Full wwPDB X-ray Structure Validation Report (i)

Dec 11, 2023 – 04:11 PM JST

PDB ID	:	8HRF
Title	:	Catalytic domain of Vibrio parahaemolyticus chitinase 1
Authors	:	Nakamura, A.
Deposited on	:	2022-12-15
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

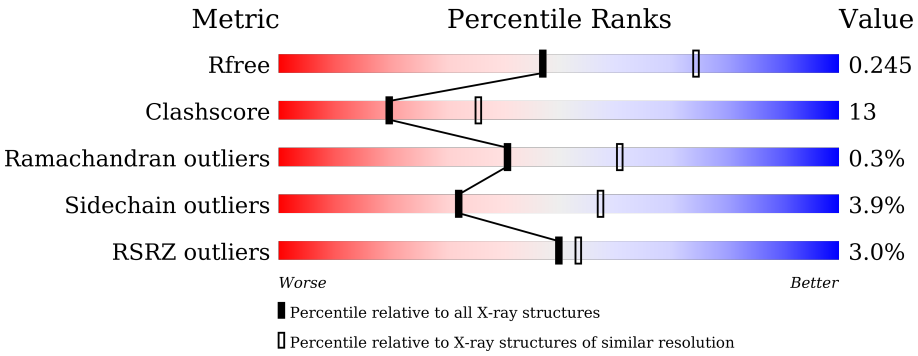
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

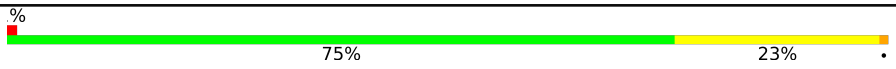
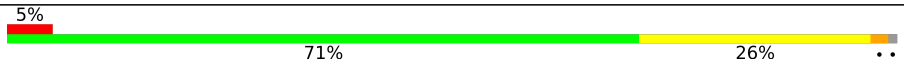
The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	571	
1	B	571	

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	ACT	A	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9432 atoms, of which 6 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.

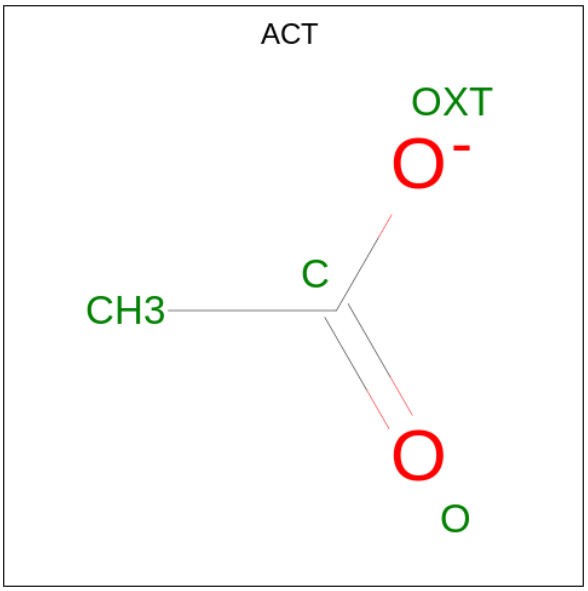
- Molecule 1 is a protein called Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	569	Total	C	N	O	S	0	0	0
			4350	2756	707	862	25			
1	B	567	Total	C	N	O	S	0	2	0
			4352	2758	705	864	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	GLY	-	expression tag	UNP A0A3E1IK76
B	21	GLY	-	expression tag	UNP A0A3E1IK76

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C H O 7 2 3 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	2	Total Ca 2 2	0	0

- Molecule 4 is water.

