W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 8, 2016 – 11:07 PM EDT

PDB ID	:	5HRA
Title	:	Crystal structure of an aspartate/glutamate racemase in complex with D-aspartate
Authors	:	Liu, X.; Gao, F.; Ma, Y.; Liu, S.; Cui, Y.; Yuan, Z.; Kang, X.
Deposited on	:	2016-01-23
Resolution	:	1.60 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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
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-20027457

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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.
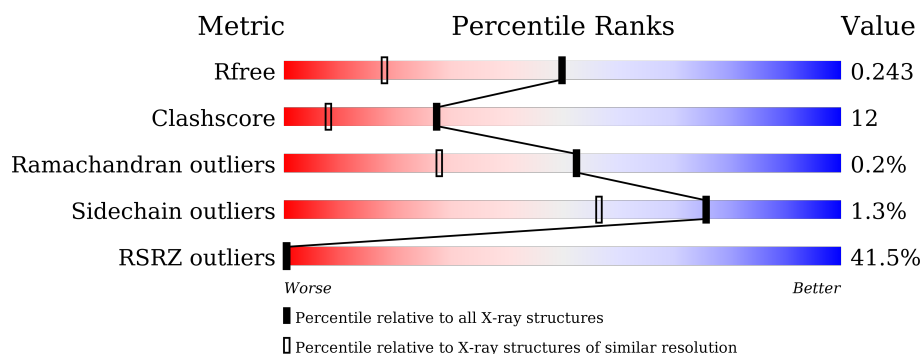
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	235	39% / 84% 15% •
1	B	235	43% / 80% 17% ••

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4052 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 aspartate/glutamate racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	1	0
			1807	1138	315	342	12			
1	B	232	Total	C	N	O	S	0	0	0
			1791	1129	311	339	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	231	LEU	-	expression tag	UNP A0A0F6FBL7
A	232	GLU	-	expression tag	UNP A0A0F6FBL7
A	233	HIS	-	expression tag	UNP A0A0F6FBL7
A	234	HIS	-	expression tag	UNP A0A0F6FBL7
A	235	HIS	-	expression tag	UNP A0A0F6FBL7
B	231	LEU	-	expression tag	UNP A0A0F6FBL7
B	232	GLU	-	expression tag	UNP A0A0F6FBL7
B	233	HIS	-	expression tag	UNP A0A0F6FBL7
B	234	HIS	-	expression tag	UNP A0A0F6FBL7
B	235	HIS	-	expression tag	UNP A0A0F6FBL7

