Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:26 am BST

PDB ID	:	3EAQ
Title	:	Novel dimerization motif in the DEAD box RNA helicase Hera form 2, complete dimer, symmetric
Authors	:	Klostermeier, D.; Rudolph, M.G.
Deposited on	:	2008-08-26
Resolution	:	2.30 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 ⓘ symbol.

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

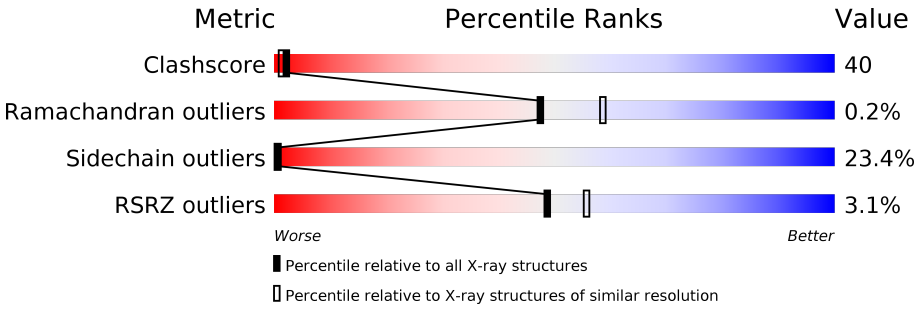
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance

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

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	212	4% 33% 51% 14%
1	B	212	2% 49% 41% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3314 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 Heat resistant RNA dependent ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1645	1033	317	294	1			
1	B	209	Total	C	N	O	S	0	0	0
			1660	1041	322	296	1			

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 3 is water.

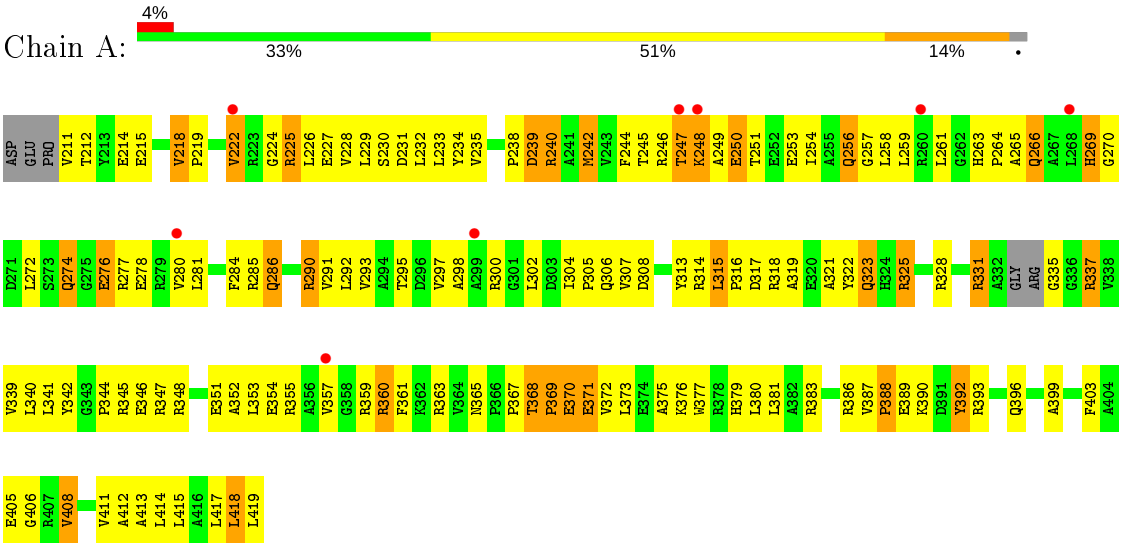
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		
3	B	6	Total	O	0	0
			6	6		

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 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.

