.42
1:A:17:LEU:HD12	1:A:214:LEU:HD11	2.01	0.42
1:A:30:ILE:HG12	1:A:54:ALA:HB3	2.00	0.42
1:A:264:THR:HG22	1:A:311:PRO:HD3	2.02	0.42
1:D:13:LEU:HD12	1:D:49:LEU:HD21	2.02	0.42
1:D:229:ASP:H	1:D:230:LEU:HD12	1.85	0.42
1:D:245:ASP:N	1:D:246:HIS:HA	2.21	0.42
1:C:90:LEU:HA	1:C:95:LEU:HD12	2.02	0.42
1:C:155:ASN:HA	1:C:156:ILE:CG2	2.42	0.42
1:D:33:VAL:HA	1:D:37:ALA:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:TYR:H	1:D:357:VAL:CA	2.32	0.41
1:D:17:LEU:HD12	1:D:214:LEU:HD11	2.03	0.41
1:C:30:ILE:HG12	1:C:54:ALA:HB3	2.01	0.41
1:B:159:HIS:HB3	1:B:160:PHE:HA	2.03	0.41
1:B:30:ILE:HG12	1:B:54:ALA:HB3	2.01	0.41
1:C:157:MET:N	1:C:189:ARG:HA	2.32	0.41
1:D:264:THR:HG22	1:D:311:PRO:HG3	2.03	0.41
1:D:90:LEU:HA	1:D:95:LEU:HD12	2.03	0.41
1:B:12:ALA:HB3	1:B:233:VAL:HG12	2.02	0.40
1:C:244:ARG:HA	1:C:245:ASP:HA	1.83	0.40
1:A:349:THR:HA	1:D:349:THR:HA	2.02	0.40
1:C:8:ILE:HA	1:C:9:ASN:CB	2.51	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	316/378 (84%)	275 (87%)	27 (8%)	14 (4%)	3	23
1	B	307/378 (81%)	253 (82%)	34 (11%)	20 (6%)	1	13
1	C	306/378 (81%)	259 (85%)	33 (11%)	14 (5%)	3	22
1	D	323/378 (85%)	273 (84%)	35 (11%)	15 (5%)	3	22
All	All	1252/1512 (83%)	1060 (85%)	129 (10%)	63 (5%)	3	20

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	154	PHE
1	A	155	ASN

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Mol	Chain	Res	Type
1	A	282	PRO
1	B	32	VAL
1	B	154	PHE
1	B	205	CYS
1	C	32	VAL
1	C	136	GLU
1	C	263	ASP
1	C	280	MET
1	D	32	VAL
1	D	175	ILE
1	D	230	LEU
1	B	9	ASN
1	B	157	MET
1	B	287	VAL
1	B	354	MET
1	C	9	ASN
1	C	155	ASN
1	C	224	VAL
1	C	321	ALA
1	D	4	ALA
1	D	192	ALA
1	D	256	ALA
1	D	321	ALA
1	A	175	ILE
1	A	187	GLY
1	A	281	ALA
1	A	321	ALA
1	B	4	ALA
1	B	176	ASP
1	B	177	LEU
1	B	285	THR
1	B	321	ALA
1	D	-12	TYR
1	D	155	ASN
1	D	313	ALA
1	A	3	ALA
1	A	115	ALA
1	A	137	MET
1	B	-5	ASN
1	B	-4	LEU
1	B	115	ALA
1	B	136	GLU

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Mol	Chain	Res	Type
1	C	0	SER
1	C	115	ALA
1	C	187	GLY
1	C	283	ASN
1	D	115	ALA
1	D	174	GLN
1	D	250	GLU
1	A	176	ASP
1	B	174	GLN
1	D	231	GLN
1	B	-2	PHE
1	C	137	MET
1	C	156	ILE
1	A	212	VAL
1	D	187	GLY
1	A	259	VAL
1	B	187	GLY
1	B	286	PRO

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	262/307 (85%)	229 (87%)	33 (13%)	5 25
1	B	262/307 (85%)	228 (87%)	34 (13%)	5 24
1	C	254/307 (83%)	219 (86%)	35 (14%)	4 21
1	D	270/307 (88%)	237 (88%)	33 (12%)	6 27
All	All	1048/1228 (85%)	913 (87%)	135 (13%)	5 24

