Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 07:24 PM JST

PDB ID	:	5H01
Title	:	The crystal structure of D-2-halacid dehalogenase mutant
Authors	:	Xue, S.; Wang, Y.
Deposited on	:	2016-10-02
Resolution	:	2.19 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 (1)) were used in the production of this report:

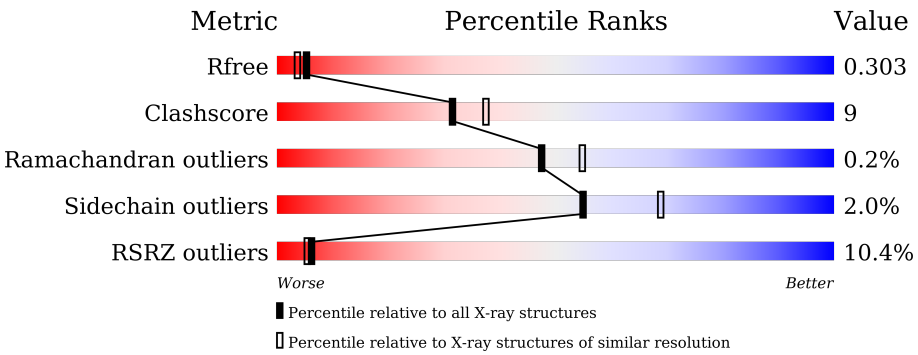
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 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	309	12% 74% 18% • 6%
1	B	309	10% 76% 17% • 6%
1	C	309	9% 77% 17% • 6%
1	D	309	8% 76% 18% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9743 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 (R)-2-haloacid dehalogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	292	2327	1491	408	418	10	0	0	0
1	B	292	2327	1491	408	418	10	0	0	0
1	C	292	2327	1491	408	418	10	0	0	0
1	D	292	2327	1491	408	418	10	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	288	ILE	LEU	engineered mutation	UNP Q52086
A	302	LEU	-	expression tag	UNP Q52086
A	303	GLU	-	expression tag	UNP Q52086
A	304	HIS	-	expression tag	UNP Q52086
A	305	HIS	-	expression tag	UNP Q52086
A	306	HIS	-	expression tag	UNP Q52086
A	307	HIS	-	expression tag	UNP Q52086
A	308	HIS	-	expression tag	UNP Q52086
A	309	HIS	-	expression tag	UNP Q52086
B	288	ILE	LEU	engineered mutation	UNP Q52086
B	302	LEU	-	expression tag	UNP Q52086
B	303	GLU	-	expression tag	UNP Q52086
B	304	HIS	-	expression tag	UNP Q52086
B	305	HIS	-	expression tag	UNP Q52086
B	306	HIS	-	expression tag	UNP Q52086
B	307	HIS	-	expression tag	UNP Q52086
B	308	HIS	-	expression tag	UNP Q52086
B	309	HIS	-	expression tag	UNP Q52086
C	288	ILE	LEU	engineered mutation	UNP Q52086
C	302	LEU	-	expression tag	UNP Q52086
C	303	GLU	-	expression tag	UNP Q52086

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Chain	Residue	Modelled	Actual	Comment	Reference
C	304	HIS	-	expression tag	UNP Q52086
C	305	HIS	-	expression tag	UNP Q52086
C	306	HIS	-	expression tag	UNP Q52086
C	307	HIS	-	expression tag	UNP Q52086
C	308	HIS	-	expression tag	UNP Q52086
C	309	HIS	-	expression tag	UNP Q52086
D	288	ILE	LEU	engineered mutation	UNP Q52086
D	302	LEU	-	expression tag	UNP Q52086
D	303	GLU	-	expression tag	UNP Q52086
D	304	HIS	-	expression tag	UNP Q52086
D	305	HIS	-	expression tag	UNP Q52086
D	306	HIS	-	expression tag	UNP Q52086
D	307	HIS	-	expression tag	UNP Q52086
D	308	HIS	-	expression tag	UNP Q52086
D	309	HIS	-	expression tag	UNP Q52086

- Molecule 2 is water.

