Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2023 – 06:34 PM EDT

PDB ID	:	3EYB
Title	:	Structural and functional insights into the ligand binding domain of a non-duplicated RXR from the invertebrate chordate amphioxus
Authors	:	Tocchini-Valentini, G.D.; Rochel, N.; Moras, D.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2008-10-20
Resolution	:	2.79 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

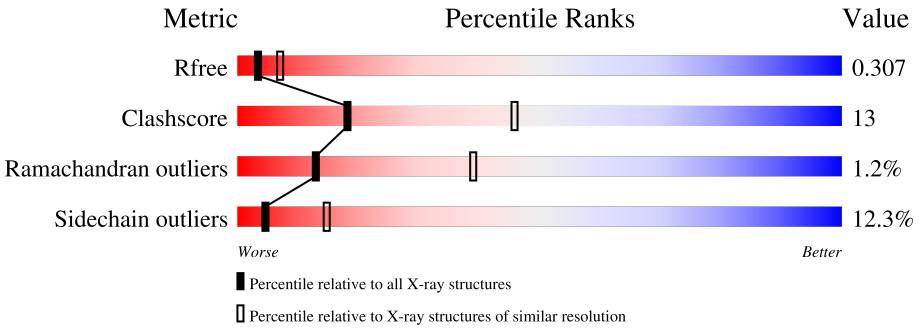
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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%

Mol	Chain	Length	Quality of chain
1	A	219	66% 20% 5% 9%
1	B	219	59% 27% 5% 9%
1	C	219	61% 26% • 9%
1	D	219	67% 21% • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6196 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 Nuclear hormone receptor RXR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1537	989	266	273	9			
1	B	199	Total	C	N	O	S	0	0	0
			1537	989	266	273	9			
1	C	199	Total	C	N	O	S	0	0	0
			1537	989	266	273	9			
1	D	199	Total	C	N	O	S	0	0	0
			1536	989	266	272	9			

- Molecule 2 is water.

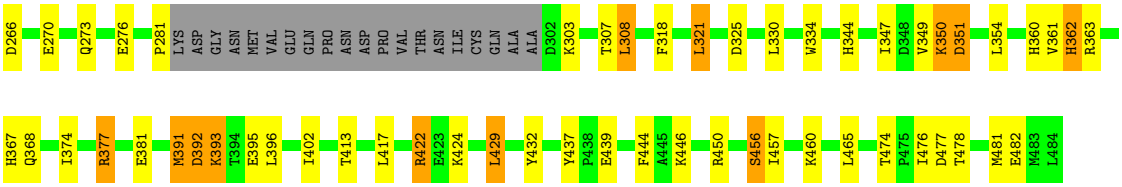
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	13	Total	O	0	0
			13	13		
2	C	10	Total	O	0	0
			10	10		
2	D	14	Total	O	0	0
			14	14		

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. 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. 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.

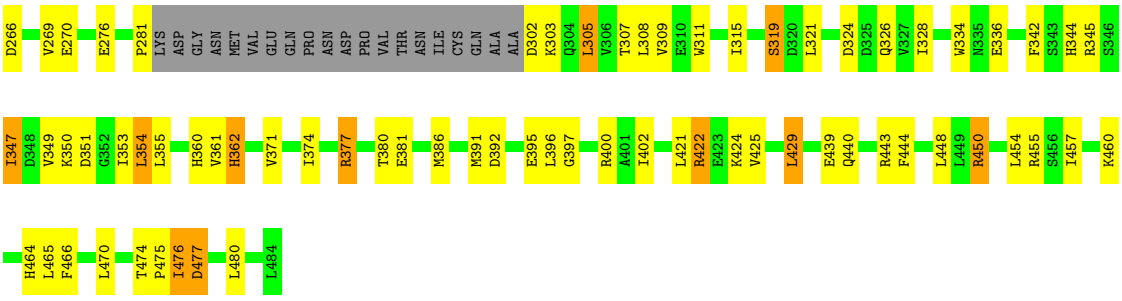
• Molecule 1: Nuclear hormone receptor RXR