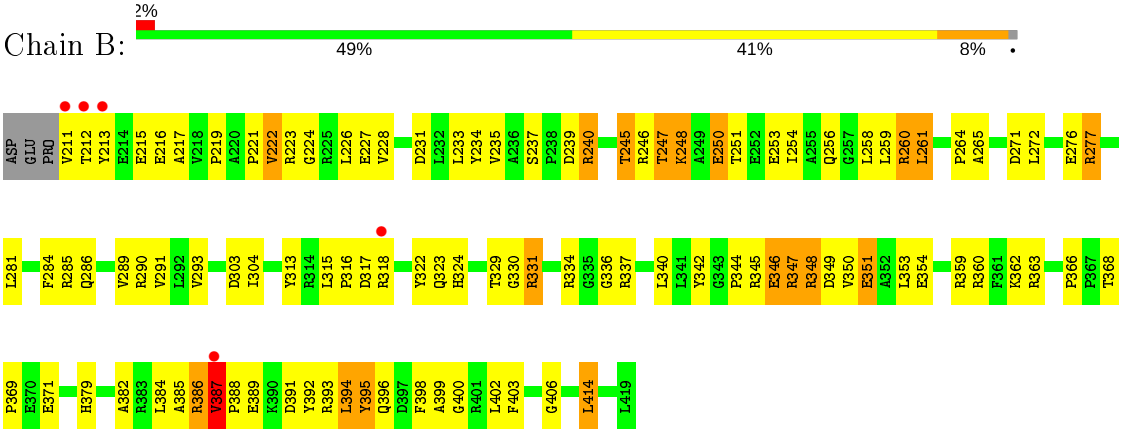
- Molecule 1: Heat resistant RNA dependent ATPase

Chain A:



- Molecule 1: Heat resistant RNA dependent ATPase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.62Å 70.78Å 101.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.88 – 2.30 42.60 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.88-2.30) 99.6 (42.60-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.29Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.218 , 0.269 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	3314	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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: CL

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	0.61	0/1673	0.78	1/2262 (0.0%)
1	B	0.80	0/1689	0.88	1/2284 (0.0%)
All	All	0.71	0/3362	0.83	2/4546 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	387	VAL	C-N-CD	-9.37	100.00	120.60
1	B	387	VAL	N-CA-C	-5.52	96.09	111.00

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	1645	0	1676	165	0
1	B	1660	0	1693	121	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	6	0	0	1	0
All	All	3314	0	3369	264	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 40.