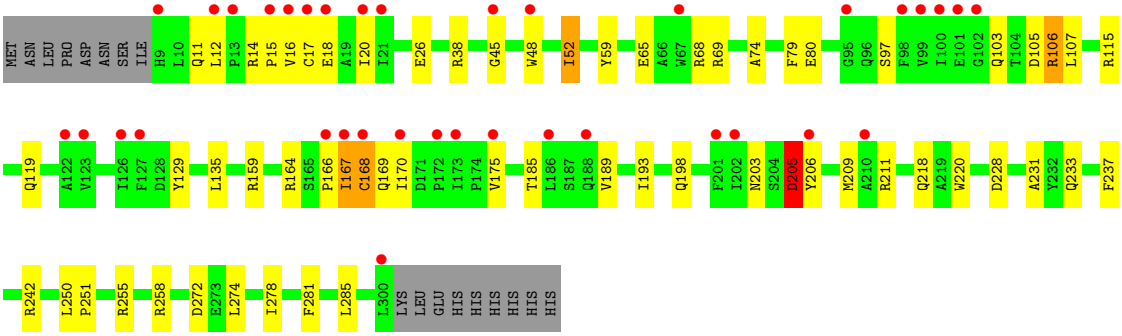
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	113	113	113	0	0
			Total	O		
2	B	108	108	108	0	0
			Total	O		
2	C	115	115	115	0	0
			Total	O		
2	D	99	99	99	0	0

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.

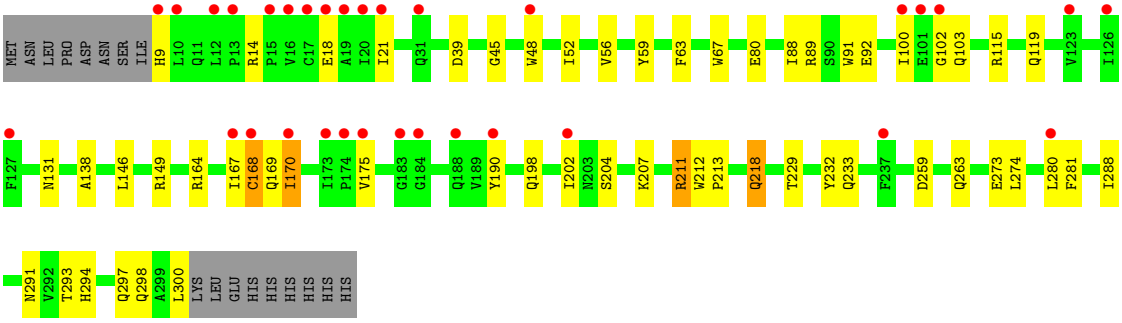
• Molecule 1: (R)-2-haloacid dehalogenase

Chain A:



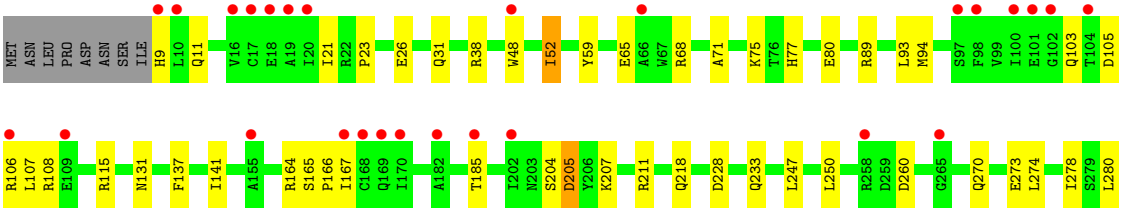
• Molecule 1: (R)-2-haloacid dehalogenase

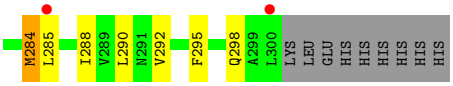
Chain B:



• Molecule 1: (R)-2-haloacid dehalogenase

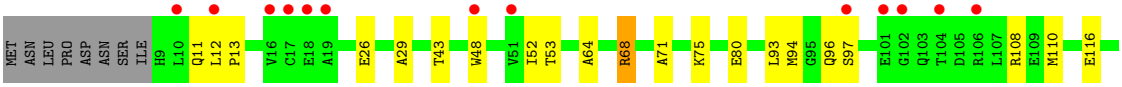
Chain C:





- Molecule 1: (R)-2-haloacid dehalogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.71Å 97.18Å 93.75Å 90.00° 107.53° 90.00°	Depositor
Resolution (Å)	48.59 – 2.19 48.59 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (48.59-2.19) 95.6 (48.59-2.19)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.253 , 0.312 0.248 , 0.303	Depositor DCC
R_{free} test set	3787 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	24.7	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.097 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9743	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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)