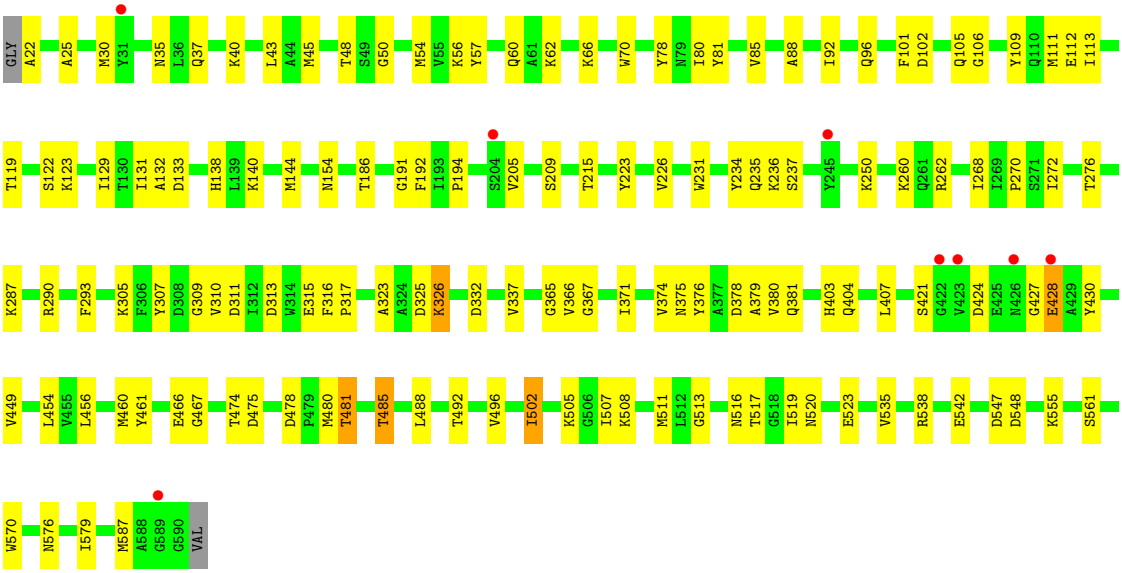
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	385	Total O 385 385	0	0
4	B	328	Total O 328 328	0	0

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.

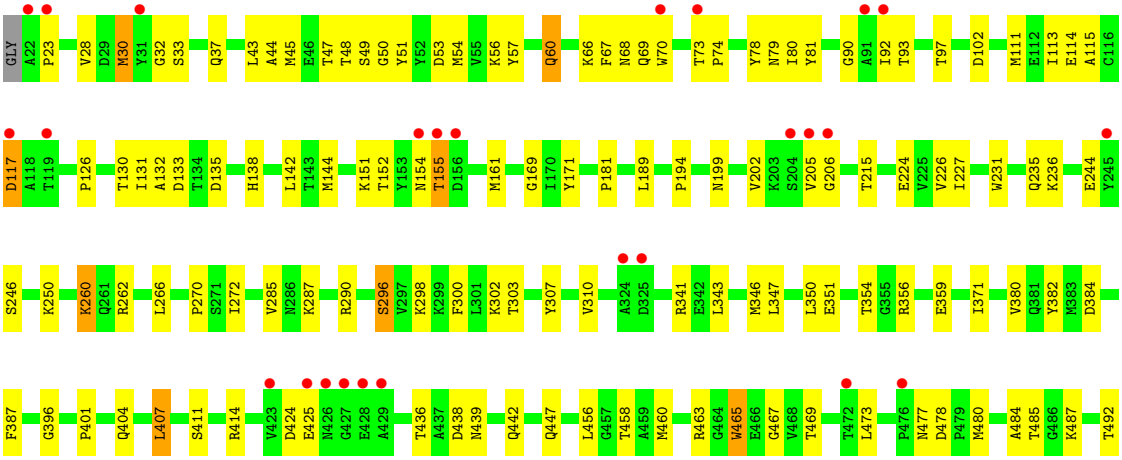
• Molecule 1: Chitinase

Chain A:



• Molecule 1: Chitinase

Chain B:




W497
G500
V501
I502
I507
K508
M511
L512
G518
F522
E523
Y524
G525
P533
W534
V535
W536
N537
R538
E542
T545
S551
V552
L553
A554
K555
G556
S557
S561
L567
I579
L580
N581
A582
M583
G586
M587
A588
GLY
GLY
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.80Å 160.00Å 75.49Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	28.70 – 2.50 28.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (28.70-2.50) 98.8 (28.70-2.50)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.30 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.161 , 0.245 0.162 , 0.245	Depositor DCC
R_{free} test set	2021 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	14.2	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9432	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT

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	0.45	0/4465	0.60	0/6078
1	B	0.42	0/4473	0.59	0/6090
All	All	0.43	0/8938	0.59	0/12168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4350	0	4087	97	0
1	B	4352	0	4089	118	0
2	A	4	3	3	3	0
2	B	4	3	3	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
4	A	385	0	0	16	0
4	B	328	0	0	11	2
All	All	9426	6	8182	215	2

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 13.

All (215) 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:475:ASP:H	1:A:481:THR:HG21	1.11	1.15
1:B:161:MET:HE1	1:B:583:MET:HB3	1.49	0.92
1:B:60:GLN:HG2	1:B:102:ASP:HB3	1.55	0.86
1:A:25:ALA:HA	1:A:122:SER:OG	1.75	0.85
1:B:300:PHE:HA	4:B:714:HOH:O	1.77	0.83
1:B:32:GLY:HA3	1:B:66:LYS:HD2	1.59	0.82
1:B:44:ALA:HB3	1:B:54:MET:HB3	1.59	0.82
1:A:502:ILE:HD13	1:A:507:ILE:HG13	1.61	0.81
1:A:62:LYS:NZ	4:A:704:HOH:O	2.12	0.79
1:B:231:TRP:HA	1:B:235:GLN:HB2	1.64	0.77
1:B:287:LYS:HD3	1:B:290:ARG:NH2	1.98	0.77
1:A:475:ASP:N	1:A:481:THR:HG21	1.95	0.76
1:A:231:TRP:HA	1:A:235:GLN:HB2	1.65	0.76
1:B:460:MET:HG2	1:B:579:ILE:HG21	1.69	0.75
1:B:23:PRO:HG3	1:B:117:ASP:HB2	1.69	0.74
1:B:523:GLU:OE2	1:B:538:ARG:NE	2.16	0.74
1:A:430:TYR:O	4:A:701:HOH:O	2.05	0.74
1:A:427:GLY:O	4:A:702:HOH:O	2.06	0.72
1:A:475:ASP:H	1:A:481:THR:CG2	1.98	0.72