- Molecule 2 is D-ASPARTIC ACID (three-letter code: DAS) (formula: $C_4H_7NO_4$).
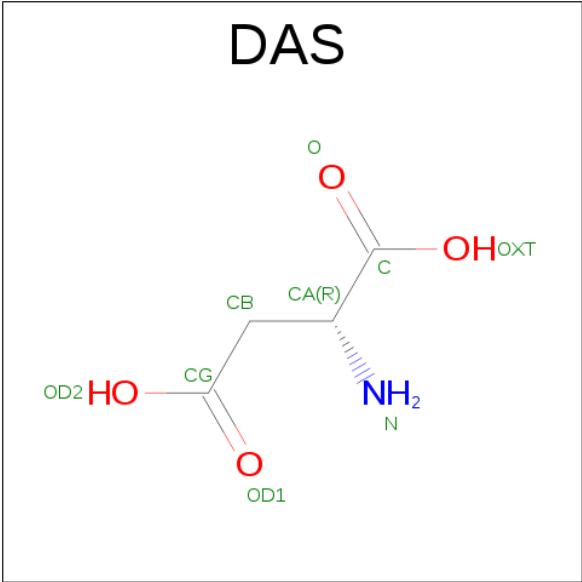
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 9	C 4	N 1	O 4	0	0
2	B	1	Total 9	C 4	N 1	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	224	Total 224	O 224	0	0
3	B	212	Total 212	O 212	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: aspartate/glutamate racemase
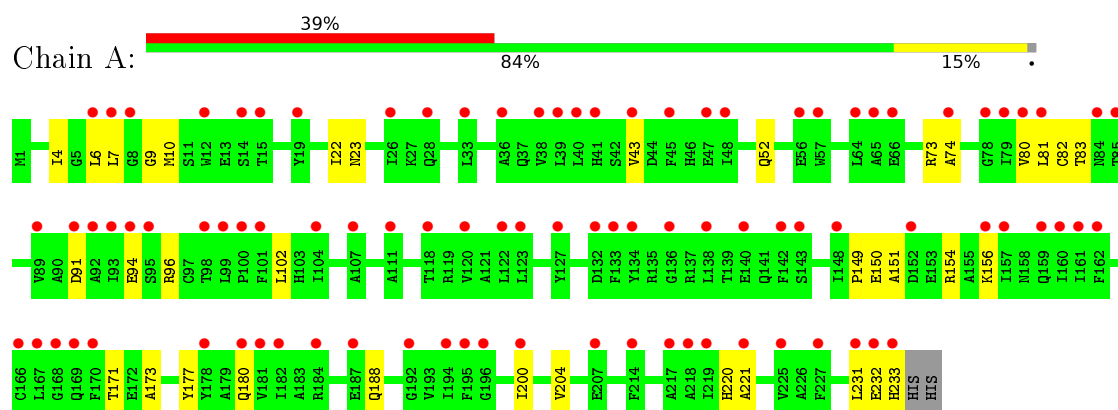
- Molecule 1: aspartate/glutamate racemase
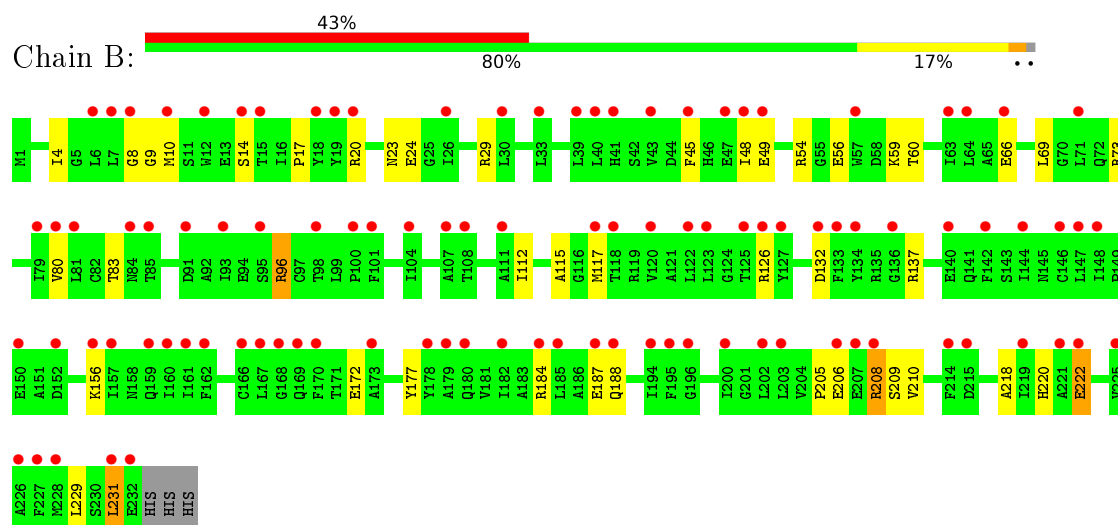
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.94Å 48.25Å 116.29Å 90.00° 92.92° 90.00°	Depositor
Resolution (Å)	32.61 – 1.60 33.62 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (32.61-1.60) 88.9 (33.62-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 1.60Å)	Xtriage
Refinement program	PHENIX (1.10pre_2090: ???)	Depositor
R, R_{free}	0.233 , 0.250 0.227 , 0.243	Depositor DCC
R_{free} test set	1840 reflections (2.99%)	DCC
Wilson B-factor (Å^2)	17.7	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 49.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -k,-h,-l 0.015 for k,h,-l 0.140 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4052	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: DAS