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	0.46	0/2388	0.60	1/3244 (0.0%)
1	B	0.50	0/2388	0.58	0/3244
1	C	0.50	1/2388 (0.0%)	0.63	3/3244 (0.1%)
1	D	0.47	0/2388	0.59	0/3244
All	All	0.48	1/9552 (0.0%)	0.60	4/12976 (0.0%)

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
1	B	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	284	MET	C-N	10.53	1.58	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	284	MET	O-C-N	-10.09	106.56	122.70
1	C	284	MET	CA-C-N	5.81	129.98	117.20
1	C	284	MET	C-N-CA	5.63	135.79	121.70
1	A	205	ASP	CB-CG-OD1	5.63	123.37	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	18	GLU	Peptide
1	C	284	MET	Mainchain

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	2327	0	2292	49	0
1	B	2327	0	2292	41	0
1	C	2327	0	2292	44	0
1	D	2327	0	2292	40	0
2	A	113	0	0	10	1
2	B	108	0	0	5	0
2	C	115	0	0	18	0
2	D	99	0	0	14	1
All	All	9743	0	9168	167	1

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 9.

All (167) 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:C:218:GLN:NE2	2:C:403:HOH:O	1.98	0.95
1:A:209:MET:HG3	2:A:428:HOH:O	1.66	0.92
1:B:14:ARG:NH1	1:B:198:GLN:O	2.02	0.92
1:C:211:ARG:NH2	2:C:404:HOH:O	2.03	0.90
1:C:228:ASP:OD1	2:C:401:HOH:O	1.90	0.89
1:A:258:ARG:NH2	1:A:272:ASP:OD1	2.08	0.87
1:A:198:GLN:NE2	2:A:401:HOH:O	2.04	0.84
1:D:148:GLY:O	2:D:402:HOH:O	1.94	0.83
1:D:96:GLN:NE2	2:D:404:HOH:O	2.11	0.82
1:D:110:MET:SD	2:D:406:HOH:O	2.37	0.82
1:D:196:THR:HG1	1:D:220:TRP:HH2	1.26	0.82
1:C:65:GLU:OE1	1:C:68:ARG:NH1	2.14	0.79
1:B:273:GLU:OE1	2:B:401:HOH:O	2.01	0.78
1:D:258:ARG:NH2	1:D:272:ASP:OD1	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:HG3	2:D:454:HOH:O	1.87	0.74
1:A:106:ARG:HG2	1:A:107:LEU:N	2.05	0.72
1:B:103:GLN:OE1	1:B:218:GLN:NE2	2.22	0.72
1:A:103:GLN:HG2	1:A:106:ARG:HD3	1.72	0.72
1:B:211:ARG:HD3	1:B:211:ARG:C	2.11	0.71
1:C:260:ASP:OD1	2:C:405:HOH:O	2.09	0.70
1:A:242:ARG:O	2:A:402:HOH:O	2.11	0.69
1:D:149:ARG:NH2	2:D:413:HOH:O	2.27	0.67
1:A:12:LEU:HD23	1:A:237:PHE:HA	1.76	0.67
1:D:121:ARG:NH1	2:D:410:HOH:O	2.23	0.67
1:C:285:LEU:HA	1:C:288:ILE:HG22	1.76	0.66
1:A:20:ILE:O	2:A:403:HOH:O	2.15	0.65
1:D:64:ALA:O	1:D:68:ARG:HG2	1.97	0.65
1:C:115:ARG:NH2	2:C:412:HOH:O	2.29	0.64
1:B:89:ARG:NH1	1:B:92:GLU:OE1	2.28	0.64
1:D:192:ASP:O	1:D:196:THR:HG23	1.97	0.64
1:A:14:ARG:NH2	1:A:17:CYS:SG	2.68	0.64
1:B:300:LEU:O	2:B:402:HOH:O	2.14	0.64
1:C:26:GLU:HG3	2:C:437:HOH:O	1.96	0.64
1:D:150:THR:OG1	2:D:403:HOH:O	2.00	0.64
1:D:116:GLU:OE2	2:D:405:HOH:O	2.15	0.63
1:B:100:ILE:HD13	1:B:297:GLN:HB3	1.80	0.62
1:A:26:GLU:OE1	2:A:404:HOH:O	2.16	0.62
1:C:52:ILE:HD11	1:C:278:ILE:HD12	1.81	0.62
1:C:298:GLN:OE1	2:C:403:HOH:O	2.16	0.61
1:A:52:ILE:HD11	1:A:278:ILE:HD12	1.83	0.61