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	GLU
1	A	-4	LEU
1	A	2	LYS

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Mol	Chain	Res	Type
1	A	9	ASN
1	A	29	ILE
1	A	73	LYS
1	A	77	LEU
1	A	105	LEU
1	A	108	LEU
1	A	110	GLN
1	A	113	LEU
1	A	121	LEU
1	A	142	GLU
1	A	154	PHE
1	A	156	ILE
1	A	159	HIS
1	A	173	GLU
1	A	174	GLN
1	A	176	ASP
1	A	177	LEU
1	A	181	LEU
1	A	206	ASP
1	A	209	ARG
1	A	240	LEU
1	A	261	ASP
1	A	269	ILE
1	A	299	ARG
1	A	303	ASP
1	A	320	GLU
1	A	336	GLN
1	A	340	ILE
1	A	354	MET
1	A	355	GLU
1	B	-3	TYR
1	B	1	MET
1	B	2	LYS
1	B	7	GLN
1	B	8	ILE
1	B	13	LEU
1	B	17	LEU
1	B	26	GLN
1	B	77	LEU
1	B	82	PHE
1	B	90	LEU
1	B	105	LEU

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Mol	Chain	Res	Type
1	B	108	LEU
1	B	113	LEU
1	B	118	VAL
1	B	123	LEU
1	B	133	ARG
1	B	142	GLU
1	B	158	THR
1	B	159	HIS
1	B	160	PHE
1	B	175	ILE
1	B	177	LEU
1	B	180	GLN
1	B	181	LEU
1	B	207	TRP
1	B	231	GLN
1	B	240	LEU
1	B	271	ILE
1	B	288	LEU
1	B	292	ARG
1	B	303	ASP
1	B	336	GLN
1	B	340	ILE
1	C	1	MET
1	C	2	LYS
1	C	7	GLN
1	C	13	LEU
1	C	29	ILE
1	C	34	LYS
1	C	73	LYS
1	C	77	LEU
1	C	82	PHE
1	C	90	LEU
1	C	105	LEU
1	C	108	LEU
1	C	113	LEU
1	C	123	LEU
1	C	127	MET
1	C	142	GLU
1	C	143	ARG
1	C	146	LYS
1	C	156	ILE
1	C	157	MET

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Mol	Chain	Res	Type
1	C	176	ASP
1	C	177	LEU
1	C	181	LEU
1	C	193	ASN
1	C	206	ASP
1	C	222	ASN
1	C	231	GLN
1	C	262	ARG
1	C	265	ARG
1	C	266	LEU
1	C	279	ARG
1	C	299	ARG
1	C	303	ASP
1	C	336	GLN
1	C	351	ARG
1	D	-6	GLU
1	D	-4	LEU
1	D	-3	TYR
1	D	9	ASN
1	D	13	LEU
1	D	26	GLN
1	D	29	ILE
1	D	73	LYS
1	D	77	LEU
1	D	82	PHE
1	D	90	LEU
1	D	105	LEU
1	D	108	LEU
1	D	113	LEU
1	D	121	LEU
1	D	123	LEU
1	D	143	ARG
1	D	156	ILE
1	D	175	ILE
1	D	180	GLN
1	D	181	LEU
1	D	207	TRP
1	D	230	LEU
1	D	231	GLN
1	D	235	THR
1	D	239	GLN
1	D	240	LEU

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Mol	Chain	Res	Type
1	D	254	TYR
1	D	271	ILE
1	D	280	MET
1	D	303	ASP
1	D	336	GLN
1	D	351	ARG

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

Mol	Chain	Res	Type
1	B	7	GLN
1	B	180	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 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	$\#\|Z\| > 2$
1	KCX	A	122	1	7,11,12	0.66	0	7,12,14	1.49	2 (28%)
1	KCX	B	122	1	7,11,12	0.58	0	7,12,14	2.02	3 (42%)
1	KCX	C	122	1	7,11,12	0.55	0	7,12,14	1.36	2 (28%)
1	KCX	D	122	1	7,11,12	0.62	0	7,12,14	1.55	2 (28%)