All (264) 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:394:LEU:HD12	1:B:394:LEU:H	1.23	1.00
1:A:414:LEU:CD2	1:B:384:LEU:HD11	1.97	0.94
1:A:413:ALA:HB1	1:B:387:VAL:HG21	1.53	0.91
1:A:245:THR:HG21	1:A:250:GLU:HB3	1.53	0.88
1:B:265:ALA:HB2	1:B:291:VAL:HB	1.51	0.88
1:A:408:VAL:HG22	1:B:399:ALA:HB3	1.55	0.88
1:A:360:ARG:HH11	1:A:360:ARG:HB2	1.37	0.86
1:A:315:LEU:H	1:A:315:LEU:HD23	1.41	0.84
1:A:269:HIS:HA	1:A:298:ALA:HB2	1.57	0.84
1:A:408:VAL:CG1	1:B:396:GLN:HB3	2.08	0.83
1:A:251:THR:HG21	1:A:295:THR:HG22	1.61	0.82
1:A:248:LYS:HD2	1:A:249:ALA:N	1.95	0.81
1:A:245:THR:CG2	1:A:250:GLU:HB3	2.10	0.81
1:B:389:GLU:OE2	1:B:393:ARG:HB2	1.81	0.80
1:A:414:LEU:HD21	1:B:384:LEU:HD11	1.63	0.79
1:B:350:VAL:O	1:B:354:GLU:HG3	1.83	0.78
1:B:231:ASP:O	1:B:235:VAL:HG23	1.84	0.77
1:B:222:VAL:HG13	1:B:223:ARG:HG3	1.67	0.77
1:B:384:LEU:O	1:B:387:VAL:HG22	1.85	0.77
1:A:406:GLY:HA2	1:B:403:PHE:CE2	2.20	0.77
1:A:337:ARG:HG2	1:A:337:ARG:HH21	1.49	0.77
1:B:264:PRO:HG2	1:B:290:ARG:HB2	1.67	0.77
1:B:322:TYR:CE1	1:B:340:LEU:HD21	2.21	0.76
1:A:242:MET:HG2	1:A:244:PHE:CE1	2.19	0.76
1:A:249:ALA:O	1:A:253:GLU:HB2	1.85	0.76
1:B:281:LEU:O	1:B:285:ARG:HG3	1.86	0.76
1:B:224:GLY:O	1:B:228:VAL:HG23	1.85	0.75
1:B:265:ALA:CB	1:B:291:VAL:HB	2.17	0.75
1:B:354:GLU:HB3	1:B:359:ARG:O	1.87	0.75
1:A:224:GLY:O	1:A:228:VAL:HG23	1.88	0.74
1:A:247:THR:HG23	1:A:250:GLU:OE2	1.88	0.73
1:A:251:THR:HG21	1:A:295:THR:CG2	2.17	0.73
1:B:322:TYR:HE1	1:B:340:LEU:HD21	1.52	0.73
1:A:259:LEU:HA	1:A:263:HIS:O	1.88	0.73
1:A:393:ARG:NH1	1:A:393:ARG:HB3	2.03	0.73
1:A:321:ALA:O	1:A:325:ARG:HG3	1.90	0.72
1:A:360:ARG:HH11	1:A:360:ARG:CB	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LEU:HD12	1:A:380:LEU:O	1.90	0.71
1:A:414:LEU:HD23	1:B:384:LEU:HD11	1.71	0.71
1:B:277:ARG:NE	1:B:303:ASP:OD1	2.24	0.71
1:B:315:LEU:HD22	1:B:315:LEU:H	1.55	0.71
1:A:368:THR:O	1:A:371:GLU:N	2.24	0.71
1:B:246:ARG:NH1	1:B:317:ASP:HB2	2.06	0.70
1:A:246:ARG:HG3	1:A:246:ARG:HH11	1.57	0.70
1:B:240:ARG:CG	1:B:331:ARG:HH21	2.05	0.70
1:A:247:THR:O	1:A:251:THR:HG23	1.93	0.69
1:A:322:TYR:HE1	1:A:340:LEU:HD21	1.56	0.69
1:B:315:LEU:HD22	1:B:315:LEU:N	2.08	0.69
1:A:368:THR:OG1	1:A:371:GLU:HG3	1.92	0.69
1:B:254:ILE:HG22	1:B:258:LEU:HD11	1.73	0.69
1:A:245:THR:HG22	1:A:251:THR:HG22	1.73	0.69
1:A:240:ARG:HG3	1:A:331:ARG:NH2	2.08	0.68
1:A:246:ARG:NH1	1:A:246:ARG:HG3	2.07	0.68
1:A:269:HIS:HA	1:A:298:ALA:CB	2.23	0.68
1:A:408:VAL:HG13	1:B:396:GLN:HB3	1.75	0.67
1:A:274:GLN:NE2	1:A:278:GLU:HG3	2.10	0.67
1:A:264:PRO:HG2	1:A:290:ARG:HB2	1.76	0.67
1:A:348:ARG:HA	1:A:351:GLU:HG3	1.77	0.67
1:A:251:THR:CG2	1:A:295:THR:HG22	2.25	0.66
1:A:244:PHE:CZ	1:A:325:ARG:HB3	2.30	0.66
1:A:212:THR:HG22	1:A:335:GLY:HA2	1.78	0.66
1:A:357:VAL:HG12	1:A:359:ARG:HG2	1.77	0.66
1:A:380:LEU:CD1	1:A:418:LEU:HD22	2.26	0.66
1:A:386:ARG:O	1:A:388:PRO:HD3	1.96	0.66
1:A:258:LEU:CD2	1:A:291:VAL:HG11	2.27	0.65
1:A:319:ALA:O	1:A:323:GLN:NE2	2.30	0.65
1:B:240:ARG:HG2	1:B:331:ARG:HH21	1.62	0.64
1:B:245:THR:HG23	1:B:246:ARG:N	2.13	0.64