1:C:211:ARG:NE	2:C:402:HOH:O	1.94	0.61
1:C:23:PRO:O	2:C:406:HOH:O	2.16	0.60
1:D:12:LEU:HD12	1:D:13:PRO:HD2	1.84	0.60
1:A:14:ARG:NH1	1:A:15:PRO:O	2.36	0.59
1:B:294:HIS:O	1:B:298:GLN:HG3	2.02	0.59
1:D:240:ASN:ND2	2:D:417:HOH:O	2.36	0.59
1:C:205:ASP:N	1:C:205:ASP:OD1	2.35	0.58
1:D:148:GLY:HA2	1:D:257:SER:HB3	1.84	0.58
1:A:168:CYS:SG	1:A:170:ILE:HG13	2.44	0.58
1:B:149:ARG:NH2	2:B:404:HOH:O	2.23	0.58
1:A:52:ILE:HD13	1:A:281:PHE:CB	2.34	0.57
1:C:105:ASP:OD1	1:C:108:ARG:NH1	2.26	0.57
1:B:204:SER:HA	1:B:207:LYS:HE2	1.87	0.56
1:A:45:GLY:HA2	1:A:168:CYS:SG	2.46	0.55
1:B:259:ASP:O	1:B:263:GLN:HG2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HD12	1:A:170:ILE:N	2.22	0.54
1:B:45:GLY:HA2	1:B:168:CYS:SG	2.47	0.54
1:A:103:GLN:HA	2:A:456:HOH:O	2.07	0.54
1:A:228:ASP:HA	1:A:233:GLN:HG3	1.90	0.54
1:D:48:TRP:HH2	1:D:131:ASN:OD1	1.90	0.53
1:B:232:TYR:OH	2:B:403:HOH:O	2.19	0.53
1:A:135:LEU:HA	1:A:285:LEU:HD13	1.91	0.53
1:D:204:SER:HA	1:D:207:LYS:HE2	1.91	0.52
1:D:43:THR:HG23	1:D:75:LYS:HG2	1.92	0.52
1:D:196:THR:HG21	1:D:224:LYS:HE3	1.91	0.52
1:B:211:ARG:HD3	1:B:211:ARG:O	2.09	0.52
1:A:106:ARG:CZ	1:A:218:GLN:OE1	2.58	0.52
1:A:52:ILE:HD13	1:A:281:PHE:HB3	1.90	0.51
1:B:56:VAL:HG12	1:B:63:PHE:HB2	1.91	0.51
1:C:80:GLU:OE1	1:C:164:ARG:HD2	2.10	0.51
1:C:247:LEU:HD12	1:C:250:LEU:HD11	1.93	0.51
1:C:31:GLN:H	1:C:31:GLN:CD	2.14	0.51
1:B:211:ARG:HD2	1:B:212:TRP:CD2	2.46	0.51
1:A:167:ILE:HD12	1:D:129:TYR:CD1	2.45	0.51
1:B:21:ILE:HD11	1:B:280:LEU:HD23	1.93	0.50
1:B:39:ASP:OD2	1:B:67:TRP:NE1	2.35	0.50
1:C:38:ARG:HD2	2:C:425:HOH:O	2.12	0.50
1:B:21:ILE:HD13	1:B:281:PHE:CE2	2.46	0.50
1:D:184:GLY:N	2:D:414:HOH:O	2.30	0.49
1:A:193:ILE:HG12	1:A:220:TRP:CE2	2.47	0.49
1:A:65:GLU:OE2	1:A:68:ARG:NH2	2.40	0.49
1:C:137:PHE:CZ	1:C:141:ILE:HD11	2.47	0.49
1:D:52:ILE:HD11	1:D:278:ILE:HD12	1.93	0.49
1:C:204:SER:HA	1:C:207:LYS:HE2	1.94	0.49
1:D:218:GLN:OE1	2:D:406:HOH:O	2.20	0.49
1:B:52:ILE:HD12	1:B:138:ALA:HB2	1.95	0.48
1:A:69:ARG:HD3	1:A:255:ARG:O	2.14	0.48
1:A:209:MET:N	2:A:428:HOH:O	2.46	0.48
1:D:148:GLY:HA2	1:D:257:SER:CB	2.43	0.48
1:A:48:TRP:CD1	1:A:48:TRP:N	2.81	0.48
1:A:105:ASP:HB2	2:A:456:HOH:O	2.14	0.48
1:B:80:GLU:HB2	1:B:164:ARG:HB2	1.95	0.48
1:A:59:TYR:CD2	1:A:274:LEU:HD13	2.49	0.47
1:B:168:CYS:SG	1:B:170:ILE:HG23	2.54	0.47
1:A:175:VAL:HG21	1:B:175:VAL:HG21	1.95	0.47
1:B:9:HIS:ND1	1:B:9:HIS:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:VAL:HA	1:D:295:PHE:CD2	2.49	0.47
1:C:38:ARG:NH1	2:C:425:HOH:O	2.48	0.47
1:D:48:TRP:CD1	1:D:48:TRP:N	2.82	0.47
2:C:412:HOH:O	1:D:29:ALA:N	2.48	0.46
1:A:103:GLN:HB3	1:A:106:ARG:NH1	2.30	0.46
1:D:142:LYS:HE2	1:D:146:LEU:HD11	1.98	0.46
1:A:97:SER:HB3	1:A:231:ALA:HB1	1.97	0.46