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	0.41	0/1837	0.60	0/2483
1	B	0.42	0/1820	0.67	4/2460 (0.2%)
All	All	0.41	0/3657	0.64	4/4943 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	ARG	NE-CZ-NH1	-9.72	115.44	120.30
1	B	210	VAL	CG1-CB-CG2	5.91	120.36	110.90
1	B	69	LEU	CB-CG-CD1	-5.87	101.03	111.00
1	B	231	LEU	CB-CG-CD2	-5.87	101.03	111.00

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	1807	0	1795	43	0
1	B	1791	0	1784	43	0
2	A	9	0	5	0	0
2	B	9	0	5	0	0
3	A	224	0	0	38	1

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	212	0	0	22	2
All	All	4052	0	3589	86	3

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 12.

All (86) 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:66:GLU:OE2	1:B:96:ARG:NH2	1.74	1.19
1:A:22:ILE:HG13	3:A:403:HOH:O	1.48	1.11
1:A:22:ILE:N	3:A:403:HOH:O	1.87	1.06
1:A:94:GLU:O	3:A:401:HOH:O	1.82	0.96
1:A:81:LEU:O	3:A:402:HOH:O	1.85	0.94
1:A:231:LEU:O	1:A:233:HIS:N	2.01	0.93
1:A:233:HIS:HA	3:A:420:HOH:O	1.67	0.93
1:A:82:CYS:SG	3:A:418:HOH:O	2.28	0.92
1:A:43:VAL:N	3:A:405:HOH:O	2.02	0.90
1:A:91:ASP:OD1	3:A:404:HOH:O	1.89	0.89
1:A:74:ALA:HA	3:A:408:HOH:O	1.74	0.86
1:A:154:ARG:NH1	3:A:406:HOH:O	2.07	0.85
1:B:206:GLU:OE2	3:B:401:HOH:O	1.94	0.85
1:B:23:ASN:ND2	3:B:403:HOH:O	2.10	0.84
1:B:115:ALA:HB3	3:B:417:HOH:O	1.76	0.84
1:B:112:ILE:HG23	3:B:578:HOH:O	1.78	0.83
1:A:9:GLY:HA3	3:A:405:HOH:O	1.78	0.83
1:B:59:LYS:HB3	3:B:410:HOH:O	1.78	0.82
1:B:66:GLU:CD	1:B:96:ARG:HH22	1.84	0.81
1:B:49:GLU:N	3:B:406:HOH:O	2.15	0.78
1:B:117:MET:SD	3:B:578:HOH:O	2.42	0.76
1:B:209:SER:O	3:B:402:HOH:O	2.03	0.76
1:A:43:VAL:O	3:A:405:HOH:O	2.03	0.74
1:A:6:LEU:HB3	3:A:418:HOH:O	1.88	0.74
1:A:149:PRO:O	3:A:406:HOH:O	2.06	0.74
1:B:60:THR:N	3:B:410:HOH:O	2.24	0.70
1:A:171:THR:OG1	3:A:407:HOH:O	2.09	0.70
1:B:9:GLY:O	3:B:404:HOH:O	2.10	0.70
1:A:73:ARG:O	3:A:408:HOH:O	2.10	0.69
1:B:205:PRO:HD2	1:B:208:ARG:HG3	1.75	0.69
1:A:96:ARG:NH1	3:A:410:HOH:O	2.16	0.69
1:B:229:LEU:CB	1:B:231:LEU:HD13	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:C	3:A:406:HOH:O	2.33	0.67
1:A:23:ASN:ND2	3:A:415:HOH:O	2.28	0.67
1:A:188:GLN:NE2	3:A:414:HOH:O	2.28	0.67
1:A:10:MET:HE2	3:A:416:HOH:O	1.94	0.67
1:A:180:GLN:NE2	3:A:413:HOH:O	2.27	0.67