1:B:436:THR:HG22	1:B:439:ASN:H	1.54	0.70
1:B:436:THR:HB	1:B:439:ASN:HB2	1.73	0.70
1:B:246:SER:O	4:B:701:HOH:O	2.10	0.69
1:A:205:VAL:HG23	1:A:276:THR:HG21	1.74	0.69
1:B:194:PRO:HD2	1:B:226:VAL:O	1.92	0.69
1:A:287:LYS:HG3	1:A:290:ARG:NH2	2.09	0.68
1:B:67:PHE:CE1	1:B:97:THR:HB	2.28	0.68
1:A:30:MET:HE3	1:A:35:ASN:HA	1.75	0.68
1:A:57:TYR:OH	1:A:305:LYS:HE2	1.94	0.66
1:B:542:GLU:OE2	4:B:702:HOH:O	2.13	0.65
1:A:365:GLY:CA	2:A:601:ACT:H1	2.27	0.65
1:A:45:MET:HB2	4:A:854:HOH:O	1.97	0.65
1:A:478:ASP:O	1:A:481:THR:HB	1.96	0.65
1:B:80:ILE:HD12	1:B:113:ILE:HG12	1.79	0.65
1:B:32:GLY:CA	1:B:66:LYS:HD2	2.28	0.64
1:A:424:ASP:N	1:A:428:GLU:O	2.25	0.64
1:A:508:LYS:HE3	1:A:513:GLY:O	1.98	0.64
1:A:112:GLU:OE2	1:A:123:LYS:HE2	2.00	0.61
1:B:67:PHE:CZ	1:B:97:THR:HB	2.35	0.61
1:A:112:GLU:CD	1:A:123:LYS:HE2	2.20	0.61
1:A:80:ILE:HB	1:A:88:ALA:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:HA3	2:A:601:ACT:H1	1.81	0.60
1:B:23:PRO:CG	1:B:117:ASP:HB2	2.31	0.60
1:A:466:GLU:HG3	1:A:485:THR:HG22	1.84	0.60
1:B:48:THR:HG22	1:B:215:THR:HG21	1.84	0.60
1:B:66:LYS:HA	1:B:97:THR:O	2.01	0.60
1:B:93:THR:O	1:B:93:THR:HG22	2.01	0.59
1:B:260:LYS:NZ	1:B:266:LEU:O	2.35	0.59
1:A:270:PRO:HD3	1:A:307:TYR:CD1	2.38	0.59
1:B:151:LYS:HG3	1:B:581:ASN:ND2	2.17	0.59
1:A:186:THR:HB	4:A:780:HOH:O	2.04	0.58
1:B:23:PRO:HD3	1:B:117:ASP:HB2	1.85	0.58
1:B:525:GLY:HA3	1:B:534:TRP:CZ2	2.38	0.58
1:A:474:THR:H	1:A:481:THR:HG23	1.69	0.58
1:A:466:GLU:CG	1:A:485:THR:HG22	2.34	0.58
1:B:244:GLU:O	1:B:250:LYS:HE2	2.04	0.56
1:B:132:ALA:HA	1:B:138:HIS:CG	2.41	0.56
1:B:557:SER:HB2	4:B:890:HOH:O	2.06	0.56
1:B:199:ASN:HB3	1:B:202:VAL:HG23	1.87	0.56
1:A:231:TRP:CZ2	1:A:236:LYS:HG3	2.41	0.56
1:A:40:LYS:HD3	1:A:133:ASP:CG	2.26	0.55
1:B:231:TRP:CE2	1:B:236:LYS:HB2	2.41	0.55
1:A:496:VAL:HG22	1:A:502:ILE:HG13	1.88	0.55
1:B:507:ILE:HG22	1:B:512:LEU:HD12	1.88	0.55
1:B:30:MET:O	1:B:33:SER:N	2.40	0.55
1:A:478:ASP:OD1	1:A:480:MET:HB2	2.08	0.54
1:A:194:PRO:HD2	1:A:226:VAL:O	2.07	0.54
1:B:199:ASN:HB3	1:B:202:VAL:CG2	2.38	0.53
1:B:92:ILE:HG22	1:B:93:THR:N	2.22	0.53