1:A:408:VAL:HG11	1:B:396:GLN:HB3	1.77	0.64
1:B:245:THR:CG2	1:B:250:GLU:HB3	2.28	0.64
1:A:297:VAL:HG22	1:A:300:ARG:NH1	2.13	0.64
1:A:337:ARG:HG2	1:A:337:ARG:NH2	2.09	0.64
1:A:257:GLY:O	1:A:261:LEU:HD12	1.96	0.64
1:B:215:GLU:OE1	1:B:359:ARG:NH1	2.31	0.64
1:B:379:HIS:O	1:B:382:ALA:HB3	1.98	0.64
1:B:394:LEU:H	1:B:394:LEU:CD1	1.94	0.63
1:A:222:VAL:HG22	1:A:225:ARG:HD3	1.81	0.62
1:A:242:MET:HB2	1:A:307:VAL:HG11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:HD22	1:B:276:GLU:CB	2.29	0.62
1:B:245:THR:HG21	1:B:250:GLU:HB3	1.81	0.62
1:A:242:MET:HG2	1:A:244:PHE:HE1	1.62	0.61
1:B:272:LEU:HD22	1:B:276:GLU:HB2	1.83	0.61
1:B:354:GLU:OE2	1:B:360:ARG:HA	2.01	0.61
1:B:254:ILE:HG22	1:B:258:LEU:CD1	2.31	0.60
1:A:304:ILE:HG21	1:A:328:ARG:HD2	1.83	0.60
1:A:403:PHE:HE1	1:B:406:GLY:HA2	1.67	0.60
1:A:228:VAL:HG12	1:A:232:LEU:HD12	1.83	0.59
1:A:354:GLU:OE1	1:A:360:ARG:HG2	2.03	0.59
1:A:419:LEU:HD23	1:B:395:TYR:OH	2.02	0.59
1:A:258:LEU:HD22	1:A:291:VAL:HG11	1.84	0.59
1:A:417:LEU:HD11	1:B:384:LEU:CD2	2.32	0.58
1:A:393:ARG:HH11	1:A:393:ARG:HB3	1.66	0.58
1:B:346:GLU:O	1:B:350:VAL:HG23	2.04	0.58
1:A:286:GLN:OE1	1:A:286:GLN:HA	2.03	0.58
1:B:277:ARG:NH2	1:B:304:ILE:HD11	2.19	0.58
1:A:417:LEU:HD11	1:B:384:LEU:HD23	1.85	0.58
1:A:353:LEU:CD1	1:A:361:PHE:HE1	2.17	0.58
1:A:351:GLU:O	1:A:355:ARG:HG3	2.03	0.57
1:A:408:VAL:HG22	1:B:399:ALA:CB	2.32	0.57
1:B:277:ARG:HG3	1:B:277:ARG:HH11	1.69	0.57
1:A:315:LEU:N	1:A:315:LEU:HD23	2.15	0.57
1:A:254:ILE:HG22	1:A:293:VAL:HG21	1.85	0.57
1:B:239:ASP:OD2	1:B:334:ARG:NH1	2.37	0.57
1:A:254:ILE:HB	1:A:293:VAL:HG11	1.86	0.57
1:A:322:TYR:CE1	1:A:340:LEU:HD21	2.40	0.56
1:A:380:LEU:HD13	1:A:418:LEU:HD22	1.86	0.56
1:A:315:LEU:H	1:A:315:LEU:CD2	2.16	0.56
1:A:265:ALA:HA	1:A:291:VAL:O	2.06	0.56
1:A:318:ARG:O	1:A:321:ALA:HB3	2.05	0.56
1:A:360:ARG:HH11	1:A:360:ARG:CG	2.18	0.56
1:B:254:ILE:HD11	1:B:313:TYR:CD2	2.41	0.55
1:B:344:PRO:O	1:B:347:ARG:HD2	2.06	0.55
1:A:297:VAL:HG22	1:A:300:ARG:HH12	1.71	0.55
1:A:254:ILE:HD11	1:A:313:TYR:CD2	2.41	0.55
1:A:270:GLY:C	1:A:272:LEU:H	2.10	0.55
1:B:368:THR:O	1:B:371:GLU:HB2	2.07	0.55
1:A:246:ARG:CG	1:A:246:ARG:HH11	2.20	0.55
1:B:246:ARG:HH12	1:B:317:ASP:CB	2.20	0.54
1:A:412:ALA:HA	1:A:415:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:CG2	1:A:293:VAL:HG11	2.38	0.54
1:B:251:THR:HA	1:B:293:VAL:CG1	2.38	0.54
1:B:260:ARG:H	1:B:260:ARG:HD2	1.73	0.54
1:B:246:ARG:HH12	1:B:317:ASP:HB2	1.71	0.54
1:B:256:GLN:O	1:B:260:ARG:HD2	2.09	0.53
1:A:212:THR:O	1:A:335:GLY:HA2	2.08	0.53
1:B:387:VAL:O	1:B:387:VAL:HG23	2.08	0.53
1:B:347:ARG:HB2	1:B:347:ARG:NH1	2.24	0.53
1:A:244:PHE:CE2	1:A:325:ARG:HB3	2.43	0.53
1:A:368:THR:HG22	1:A:369:PRO:CD	2.38	0.53
1:A:281:LEU:HD22	1:A:305:PRO:HD3	1.91	0.53
1:A:413:ALA:CB	1:B:387:VAL:HG21	2.32	0.53
1:A:234:TYR:OH	1:A:261:LEU:O	2.25	0.52
1:A:231:ASP:O	1:A:235:VAL:HG23	2.10	0.52
1:A:245:THR:HG21	1:A:251:THR:N	2.25	0.52
1:A:256:GLN:HA	1:A:256:GLN:OE1	2.08	0.52
1:A:353:LEU:HD12	1:A:361:PHE:HE1	1.72	0.52