1:A:204:VAL:N	3:A:409:HOH:O	2.14	0.66
1:B:117:MET:HB2	3:B:578:HOH:O	1.96	0.65
1:A:221:ALA:HB1	3:A:403:HOH:O	1.97	0.65
1:A:200:ILE:O	3:A:409:HOH:O	2.15	0.65
1:A:7:LEU:N	3:A:418:HOH:O	2.29	0.65
1:B:222:GLU:OE2	3:B:405:HOH:O	2.14	0.64
1:B:126:ARG:HG2	3:B:416:HOH:O	1.98	0.63
1:A:231:LEU:C	1:A:233:HIS:H	1.99	0.61
1:B:184:ARG:O	1:B:187:GLU:HG2	2.01	0.61
1:B:229:LEU:HB2	1:B:231:LEU:HD13	1.82	0.60
1:B:132:ASP:OD1	3:B:407:HOH:O	2.16	0.59
1:A:171:THR:CB	3:A:407:HOH:O	2.52	0.58
1:B:54:ARG:HB2	1:B:56:GLU:HG3	1.85	0.58
1:B:172:GLU:CD	1:B:208:ARG:HH22	2.09	0.56
1:B:172:GLU:OE1	1:B:208:ARG:NH2	2.39	0.55
1:A:151:ALA:N	3:A:406:HOH:O	2.42	0.53
1:B:60:THR:HG23	3:B:410:HOH:O	2.08	0.52
1:B:229:LEU:HB3	1:B:231:LEU:HD13	1.90	0.52
1:A:150:GLU:CA	3:A:406:HOH:O	2.58	0.52
1:A:6:LEU:CA	3:A:418:HOH:O	2.57	0.52
1:A:171:THR:HB	3:A:407:HOH:O	2.09	0.52
1:B:188:GLN:HG2	3:B:591:HOH:O	2.09	0.51
1:A:22:ILE:CA	3:A:403:HOH:O	2.47	0.51
1:B:205:PRO:O	1:B:208:ARG:HB2	2.12	0.50
1:A:231:LEU:C	1:A:233:HIS:N	2.59	0.49
1:B:10:MET:HA	1:B:45:PHE:CD1	2.47	0.49
1:A:80:VAL:HG13	1:A:220:HIS:CE1	2.47	0.49
1:B:48:ILE:HB	3:B:406:HOH:O	2.14	0.48
1:B:8:GLY:O	3:B:408:HOH:O	2.20	0.47
1:A:52:GLN:HG3	3:A:424:HOH:O	2.14	0.47
1:B:156:LYS:HD3	1:B:177:TYR:CZ	2.49	0.47
1:B:80:VAL:HG13	1:B:220:HIS:CE1	2.50	0.47
1:A:156:LYS:HD3	1:A:177:TYR:CZ	2.50	0.47
1:B:218:ALA:O	1:B:222:GLU:OE1	2.32	0.46
1:B:45:PHE:CE1	3:B:406:HOH:O	2.66	0.46
1:B:49:GLU:HB2	3:B:406:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:NH2	3:B:420:HOH:O	2.42	0.45
1:A:150:GLU:HA	3:A:406:HOH:O	2.16	0.44
3:A:408:HOH:O	1:B:73:ARG:NE	2.50	0.44
1:B:209:SER:O	3:B:409:HOH:O	2.21	0.43
1:A:73:ARG:C	3:A:408:HOH:O	2.54	0.42
1:A:82:CYS:HA	3:A:402:HOH:O	2.20	0.42
1:B:20:ARG:O	1:B:24:GLU:HG3	2.20	0.42
1:B:59:LYS:HB2	1:B:59:LYS:HE3	1.72	0.41
1:B:29:ARG:CD	1:B:231:LEU:HD21	2.51	0.41
1:B:4:ILE:HD12	1:B:4:ILE:HA	1.97	0.41
1:B:14:SER:C	1:B:17:PRO:HD2	2.41	0.40
1:A:4:ILE:HA	1:A:4:ILE:HD12	1.92	0.40
1:A:173:ALA:HB3	3:A:407:HOH:O	2.21	0.40

All (3) 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)
3:B:587:HOH:O	3:B:597:HOH:O[2_554]	2.10	0.10
3:B:536:HOH:O	3:B:576:HOH:O[2_544]	2.11	0.09
3:A:531:HOH:O	3:A:562:HOH:O[2_545]	2.14	0.06