1:A:154:ASN:ND2	4:A:713:HOH:O	2.36	0.53
1:A:367:GLY:O	1:A:371:ILE:HG13	2.08	0.53
1:A:381:GLN:HG3	4:A:984:HOH:O	2.09	0.53
1:B:80:ILE:CD1	1:B:113:ILE:HG12	2.39	0.53
1:B:133:ASP:HB3	1:B:135:ASP:OD1	2.09	0.53
1:B:181:PRO:HG2	1:B:580:LEU:CD2	2.38	0.53
1:A:43:LEU:HD13	1:A:234:TYR:CD1	2.44	0.52
1:A:109:TYR:HB2	1:A:129:ILE:HG22	1.91	0.52
1:B:285:VAL:HG13	4:B:857:HOH:O	2.09	0.52
1:B:142:LEU:HD23	1:B:144:MET:SD	2.49	0.52
1:B:341:ARG:NH2	4:B:708:HOH:O	2.30	0.52
1:B:460:MET:HG2	1:B:579:ILE:CG2	2.40	0.52
1:B:23:PRO:CD	1:B:117:ASP:HB2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:GLU:OE2	1:A:538:ARG:NE	2.41	0.51
1:A:516:ASN:HB3	4:A:711:HOH:O	2.10	0.51
1:B:142:LEU:O	1:B:262:ARG:HD2	2.11	0.51
1:A:502:ILE:HD13	1:A:507:ILE:CG1	2.38	0.51
1:B:205:VAL:HG12	1:B:205:VAL:O	2.10	0.51
1:B:93:THR:O	1:B:93:THR:CG2	2.59	0.51
1:B:465:TRP:O	1:B:542:GLU:HA	2.10	0.51
1:A:516:ASN:ND2	4:A:725:HOH:O	2.44	0.51
1:B:244:GLU:OE2	1:B:246:SER:HB3	2.11	0.51
1:B:343:LEU:O	1:B:347:LEU:HG	2.11	0.50
1:B:407:LEU:O	1:B:436:THR:HG23	2.11	0.50
1:B:492:THR:HB	1:B:497:TRP:CZ3	2.46	0.50
1:B:473:LEU:N	1:B:473:LEU:HD23	2.26	0.50
1:A:101:PHE:HB2	4:A:904:HOH:O	2.11	0.50
1:B:161:MET:HE1	1:B:583:MET:CB	2.33	0.50
1:A:70:TRP:NE1	4:A:705:HOH:O	2.19	0.49
1:B:351:GLU:HG2	1:B:356:ARG:O	2.12	0.49
1:B:224:GLU:HG2	1:B:296:SER:HB3	1.93	0.49
1:A:481:THR:HG23	1:A:481:THR:O	2.11	0.49
1:A:488:LEU:HD12	1:A:542:GLU:HG2	1.95	0.49
1:B:467:GLY:HA3	1:B:485:THR:HG23	1.95	0.49
1:A:376:TYR:O	1:A:380:VAL:HB	2.12	0.49
1:B:518:GLY:HA3	1:B:522:PHE:O	2.13	0.49
1:A:474:THR:H	1:A:481:THR:CG2	2.26	0.48
1:B:53:ASP:HB2	4:B:933:HOH:O	2.12	0.48
1:B:154:ASN:O	1:B:155:THR:O	2.32	0.48
1:A:66:LYS:HE2	1:A:96:GLN:HG2	1.94	0.48
1:A:50:GLY:O	1:A:54:MET:HG3	2.13	0.48
1:B:81:TYR:O	1:B:111:MET:HA	2.13	0.48
1:A:519:ILE:HD12	1:A:520:ASN:OD1	2.13	0.48
1:B:460:MET:CG	1:B:579:ILE:HG21	2.42	0.48
1:B:553:LEU:HA	1:B:586:GLY:HA3	1.96	0.48
1:A:375:ASN:ND2	1:A:378:ASP:OD2	2.46	0.47
1:A:66:LYS:CE	1:A:96:GLN:HG2	2.43	0.47
1:A:460:MET:HE2	1:A:579:ILE:HB	1.96	0.47
1:B:78:TYR:CE2	1:B:90:GLY:HA3	2.49	0.47