1:A:212:THR:O	1:A:212:THR:HG22	2.10	0.52
1:A:380:LEU:HD11	1:A:418:LEU:HD22	1.90	0.52
1:A:380:LEU:HD12	1:A:380:LEU:C	2.29	0.52
1:A:388:PRO:HB2	1:A:390:LYS:HG2	1.92	0.51
1:B:256:GLN:HB3	1:B:260:ARG:NH1	2.25	0.51
1:A:315:LEU:N	1:A:315:LEU:CD2	2.74	0.51
1:B:348:ARG:O	1:B:351:GLU:HG3	2.10	0.51
1:B:254:ILE:O	1:B:258:LEU:HG	2.10	0.51
1:B:245:THR:HG21	1:B:251:THR:HG23	1.92	0.51
1:B:246:ARG:HB3	1:B:250:GLU:OE2	2.10	0.50
1:B:347:ARG:CG	1:B:347:ARG:HH11	2.24	0.50
1:A:222:VAL:HG23	1:A:225:ARG:HH11	1.75	0.50
1:A:238:PRO:HB2	1:A:308:ASP:HB2	1.93	0.50
1:A:284:PHE:CD2	1:A:292:LEU:HD22	2.47	0.50
1:A:306:GLN:HE22	1:A:328:ARG:HA	1.76	0.50
1:B:394:LEU:HD12	1:B:394:LEU:N	2.07	0.50
1:A:389:GLU:O	1:A:393:ARG:HB2	2.11	0.49
1:A:352:ALA:HA	1:A:355:ARG:NH1	2.28	0.49
1:A:244:PHE:CE1	1:A:325:ARG:HB3	2.47	0.49
1:A:222:VAL:HA	1:A:225:ARG:HD3	1.95	0.49
1:A:274:GLN:HE21	1:A:278:GLU:HG3	1.78	0.49
1:B:245:THR:CG2	1:B:247:THR:O	2.60	0.49
1:B:315:LEU:CD2	1:B:315:LEU:H	2.23	0.49
1:B:316:PRO:HG2	1:B:322:TYR:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ALA:HB1	1:B:342:TYR:CE1	2.47	0.49
1:A:269:HIS:CA	1:A:298:ALA:HB2	2.38	0.48
1:B:216:GLU:OE1	1:B:337:ARG:NH2	2.45	0.48
1:B:221:PRO:HD2	1:B:228:VAL:HG21	1.95	0.48
1:A:340:LEU:N	1:A:340:LEU:HD12	2.28	0.48
1:B:245:THR:CG2	1:B:251:THR:HG23	2.44	0.48
1:B:245:THR:CG2	1:B:246:ARG:N	2.76	0.48
1:B:385:ALA:C	1:B:386:ARG:HG3	2.34	0.48
1:A:418:LEU:HD13	1:B:414:LEU:CD2	2.43	0.48
1:A:222:VAL:CG2	1:A:225:ARG:HD3	2.43	0.48
1:A:344:PRO:O	1:A:347:ARG:HG3	2.13	0.48
1:A:218:VAL:CG2	1:A:339:VAL:HG13	2.44	0.47
1:A:272:LEU:HD12	1:A:276:GLU:OE1	2.14	0.47
1:A:280:VAL:HG12	1:A:281:LEU:N	2.28	0.47
1:A:393:ARG:CB	1:A:393:ARG:CZ	2.92	0.47
1:A:368:THR:HG22	1:A:369:PRO:HD2	1.95	0.47
1:B:398:PHE:CE2	1:B:402:LEU:HD11	2.49	0.47
1:A:272:LEU:HD12	1:A:276:GLU:CD	2.35	0.47
1:B:234:TYR:OH	1:B:261:LEU:O	2.14	0.47
1:B:347:ARG:HG3	1:B:347:ARG:HH11	1.80	0.47
1:A:277:ARG:O	1:A:277:ARG:HG2	2.15	0.47
1:A:263:HIS:HA	1:A:264:PRO:HD2	1.84	0.47
1:A:351:GLU:HA	1:A:354:GLU:OE2	2.15	0.47
1:B:251:THR:HA	1:B:293:VAL:HG12	1.95	0.47
1:A:376:LYS:HB2	1:A:419:LEU:HD11	1.97	0.46
1:A:357:VAL:CG1	1:A:359:ARG:HG2	2.44	0.46
1:A:370:GLU:HG2	1:A:370:GLU:H	1.48	0.46
1:B:213:TYR:HB2	1:B:336:GLY:O	2.16	0.46
1:B:277:ARG:HE	1:B:303:ASP:CG	2.17	0.46
1:A:251:THR:HA	1:A:293:VAL:HG12	1.97	0.46
1:B:277:ARG:CG	1:B:277:ARG:HH11	2.28	0.46
1:A:377:TRP:HA	1:A:419:LEU:HD13	1.97	0.46
1:A:360:ARG:CG	1:A:360:ARG:NH1	2.78	0.45
1:A:235:VAL:HG21	1:A:367:PRO:HB3	1.98	0.45
1:B:384:LEU:C	1:B:386:ARG:H	2.19	0.45
1:A:218:VAL:HG23	1:A:339:VAL:HG13	1.98	0.45
1:A:375:ALA:O	1:A:379:HIS:ND1	2.48	0.45
1:B:245:THR:HG21	1:B:247:THR:O	2.16	0.45
1:A:406:GLY:CA	1:B:403:PHE:CE2	2.96	0.45
1:B:240:ARG:CG	1:B:331:ARG:NH2	2.78	0.45
1:A:274:GLN:NE2	1:A:278:GLU:CG	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:ARG:O	1:A:246:ARG:HG2	2.16	0.45
1:B:315:LEU:N	1:B:315:LEU:CD2	2.79	0.45
1:A:248:LYS:C	1:A:248:LYS:HD2	2.36	0.45
1:A:251:THR:HB	1:A:293:VAL:O	2.17	0.45