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	232/235 (99%)	228 (98%)	3 (1%)	1 (0%)	39	17
1	B	230/235 (98%)	226 (98%)	4 (2%)	0	100	100
All	All	462/470 (98%)	454 (98%)	7 (2%)	1 (0%)	52	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	232	GLU

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	187/188 (100%)	185 (99%)	2 (1%)	80	63
1	B	185/188 (98%)	182 (98%)	3 (2%)	70	47
All	All	372/376 (99%)	367 (99%)	5 (1%)	76	56

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	THR
1	A	102	LEU
1	B	83	THR
1	B	96	ARG
1	B	222	GLU

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	180	GLN
1	B	131	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	DAS	A	301	-	2,8,8	0.50	0	1,10,10	0.34	0
2	DAS	B	301	-	2,8,8	0.54	0	1,10,10	0.50	0

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	DAS	A	301	-	-	0/2/8/8	0/0/0/0
2	DAS	B	301	-	-	0/2/8/8	0/0/0/0

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 (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	233/235 (99%)	1.96	92 (39%)	0	0	9, 15, 28, 38	0
1	B	232/235 (98%)	2.03	101 (43%)	0	0	9, 17, 30, 40	0
All	All	465/470 (98%)	1.99	193 (41%)	0	0	9, 16, 29, 40	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	LEU	7.4
1	A	232	GLU	7.4
1	A	233	HIS	7.1
1	A	6	LEU	6.5
1	B	132	ASP	6.1
1	B	81	LEU	5.9
1	B	231	LEU	5.8
1	B	142	PHE	5.2
1	A	57	TRP	5.2
1	B	152	ASP	5.1
1	B	122	LEU	5.0
1	B	200	ILE	4.9
1	B	161	ILE	4.8
1	B	170	PHE	4.7
1	B	208	ARG	4.7
1	B	91	ASP	4.7
1	B	120	VAL	4.6
1	B	214	PHE	4.6
1	B	207	GLU	4.6
1	B	225	VAL	4.6
1	A	28	GLN	4.6
1	A	200	ILE	4.5
1	B	98	THR	4.5
1	B	6	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	173	ALA	4.4
1	B	219	ILE	4.4
1	A	93	ILE	4.3
1	A	12	TRP	4.3
1	B	188	GLN	4.3
1	A	214	PHE	4.1
1	B	232	GLU	4.2
1	B	203	LEU	4.1
1	A	140	GLU	4.1
1	B	48	ILE	4.0
1	A	170	PHE	4.0
1	B	178	TYR	3.9
1	A	64	LEU	3.9
1	A	81	LEU	3.9
1	A	178	TYR	3.9
1	B	12	TRP	3.8
1	A	91	ASP	3.8
1	B	71	LEU	3.7
1	A	182	ILE	3.7
1	A	148	ILE	3.7
1	A	219	ILE	3.7
1	A	40	LEU	3.7
1	A	43	VAL	3.6
1	A	104	ILE	3.6
1	A	142	PHE	3.6
1	B	167	LEU	3.6
1	A	45	PHE	3.5
1	B	41	HIS	3.5
1	A	166	CYS	3.5
1	A	161	ILE	3.5
1	B	134	TYR	3.5
1	B	169	GLN	3.5
1	A	26	ILE	3.5
1	A	207	GLU	3.5
1	A	80	VAL	3.5
1	B	187	GLU	3.4
1	A	152	ASP	3.4
1	B	182	ILE	3.4
1	A	134	TYR	3.4
1	B	227	PHE	3.4
1	B	107	ALA	3.3
1	B	144	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	120	VAL	3.3
1	B	104	ILE	3.2