1:A:45:MET:SD	1:A:250:LYS:HE3	2.55	0.47
1:A:461:TYR:CE1	1:A:570:TRP:HD1	2.32	0.47
1:A:337:VAL:HG22	1:A:379:ALA:HB2	1.97	0.47
1:B:78:TYR:HA	1:B:114:GLU:O	2.14	0.47
1:B:533:PRO:HD3	1:B:551:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ASP:OD2	1:A:313:ASP:OD1	2.32	0.47
1:A:365:GLY:HA2	2:A:601:ACT:H1	1.96	0.47
1:B:270:PRO:HD3	1:B:307:TYR:CD1	2.50	0.47
1:B:189:LEU:HD11	1:B:387:PHE:CE2	2.50	0.47
1:A:315:GLU:HG2	1:A:316:PHE:CE2	2.50	0.47
1:A:502:ILE:HG23	1:A:502:ILE:O	2.15	0.46
1:A:523:GLU:CD	1:A:538:ARG:HE	2.19	0.46
1:B:78:TYR:CZ	1:B:90:GLY:HA3	2.50	0.46
1:A:106:GLY:HA2	1:A:131:ILE:HG22	1.98	0.46
1:A:366:VAL:HA	1:A:371:ILE:HD11	1.97	0.46
1:B:272:ILE:HD12	1:B:310:VAL:HG23	1.97	0.46
1:B:341:ARG:HB2	1:B:382:TYR:CE2	2.50	0.46
1:A:140:LYS:HD3	1:A:140:LYS:HA	1.65	0.46
1:A:60:GLN:HB3	1:A:102:ASP:HB3	1.97	0.46
1:A:191:GLY:HA2	1:A:192:PHE:HA	1.77	0.46
1:B:456:LEU:HD23	1:B:567:LEU:CD2	2.46	0.45
1:B:272:ILE:CD1	1:B:310:VAL:HG23	2.47	0.45
1:B:396:GLY:O	1:B:487:LYS:HE2	2.16	0.45
1:A:323:ALA:C	1:A:325:ASP:H	2.19	0.45
1:A:505:LYS:HB3	1:A:576:ASN:HB3	1.99	0.45
1:B:272:ILE:HD12	1:B:310:VAL:CG2	2.47	0.45
1:A:48:THR:HG22	1:A:215:THR:HG21	1.98	0.45
1:B:407:LEU:HD22	1:B:555:LYS:HG2	1.99	0.45
1:B:478:ASP:OD1	1:B:480:MET:HB2	2.17	0.45
1:B:436:THR:HG22	1:B:438:ASP:N	2.32	0.45
1:B:51:TYR:HE1	1:B:227:ILE:HD12	1.82	0.44
1:A:70:TRP:HA	1:A:70:TRP:CE3	2.52	0.44
1:A:111:MET:HG2	1:A:112:GLU:N	2.32	0.44
1:A:270:PRO:HD3	1:A:307:TYR:CG	2.53	0.44
1:A:78:TYR:HB3	1:A:92:ILE:HD11	2.00	0.44
1:A:81:TYR:HA	1:A:85:VAL:O	2.17	0.44
1:A:272:ILE:CD1	1:A:310:VAL:CG1	2.95	0.44
1:A:234:TYR:HA	1:A:250:LYS:O	2.17	0.43
1:B:68:ASN:OD1	1:B:68:ASN:N	2.51	0.43
1:A:456:LEU:HD23	1:A:555:LYS:HB3	2.01	0.43
1:A:421:SER:HA	4:A:877:HOH:O	2.17	0.43
1:B:66:LYS:HE2	1:B:66:LYS:HB3	1.84	0.43
1:B:438:ASP:O	1:B:442:GLN:HG2	2.18	0.43
1:A:223:TYR:O	1:A:293:PHE:HA	2.18	0.43
1:A:144:MET:HG2	1:A:262:ARG:NE	2.34	0.43
1:B:57:TYR:HB2	1:B:303:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:LYS:HD3	1:A:268:ILE:HD12	2.01	0.43
1:B:79:ASN:HB2	1:B:114:GLU:HB3	2.00	0.43