1:B:247:THR:OG1	1:B:248:LYS:N	2.50	0.45
1:A:368:THR:HG22	1:A:369:PRO:HD3	1.99	0.44
1:B:304:ILE:HD13	1:B:304:ILE:N	2.32	0.44
1:A:304:ILE:HD13	1:A:304:ILE:HA	1.80	0.44
1:A:353:LEU:CD1	1:A:361:PHE:CE1	2.99	0.44
1:A:396:GLN:O	1:A:399:ALA:HB3	2.17	0.44
1:B:246:ARG:NH1	1:B:317:ASP:CB	2.78	0.44
1:A:266:GLN:HE21	1:A:266:GLN:HB3	1.55	0.44
1:A:222:VAL:HA	1:A:225:ARG:CD	2.48	0.43
1:A:408:VAL:HG13	1:B:396:GLN:CB	2.45	0.43
1:B:388:PRO:HD2	1:B:391:ASP:OD1	2.18	0.43
1:B:368:THR:HA	1:B:369:PRO:HD3	1.84	0.43
1:A:251:THR:HG21	1:A:295:THR:HG23	2.00	0.43
1:A:393:ARG:NH1	1:A:393:ARG:CB	2.79	0.43
1:A:239:ASP:HB3	1:A:331:ARG:NH2	2.33	0.43
1:A:408:VAL:CG2	1:B:400:GLY:N	2.82	0.43
1:B:211:VAL:HG12	1:B:211:VAL:O	2.19	0.43
1:B:395:TYR:HA	3:B:421:HOH:O	2.19	0.43
1:A:212:THR:HG22	1:A:335:GLY:CA	2.48	0.43
1:A:222:VAL:HG23	1:A:225:ARG:NH1	2.34	0.43
1:B:396:GLN:O	1:B:399:ALA:HB3	2.18	0.43
1:A:315:LEU:HA	1:A:316:PRO:HD3	1.76	0.43
1:B:248:LYS:HE2	1:B:248:LYS:HB2	1.76	0.43
1:A:251:THR:HA	1:A:293:VAL:CG1	2.49	0.42
1:A:218:VAL:O	1:A:341:LEU:HA	2.18	0.42
1:A:347:ARG:O	1:A:351:GLU:HG3	2.19	0.42
1:A:368:THR:O	1:A:371:GLU:HB2	2.19	0.42
1:A:389:GLU:HG2	1:A:393:ARG:HD3	2.00	0.42
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.91	0.42
1:B:329:THR:OG1	1:B:330:GLY:N	2.52	0.42
1:A:245:THR:HG22	1:A:251:THR:CG2	2.47	0.42
1:B:284:PHE:HD1	1:B:289:VAL:HG12	1.84	0.42
1:B:322:TYR:CD1	1:B:340:LEU:HD21	2.55	0.42
1:A:218:VAL:HA	1:A:219:PRO:HD2	1.72	0.42
1:A:342:TYR:HB2	1:A:346:GLU:HB3	2.02	0.42
1:A:368:THR:N	1:A:371:GLU:HB2	2.34	0.42
1:B:389:GLU:HA	1:B:392:TYR:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:TYR:CD1	1:A:392:TYR:C	2.94	0.42
1:A:230:SER:O	1:A:233:LEU:HB2	2.20	0.41
1:B:251:THR:CB	1:B:293:VAL:HG12	2.50	0.41
1:B:265:ALA:HA	1:B:291:VAL:O	2.20	0.41
1:B:348:ARG:HA	1:B:351:GLU:HG3	2.01	0.41
1:A:411:VAL:O	1:A:415:LEU:HD12	2.20	0.41
1:B:245:THR:CG2	1:B:250:GLU:CB	2.98	0.41
1:B:347:ARG:CB	1:B:347:ARG:CZ	2.99	0.41
1:A:337:ARG:HH21	1:A:337:ARG:CG	2.21	0.41
1:B:316:PRO:HB2	1:B:318:ARG:O	2.21	0.41
1:A:417:LEU:CD1	1:B:384:LEU:HD21	2.51	0.41
1:A:414:LEU:HD23	1:B:384:LEU:HD21	2.02	0.41
1:B:251:THR:HA	1:B:293:VAL:HG11	2.03	0.41
1:B:347:ARG:CB	1:B:347:ARG:NH1	2.84	0.41
1:B:402:LEU:HD23	1:B:402:LEU:HA	1.94	0.41
1:A:226:LEU:O	1:A:229:LEU:HB3	2.21	0.41
1:B:219:PRO:HG2	1:B:366:PRO:HD3	2.03	0.41
1:A:417:LEU:HD11	1:B:384:LEU:HD21	2.02	0.41
1:B:213:TYR:C	1:B:213:TYR:CD1	2.95	0.41
1:A:254:ILE:CB	1:A:293:VAL:HG11	2.49	0.40
1:B:254:ILE:CG2	1:B:258:LEU:HD11	2.48	0.40
1:B:345:ARG:HH11	1:B:345:ARG:CG	2.34	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	203/212 (96%)	186 (92%)	16 (8%)	1 (0%)	29 35
1	B	207/212 (98%)	185 (89%)	22 (11%)	0	100 100
All	All	410/424 (97%)	371 (90%)	38 (9%)	1 (0%)	47 58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	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	166/170 (98%)	121 (73%)	45 (27%)	0 0
1	B	167/170 (98%)	134 (80%)	33 (20%)	1 1
All	All	333/340 (98%)	255 (77%)	78 (23%)	1 0