Chain A:



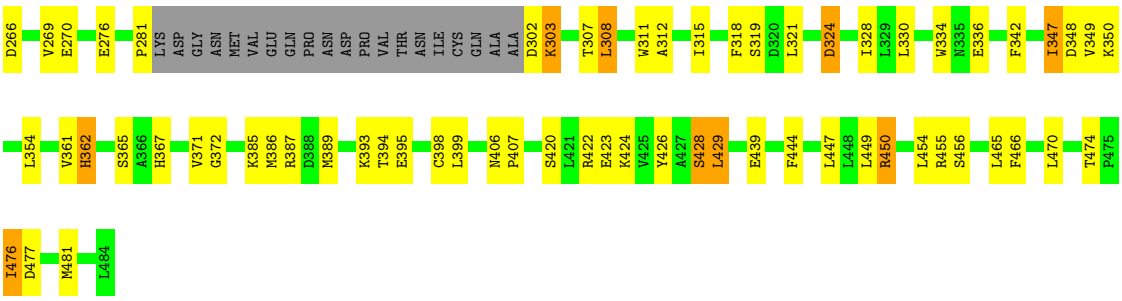
• Molecule 1: Nuclear hormone receptor RXR

Chain B:



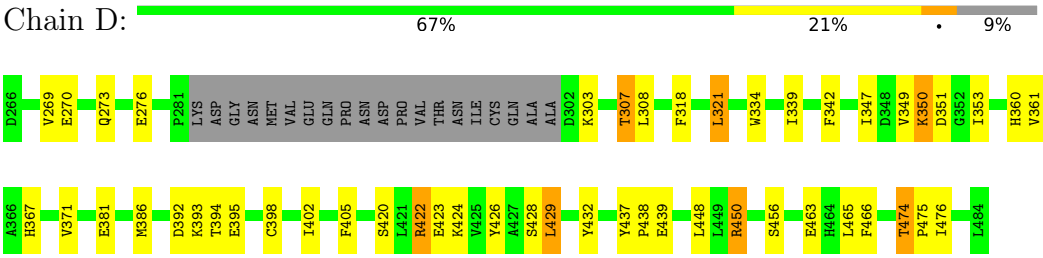
• Molecule 1: Nuclear hormone receptor RXR

Chain C:



• Molecule 1: Nuclear hormone receptor RXR

Chain D:


67%
21%
9%
D266 V269 E270 Q273 E276 P281 LYS ASP GLY ASN MET VAL GLU GLN PRO ASN ASP PRO VAL THR ASN ILE CYS GLN ALA ALA D302 K303 T307 L308 F318 L321 W334 I339 F342 I347 D348 V349 K350 D351 G352 I353 H360 V361 H362 R363 S364 S365
A366 H367 V371 E381 M386 D392 K393 T394 E395 C398 I402 F405 S420 L421 R422 E423 K424 V425 Y426 A427 S428 L429 Y432 Y437 P438 E439 L448 L449 R450 S456 E463 H464 L465 F466 T474 P475 I476 L484

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.72Å 96.12Å 131.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.79 14.97 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.79) 90.3 (14.97-2.79)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	7.56 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, R_{free}	0.202 , 0.257 0.253 , 0.307	Depositor DCC
R_{free} test set	1192 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	1.085	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6196	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.94% 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

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	0.76	0/1566	0.88	2/2116 (0.1%)
1	B	0.70	0/1566	0.82	2/2116 (0.1%)
1	C	0.76	2/1566 (0.1%)	0.82	4/2116 (0.2%)
1	D	0.74	0/1565	0.85	0/2116
All	All	0.74	2/6263 (0.0%)	0.85	8/8464 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	303	LYS	CE-NZ	14.87	1.86	1.49
1	C	303	LYS	CD-CE	5.48	1.65	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	303	LYS	CD-CE-NZ	-7.70	93.99	111.70
1	B	281	PRO	N-CA-CB	6.27	110.82	103.30
1	C	281	PRO	N-CA-CB	6.10	110.62	103.30
1	A	281	PRO	N-CA-CB	5.85	110.32	103.30
1	A	392	ASP	CB-CA-C	-5.46	99.49	110.40
1	C	455	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	377	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	450	ARG	NE-CZ-NH1	5.12	122.86	120.30