1:B:161:MET:HG2	4:B:728:HOH:O	2.18	0.43
1:B:350:LEU:O	1:B:354:THR:HG23	2.18	0.43
1:B:50:GLY:O	1:B:54:MET:HG3	2.18	0.43
1:B:298:LYS:HE3	1:B:350:LEU:HD13	2.00	0.43
1:B:583:MET:O	1:B:587:MET:HB2	2.18	0.43
1:A:449:VAL:HG11	1:A:454:LEU:HD21	2.01	0.42
1:A:517:THR:O	4:A:706:HOH:O	2.21	0.42
1:B:28:VAL:HG22	1:B:113:ILE:HD12	2.00	0.42
1:A:56:LYS:NZ	4:A:740:HOH:O	2.52	0.42
1:A:467:GLY:HA3	1:A:485:THR:HB	2.01	0.42
1:B:67:PHE:CE1	1:B:97:THR:CB	3.00	0.42
1:A:523:GLU:O	1:A:535:VAL:HA	2.20	0.42
1:B:414:ARG:NH1	1:B:424:ASP:C	2.73	0.42
1:B:401:PRO:HA	1:B:465:TRP:CH2	2.54	0.42
1:A:22:ALA:N	1:A:119:THR:HG1	2.17	0.42
1:A:317:PRO:HB3	1:A:332:ASP:HB3	2.01	0.42
1:B:502:ILE:HG23	1:B:507:ILE:HD11	2.02	0.42
1:A:374:VAL:HB	1:A:376:TYR:CE2	2.55	0.42
1:B:37:GLN:HE21	1:B:130:THR:HB	1.85	0.42
1:B:298:LYS:HD2	1:B:346:MET:HG2	2.02	0.41
1:A:35:ASN:O	1:A:37:GLN:HG2	2.20	0.41
1:B:425:GLU:OE2	1:B:425:GLU:HA	2.20	0.41
1:B:463:ARG:HA	1:B:500:GLY:O	2.20	0.41
1:A:326:LYS:HG3	4:A:1061:HOH:O	2.20	0.41
1:A:403:HIS:HD2	4:A:722:HOH:O	2.03	0.41
1:B:23:PRO:HG3	1:B:117:ASP:CB	2.43	0.41
1:B:68:ASN:ND2	1:B:70:TRP:CH2	2.88	0.41
1:B:154:ASN:O	1:B:154:ASN:OD1	2.39	0.41
1:A:131:ILE:HG22	1:A:131:ILE:O	2.20	0.41
1:B:359:GLU:HA	1:B:384:ASP:OD2	2.20	0.41
1:B:508:LYS:HA	1:B:512:LEU:HB2	2.03	0.41
1:B:43:LEU:HA	1:B:54:MET:O	2.20	0.41
1:B:169:GLY:HA3	4:B:884:HOH:O	2.19	0.41
1:A:25:ALA:CA	1:A:122:SER:OG	2.60	0.41
1:A:132:ALA:HA	1:A:138:HIS:CG	2.56	0.41
1:A:270:PRO:HD2	1:A:309:GLY:O	2.21	0.41
1:B:171:TYR:OH	1:B:231:TRP:HD1	2.03	0.41
1:B:47:THR:HG22	1:B:48:THR:H	1.85	0.41
1:B:371:ILE:HG22	1:B:447:GLN:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:LYS:HE3	4:B:788:HOH:O	2.20	0.40
1:B:465:TRP:HB3	1:B:484:ALA:HB1	2.04	0.40
1:A:323:ALA:C	1:A:325:ASP:N	2.75	0.40
1:B:152:THR:HA	4:B:706:HOH:O	2.20	0.40
1:B:511:MET:SD	1:B:511:MET:N	2.94	0.40
1:B:37:GLN:NE2	1:B:130:THR:HB	2.36	0.40
1:B:49:SER:HB3	1:B:53:ASP:OD2	2.22	0.40
1:B:69:GLN:HE22	1:B:115:ALA:CB	2.35	0.40
1:B:73:THR:HA	1:B:74:PRO:HD3	1.93	0.40
1:B:111:MET:O	1:B:126:PRO:HA	2.22	0.40
1:B:473:LEU:HD11	1:B:536:TRP:CH2	2.56	0.40