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	VAL
1	A	214	GLU
1	A	215	GLU
1	A	218	VAL
1	A	222	VAL
1	A	225	ARG
1	A	227	GLU
1	A	239	ASP
1	A	240	ARG
1	A	242	MET
1	A	247	THR
1	A	248	LYS
1	A	250	GLU
1	A	256	GLN
1	A	266	GLN
1	A	269	HIS
1	A	274	GLN
1	A	276	GLU
1	A	285	ARG
1	A	286	GLN
1	A	290	ARG
1	A	302	LEU

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Mol	Chain	Res	Type
1	A	314	ARG
1	A	315	LEU
1	A	317	ASP
1	A	323	GLN
1	A	325	ARG
1	A	331	ARG
1	A	337	ARG
1	A	345	ARG
1	A	360	ARG
1	A	363	ARG
1	A	365	ASN
1	A	368	THR
1	A	369	PRO
1	A	370	GLU
1	A	371	GLU
1	A	372	VAL
1	A	373	LEU
1	A	381	LEU
1	A	383	ARG
1	A	392	TYR
1	A	405	GLU
1	A	408	VAL
1	A	418	LEU
1	B	212	THR
1	B	222	VAL
1	B	226	LEU
1	B	227	GLU
1	B	237	SER
1	B	240	ARG
1	B	245	THR
1	B	247	THR
1	B	248	LYS
1	B	250	GLU
1	B	253	GLU
1	B	259	LEU
1	B	260	ARG
1	B	261	LEU
1	B	271	ASP
1	B	277	ARG
1	B	286	GLN
1	B	323	GLN
1	B	324	HIS