1:C:141:ILE:HA	2:C:432:HOH:O	2.16	0.46
1:A:11:GLN:N	2:A:411:HOH:O	2.29	0.45
1:D:80:GLU:HB2	1:D:164:ARG:HB2	1.99	0.45
1:D:238:ASP:O	1:D:242:ARG:HG2	2.16	0.45
1:A:129:TYR:HB2	1:D:166:PRO:HG2	1.98	0.45
1:B:164:ARG:NH2	2:B:421:HOH:O	2.50	0.45
1:C:274:LEU:O	1:C:278:ILE:HG22	2.16	0.45
1:C:21:ILE:HD11	1:C:280:LEU:HD23	1.98	0.45
1:C:103:GLN:HG3	2:C:403:HOH:O	2.16	0.45
1:A:185:THR:O	1:A:189:VAL:HG23	2.16	0.45
1:A:38:ARG:NH1	1:A:170:ILE:HG22	2.32	0.45
1:C:11:GLN:HG2	2:C:450:HOH:O	2.17	0.45
1:C:71:ALA:O	1:C:75:LYS:HG3	2.16	0.45
1:C:94:MET:SD	1:C:290:LEU:HD22	2.57	0.45
1:C:165:SER:HA	1:C:166:PRO:HD3	1.82	0.44
1:D:97:SER:HB3	1:D:231:ALA:HB1	1.99	0.44
1:B:229:THR:O	1:B:233:GLN:HG3	2.17	0.44
1:C:9:HIS:ND1	2:C:407:HOH:O	2.19	0.44
1:D:11:GLN:NE2	2:D:409:HOH:O	2.26	0.44
1:D:71:ALA:O	1:D:75:LYS:HG3	2.18	0.44
1:C:11:GLN:OE1	1:C:233:GLN:NE2	2.50	0.44
1:A:80:GLU:OE1	1:A:164:ARG:HD2	2.18	0.44
1:A:115:ARG:NE	2:A:431:HOH:O	2.50	0.44
1:A:205:ASP:N	1:A:205:ASP:OD1	2.51	0.44
1:A:250:LEU:HA	1:A:251:PRO:HD3	1.80	0.44
1:C:48:TRP:CD1	1:C:48:TRP:N	2.86	0.44
1:B:91:TRP:CZ3	1:B:297:GLN:HG2	2.52	0.44
1:B:293:THR:O	1:B:297:GLN:HG3	2.18	0.44
1:A:211:ARG:NE	1:B:175:VAL:HG13	2.33	0.44
1:C:292:VAL:HA	1:C:295:PHE:CD2	2.52	0.44
1:A:115:ARG:O	1:A:119:GLN:HG3	2.18	0.43
1:A:159:ARG:HE	1:A:159:ARG:HB2	1.69	0.43
1:C:80:GLU:HB2	1:C:164:ARG:HB2	2.00	0.43
1:C:89:ARG:O	1:C:93:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASN:HB2	1:A:206:TYR:CD2	2.53	0.43
1:A:211:ARG:HE	1:B:175:VAL:HG13	1.84	0.43
1:C:107:LEU:HD23	1:C:107:LEU:HA	1.77	0.43
1:A:74:ALA:HA	1:A:79:PHE:CD2	2.54	0.43
1:C:270:GLN:OE1	2:C:408:HOH:O	2.21	0.43
1:B:146:LEU:HD23	1:B:146:LEU:HA	1.89	0.43
1:C:103:GLN:OE1	1:C:106:ARG:NH1	2.52	0.43
1:A:14:ARG:HE	1:A:198:GLN:HB3	1.84	0.43
1:B:88:ILE:HG13	1:C:77:HIS:CE1	2.54	0.43
1:D:203:ASN:HD22	1:D:206:TYR:HE2	1.67	0.42
1:B:169:GLN:H	1:C:167:ILE:HD11	1.83	0.42
1:D:196:THR:OG1	1:D:220:TRP:HH2	1.92	0.42
1:C:211:ARG:NH1	2:C:410:HOH:O	2.27	0.42
1:B:190:TYR:O	1:B:202:ILE:HD11	2.20	0.42
1:D:94:MET:SD	1:D:290:LEU:HD22	2.60	0.42
1:B:288:ILE:HA	1:B:291:ASN:HB2	2.01	0.42
1:C:48:TRP:HH2	1:C:131:ASN:OD1	2.03	0.42
1:D:250:LEU:HA	1:D:251:PRO:HD3	1.84	0.42
1:B:149:ARG:HE	1:B:149:ARG:HB3	1.56	0.41
1:A:16:VAL:HG22	1:A:18:GLU:HG3	2.02	0.41
1:D:229:THR:O	1:D:233:GLN:HG3	2.20	0.41
1:A:106:ARG:NH2	1:A:218:GLN:HE22	2.19	0.41
1:B:211:ARG:C	1:B:213:PRO:HD3	2.41	0.41
1:B:115:ARG:O	1:B:119:GLN:HG3	2.21	0.41
1:C:59:TYR:OH	1:C:273:GLU:OE1	2.38	0.41
1:B:103:GLN:HB3	1:B:218:GLN:NE2	2.36	0.40
1:B:48:TRP:HH2	1:B:131:ASN:OD1	2.04	0.40
1:B:59:TYR:CD1	1:B:274:LEU:HD13	2.56	0.40
1:C:185:THR:HG21	2:D:414:HOH:O	2.21	0.40
1:D:108:ARG:HB2	2:D:444:HOH:O	2.21	0.40