All (2) 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:B:735:HOH:O	4:B:896:HOH:O[1_655]	2.15	0.05
4:B:754:HOH:O	4:B:954:HOH:O[1_655]	2.16	0.04

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	567/571 (99%)	542 (96%)	25 (4%)	0	100	100
1	B	567/571 (99%)	530 (94%)	34 (6%)	3 (0%)	29	48
All	All	1134/1142 (99%)	1072 (94%)	59 (5%)	3 (0%)	41	61

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	155	THR

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Mol	Chain	Res	Type
1	B	30	MET
1	B	206	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	449/450 (100%)	432 (96%)	17 (4%)	33	58
1	B	451/450 (100%)	433 (96%)	18 (4%)	31	56
All	All	900/900 (100%)	865 (96%)	35 (4%)	32	57

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	A	113	ILE
1	A	209	SER
1	A	237	SER
1	A	326	LYS
1	A	404	GLN
1	A	407	LEU
1	A	428	GLU
1	A	481	THR
1	A	485	THR
1	A	492	THR
1	A	502	ILE
1	A	511	MET
1	A	547	ASP
1	A	548	ASP
1	A	561	SER
1	A	587	MET
1	B	45	MET
1	B	56	LYS
1	B	60	GLN
1	B	117	ASP

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Mol	Chain	Res	Type
1	B	131	ILE
1	B	260	LYS
1	B	296	SER
1	B	380	VAL
1	B	404	GLN
1	B	407	LEU
1	B	411	SER
1	B	458	THR
1	B	465	TRP
1	B	469	THR
1	B	477	ASN
1	B	511	MET
1	B	545	THR
1	B	561	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	96	GLN
1	A	184	ASN
1	A	214	GLN
1	A	403	HIS
1	B	37	GLN
1	B	69	GLN
1	B	145	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)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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	ACT	B	601	-	3,3,3	1.39	0	3,3,3	1.62	1 (33%)
2	ACT	A	601	-	3,3,3	0.71	0	3,3,3	2.38	2 (66%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	ACT	O-C-CH3	-3.14	110.12	122.33
2	A	601	ACT	OXT-C-O	2.57	131.52	122.05
2	B	601	ACT	OXT-C-O	2.16	130.00	122.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ACT	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

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	569/571 (99%)	-0.27	8 (1%) 75 77	5, 13, 27, 49	0
1	B	567/571 (99%)	-0.00	26 (4%) 32 34	6, 18, 40, 58	0
All	All	1136/1142 (99%)	-0.14	34 (2%) 50 53	5, 15, 35, 58	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	117	ASP	4.2
1	B	476	PRO	4.1
1	B	70	TRP	3.7
1	B	425	GLU	3.7
1	B	204	SER	3.6
1	A	426	ASN	3.5
1	B	426	ASN	3.5
1	B	119	THR	3.2
1	A	589	GLY	3.0
1	B	245	TYR	2.9
1	A	204	SER	2.9
1	B	31	TYR	2.8
1	A	428	GLU	2.7
1	B	154	ASN	2.7
1	B	92	ILE	2.6
1	A	31	TYR	2.6
1	B	73	THR	2.5
1	B	206	GLY	2.5
1	B	325	ASP	2.4
1	A	423	VAL	2.3
1	B	428	GLU	2.3
1	B	427	GLY	2.3
1	B	205	VAL	2.3
1	B	155	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	423	VAL	2.1
1	B	324	ALA	2.1
1	A	422	GLY	2.1
1	B	429	ALA	2.1
1	B	156	ASP	2.1
1	B	91	ALA	2.1
1	B	22	ALA	2.1
1	B	472	THR	2.1
1	A	245	TYR	2.0
1	B	23	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
2	ACT	A	601	4/4	0.87	0.25	13,25,30,30	0
2	ACT	B	601	4/4	0.93	0.24	10,12,15,22	0
3	CA	B	603	1/1	0.96	0.10	28,28,28,28	0
3	CA	B	602	1/1	0.99	0.04	15,15,15,15	0
3	CA	A	602	1/1	1.00	0.03	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.