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Mol	Chain	Res	Type
1	B	331	ARG
1	B	346	GLU
1	B	347	ARG
1	B	348	ARG
1	B	349	ASP
1	B	351	GLU
1	B	353	LEU
1	B	362	LYS
1	B	363	ARG
1	B	386	ARG
1	B	387	VAL
1	B	394	LEU
1	B	395	TYR
1	B	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	266	GLN
1	A	274	GLN
1	A	306	GLN
1	A	323	GLN
1	B	365	ASN
1	B	396	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

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	207/212 (97%)	0.35	8 (3%) 39 46	38, 72, 94, 118	0
1	B	209/212 (98%)	0.17	5 (2%) 59 66	31, 58, 87, 106	0
All	All	416/424 (98%)	0.26	13 (3%) 49 56	31, 66, 93, 118	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	211	VAL	4.3
1	B	212	THR	4.3
1	A	357	VAL	3.3
1	A	299	ALA	3.0
1	B	318	ARG	2.9
1	B	387	VAL	2.8
1	A	280	VAL	2.4
1	A	222	VAL	2.4
1	A	260	ARG	2.3
1	B	213	TYR	2.3
1	A	247	THR	2.1
1	A	248	LYS	2.1
1	A	268	LEU	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	CL	A	2	1/1	0.62	0.22	113,113,113,113	0
2	CL	B	1	1/1	0.87	0.24	101,101,101,101	0

6.5 Other polymers

There are no such residues in this entry.