All (1) 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)
2:A:414:HOH:O	2:D:487:HOH:O[2_757]	2.17	0.03

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	290/309 (94%)	281 (97%)	8 (3%)	1 (0%)	41	46
1	B	290/309 (94%)	281 (97%)	8 (3%)	1 (0%)	41	46
1	C	290/309 (94%)	282 (97%)	8 (3%)	0	100	100
1	D	290/309 (94%)	286 (99%)	4 (1%)	0	100	100
All	All	1160/1236 (94%)	1130 (97%)	28 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	PRO
1	B	102	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	240/257 (93%)	234 (98%)	6 (2%)	47	60
1	B	240/257 (93%)	235 (98%)	5 (2%)	53	67
1	C	240/257 (93%)	238 (99%)	2 (1%)	81	90
1	D	240/257 (93%)	234 (98%)	6 (2%)	47	60
All	All	960/1028 (93%)	941 (98%)	19 (2%)	55	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ILE
1	A	106	ARG
1	A	167	ILE
1	A	168	CYS
1	A	169	GLN
1	A	205	ASP
1	B	167	ILE
1	B	168	CYS
1	B	170	ILE
1	B	211	ARG
1	B	218	GLN
1	C	52	ILE
1	C	205	ASP
1	D	53	THR
1	D	68	ARG
1	D	93	LEU
1	D	169	GLN
1	D	211	ARG
1	D	218	GLN