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
1	KCX	A	122	1	-	0/6/10/12	0/0/0/0
1	KCX	B	122	1	-	0/6/10/12	0/0/0/0
1	KCX	C	122	1	-	0/6/10/12	0/0/0/0
1	KCX	D	122	1	-	0/6/10/12	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	122	KCX	O-C-CA	-2.37	119.30	125.49
1	B	122	KCX	O-C-CA	-2.35	119.36	125.49
1	C	122	KCX	O-C-CA	-2.35	119.37	125.49
1	A	122	KCX	O-C-CA	-2.23	119.68	125.49
1	B	122	KCX	CG-CB-CA	-2.12	105.23	114.16
1	C	122	KCX	CB-CA-N	2.36	117.22	110.52
1	A	122	KCX	CB-CA-N	2.39	117.31	110.52
1	D	122	KCX	CB-CA-N	2.54	117.75	110.52
1	B	122	KCX	CB-CA-N	3.98	121.85	110.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	122	KCX	1	0
1	B	122	KCX	2	0
1	C	122	KCX	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	324/378 (85%)	0.42	22 (6%)	20	15	62, 100, 147, 217	0
1	B	319/378 (84%)	0.47	16 (5%)	32	24	74, 107, 166, 252	0
1	C	316/378 (83%)	0.39	19 (6%)	25	18	64, 106, 173, 251	0
1	D	335/378 (88%)	0.51	26 (7%)	16	11	56, 112, 215, 253	0
All	All	1294/1512 (85%)	0.45	83 (6%)	23	17	56, 106, 183, 253	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	ASP	7.0
1	B	310	GLY	5.6
1	D	357	VAL	5.3
1	D	-7	THR	4.6
1	A	147	CYS	4.5
1	A	146	LYS	4.4
1	A	327	GLY	4.3
1	C	357	VAL	4.2
1	B	320	GLU	4.1
1	B	289	VAL	4.1
1	A	208	VAL	3.9
1	C	135	ASP	3.8
1	D	123	LEU	3.7
1	B	321	ALA	3.6
1	B	223	THR	3.5
1	D	187	GLY	3.4
1	B	158	THR	3.4
1	C	245	ASP	3.4
1	A	328	LEU	3.3
1	A	274	GLY	3.3
1	C	198	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	291	GLY	3.2
1	D	227	ASP	3.2
1	D	226	ALA	3.1
1	D	-8	THR	3.1
1	A	253	GLY	3.1
1	C	0	SER	3.0
1	D	-5	ASN	3.0
1	C	265	ARG	2.9
1	A	182	THR	2.9
1	A	107	ALA	2.9
1	C	315	ASP	2.9
1	B	213	ILE	2.8
1	A	255	GLY	2.8
1	D	254	TYR	2.8
1	B	-7	THR	2.8
1	D	349	THR	2.7
1	A	144	LEU	2.7
1	D	307	VAL	2.6
1	C	229	ASP	2.6
1	C	240	LEU	2.5
1	A	186	LEU	2.5
1	A	187	GLY	2.5
1	D	229	ASP	2.5
1	D	213	ILE	2.5
1	C	17	LEU	2.4
1	D	-1	GLN	2.4
1	D	-3	TYR	2.4
1	B	264	THR	2.3
1	A	183	ALA	2.3
1	D	241	ILE	2.3
1	B	160	PHE	2.3
1	D	230	LEU	2.3
1	A	305	THR	2.3
1	D	3	ALA	2.3
1	D	251	PRO	2.2
1	C	38	TYR	2.2
1	A	207	TRP	2.2
1	B	22	ARG	2.2
1	D	186	LEU	2.2
1	C	207	TRP	2.2
1	B	270	ALA	2.2
1	C	-1	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	247	LYS	2.1
1	C	318	GLY	2.1
1	C	197	ILE	2.1
1	A	269	ILE	2.1
1	A	256	ALA	2.1
1	D	321	ALA	2.1
1	A	185	LEU	2.1
1	D	-2	PHE	2.1
1	B	328	LEU	2.1
1	A	225	ALA	2.1
1	C	239	GLN	2.1
1	B	228	TYR	2.1
1	A	267	GLY	2.1
1	C	312	GLY	2.1
1	D	-13	ASP	2.0
1	D	22	ARG	2.0
1	B	218	SER	2.0
1	C	262	ARG	2.0
1	A	320	GLU	2.0
1	D	240	LEU	2.0

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. 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
1	KCX	C	122	12/13	0.88	0.19	-	85,90,96,96	0
1	KCX	B	122	12/13	0.70	0.39	-	92,105,112,124	0
1	KCX	D	122	12/13	0.80	0.27	-	90,92,95,96	0
1	KCX	A	122	12/13	0.89	0.28	-	67,68,69,71	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.