1	B	19	TYR	3.2
1	B	195	PHE	3.2
1	B	168	GLY	3.2
1	A	133	PHE	3.2
1	A	41	HIS	3.2
1	A	7	LEU	3.2
1	B	64	LEU	3.2
1	B	80	VAL	3.2
1	A	74	ALA	3.1
1	A	48	ILE	3.1
1	A	194	ILE	3.1
1	B	15	THR	3.1
1	A	122	LEU	3.0
1	A	95[A]	SER	3.0
1	A	195	PHE	3.0
1	A	136	GLY	3.0
1	B	30	LEU	3.0
1	A	169	GLN	3.0
1	B	133	PHE	3.0
1	B	180	GLN	3.0
1	A	101	PHE	2.9
1	B	43	VAL	2.9
1	B	45	PHE	2.9
1	B	140	GLU	2.9
1	B	136	GLY	2.9
1	B	157	ILE	2.9
1	A	156	LYS	2.9
1	B	39	LEU	2.9
1	B	179	ALA	2.9
1	B	49	GLU	2.8
1	B	215	ASP	2.8
1	A	15	THR	2.8
1	A	157	ILE	2.8
1	B	100	PRO	2.8
1	A	92	ALA	2.8
1	A	218	ALA	2.8
1	B	162	PHE	2.8
1	B	221	ALA	2.7
1	A	162	PHE	2.7
1	A	8	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	107	ALA	2.7
1	A	187	GLU	2.7
1	B	101	PHE	2.7
1	B	40	LEU	2.7
1	B	166	CYS	2.7
1	A	123	LEU	2.7
1	B	108	THR	2.6
1	A	66	GLU	2.6
1	B	194	ILE	2.6
1	A	38	VAL	2.6
1	B	85	THR	2.6
1	B	95	SER	2.6
1	A	98	THR	2.6
1	B	66	GLU	2.6
1	B	118	THR	2.6
1	B	63	ILE	2.6
1	A	221	ALA	2.5
1	B	93	ILE	2.5
1	B	222	GLU	2.5
1	A	180	GLN	2.5
1	A	227	PHE	2.5
1	A	89	VAL	2.5
1	B	202	LEU	2.5
1	A	132	ASP	2.4
1	A	168	GLY	2.4
1	A	192	GLY	2.4
1	B	228	MET	2.4
1	A	181	VAL	2.4
1	A	167	LEU	2.4
1	B	14	SER	2.4
1	B	84	ASN	2.4
1	A	19	TYR	2.4
1	A	127	TYR	2.4
1	B	184	ARG	2.4
1	A	56	GLU	2.4
1	B	146	CYS	2.4
1	A	14	SER	2.3
1	A	47	GLU	2.3
1	A	159	GLN	2.3
1	B	148	ILE	2.3
1	A	184	ARG	2.3
1	B	125	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	156	LYS	2.3
1	A	217	ALA	2.3
1	B	111	ALA	2.3
1	A	118	THR	2.3
1	A	138	LEU	2.3
1	B	47	GLU	2.3
1	B	18	TYR	2.3
1	B	159	GLN	2.3
1	A	79	ILE	2.2
1	A	39	LEU	2.2
1	B	7	LEU	2.2
1	A	78	GLY	2.2
1	B	57	TRP	2.2
1	A	111	ALA	2.2
1	B	117	MET	2.2
1	A	143	SER	2.2
1	A	99	LEU	2.2
1	B	123	LEU	2.2
1	B	196	GLY	2.2
1	B	33	LEU	2.2
1	B	160	ILE	2.2
1	A	94	GLU	2.2
1	A	33	LEU	2.1
1	A	84	ASN	2.1
1	B	20	ARG	2.1
1	A	65	ALA	2.1
1	B	10	MET	2.1
1	B	147	LEU	2.1
1	B	185	LEU	2.1
1	B	26	ILE	2.1
1	A	196	GLY	2.1
1	A	36	ALA	2.1
1	A	225	VAL	2.1
1	A	85	THR	2.1
1	B	79	ILE	2.0
1	B	150	GLU	2.0
1	B	126	ARG	2.0
1	B	127	TYR	2.0
1	B	8	GLY	2.0
1	B	226	ALA	2.0
1	B	206	GLU	2.0
1	A	160	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	100	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. 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
2	DAS	B	301	9/9	0.70	0.20	1.19	15,15,21,22	0
2	DAS	A	301	9/9	0.77	0.18	0.64	10,13,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.