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

Mol	Chain	Res	Type
1	A	31	GLN
1	B	218	GLN
1	C	198	GLN
1	C	233	GLN
1	D	240	ASN

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 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	292/309 (94%)	1.03	36 (12%)	4	3	20, 30, 48, 68	0
1	B	292/309 (94%)	0.99	32 (10%)	5	4	22, 30, 47, 70	0
1	C	292/309 (94%)	0.94	29 (9%)	7	6	21, 30, 46, 64	0
1	D	292/309 (94%)	0.94	24 (8%)	11	10	20, 30, 47, 66	0
All	All	1168/1236 (94%)	0.97	121 (10%)	6	5	20, 30, 47, 70	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	155	ALA	7.5
1	D	155	ALA	6.1
1	C	167	ILE	5.8
1	B	18	GLU	5.6
1	B	16	VAL	5.4
1	A	17	CYS	5.4
1	B	9	HIS	5.0
1	D	167	ILE	5.0
1	B	168	CYS	4.8
1	A	167	ILE	4.6
1	A	12	LEU	4.4
1	D	97	SER	4.4
1	A	48	TRP	4.4
1	B	21	ILE	4.3
1	C	300	LEU	4.3
1	B	100	ILE	4.3
1	C	19	ALA	4.2
1	A	168	CYS	4.2
1	A	18	GLU	4.1
1	A	15	PRO	4.1
1	A	9	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	18	GLU	4.0
1	A	300	LEU	3.9
1	B	48	TRP	3.9
1	B	20	ILE	3.9
1	B	167	ILE	3.8
1	D	10	LEU	3.8
1	B	184	GLY	3.7
1	A	21	ILE	3.7
1	B	19	ALA	3.6
1	C	16	VAL	3.5
1	D	184	GLY	3.5
1	A	170	ILE	3.4
1	D	19	ALA	3.4
1	D	300	LEU	3.4
1	C	285	LEU	3.4
1	B	183	GLY	3.4
1	A	202	ILE	3.3
1	C	104	THR	3.3
1	B	123	VAL	3.3
1	D	104	THR	3.2
1	A	16	VAL	3.2
1	B	10	LEU	3.2
1	D	16	VAL	3.2
1	D	168	CYS	3.1
1	C	98	PHE	3.1
1	D	48	TRP	3.1
1	C	168	CYS	3.1
1	B	126	ILE	3.1
1	D	106	ARG	3.1
1	B	202	ILE	3.0
1	A	13	PRO	3.0
1	B	173	ILE	3.0
1	C	100	ILE	2.9
1	A	102	GLY	2.9
1	D	219	ALA	2.9
1	A	101	GLU	2.9
1	C	17	CYS	2.9
1	A	99	VAL	2.8
1	C	101	GLU	2.8
1	A	95	GLY	2.8
1	A	20	ILE	2.8
1	A	123	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	97	SER	2.7
1	B	15	PRO	2.7
1	A	173	ILE	2.7
1	D	249	ALA	2.7
1	C	169	GLN	2.6
1	B	170	ILE	2.6
1	D	101	GLU	2.5
1	C	170	ILE	2.5
1	B	17	CYS	2.5
1	A	175	VAL	2.5
1	B	101	GLU	2.5
1	C	9	HIS	2.5
1	D	183	GLY	2.5
1	A	186	LEU	2.4
1	A	172	PRO	2.4
1	D	12	LEU	2.4
1	A	100	ILE	2.4
1	C	48	TRP	2.4
1	D	215	TYR	2.4
1	B	12	LEU	2.3
1	A	98	PHE	2.3
1	C	10	LEU	2.3
1	A	67	TRP	2.3
1	D	17	CYS	2.3
1	B	127	PHE	2.3
1	D	18	GLU	2.3
1	A	166	PRO	2.3
1	C	265	GLY	2.3
1	C	20	ILE	2.2
1	A	210	ALA	2.2
1	B	31	GLN	2.2
1	D	254	TYR	2.2
1	B	175	VAL	2.2
1	A	188	GLN	2.2
1	D	102	GLY	2.2
1	C	109	GLU	2.1
1	A	206	TYR	2.1
1	A	126	ILE	2.1
1	C	106	ARG	2.1
1	B	102	GLY	2.1
1	C	66	ALA	2.1
1	C	202	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	190	TYR	2.1
1	B	188	GLN	2.1
1	A	127	PHE	2.1
1	B	174	PRO	2.1
1	B	237	PHE	2.1
1	C	102	GLY	2.1
1	B	280	LEU	2.1
1	C	182	ALA	2.1
1	C	185	THR	2.1
1	A	45	GLY	2.1
1	D	135	LEU	2.0
1	A	122	ALA	2.0
1	A	201	PHE	2.0
1	B	13	PRO	2.0
1	C	258	ARG	2.0
1	D	51	VAL	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 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.