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	1537	0	1543	36	0
1	B	1537	0	1543	50	0
1	C	1537	0	1543	47	0
1	D	1536	0	1543	33	0
2	A	12	0	0	4	0
2	B	13	0	0	3	0
2	C	10	0	0	2	0
2	D	14	0	0	4	0
All	All	6196	0	6172	165	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 13.

All (165) 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:303:LYS:CE	1:C:303:LYS:NZ	1.86	1.37
1:C:476:ILE:H	1:C:476:ILE:HD13	1.05	1.14
1:B:476:ILE:H	1:B:476:ILE:HD13	1.15	1.06
1:B:422:ARG:HG3	1:B:422:ARG:HH11	1.15	1.04
1:C:407:PRO:HD2	1:C:422:ARG:NH1	1.74	1.03
1:B:450:ARG:HH11	1:B:450:ARG:HG3	1.29	0.96
1:D:347:ILE:HD11	1:D:386:MET:HB3	1.46	0.96
1:A:422:ARG:HH11	1:A:422:ARG:HG3	1.27	0.94
1:C:361:VAL:O	1:C:362:HIS:HB2	1.69	0.92
1:A:361:VAL:O	1:A:362:HIS:HB2	1.70	0.91
1:D:361:VAL:O	1:D:362:HIS:HB2	1.69	0.90
1:C:476:ILE:H	1:C:476:ILE:CD1	1.85	0.90
1:C:476:ILE:HD13	1:C:476:ILE:N	1.87	0.88
1:C:407:PRO:CD	1:C:422:ARG:HH11	1.92	0.82
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.44	0.81
1:B:476:ILE:H	1:B:476:ILE:CD1	1.93	0.81
1:A:392:ASP:OD2	1:A:432:TYR:OH	1.99	0.80
1:B:476:ILE:HD13	1:B:476:ILE:N	1.95	0.80
1:C:407:PRO:CD	1:C:422:ARG:NH1	2.45	0.79
1:C:361:VAL:HG21	1:C:470:LEU:HD21	1.66	0.77
1:A:482:GLU:N	2:A:34:HOH:O	2.16	0.76
1:A:273:GLN:CB	2:A:48:HOH:O	2.34	0.76
1:B:450:ARG:HG3	1:B:450:ARG:NH1	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ILE:O	1:B:422:ARG:NH1	2.17	0.75
1:B:360:HIS:HE1	2:B:6:HOH:O	1.68	0.75
1:B:266:ASP:N	1:B:424:LYS:HZ1	1.85	0.74
1:D:360:HIS:CE1	2:D:59:HOH:O	2.41	0.73
1:B:422:ARG:HG3	1:B:422:ARG:NH1	1.95	0.72
1:D:360:HIS:HE1	2:D:59:HOH:O	1.73	0.72
1:B:305:LEU:HD11	1:B:475:PRO:HB3	1.72	0.71
1:B:336:GLU:HG2	1:B:454:LEU:HG	1.73	0.71
1:A:422:ARG:HG3	1:A:422:ARG:NH1	2.04	0.70
1:B:361:VAL:HG21	1:B:470:LEU:HD21	1.72	0.69
1:C:303:LYS:NZ	1:C:303:LYS:CD	2.57	0.68
1:A:402:ILE:O	1:A:422:ARG:NH1	2.29	0.65
1:C:407:PRO:HD2	1:C:422:ARG:HH12	1.60	0.64
1:B:345:ARG:HG2	1:B:354:LEU:HD23	1.81	0.63
1:C:312:ALA:HA	1:C:315:ILE:HD13	1.79	0.63
1:B:429:LEU:HD13	1:B:444:PHE:CD1	2.34	0.63
1:B:302:ASP:HB3	2:B:25:HOH:O	1.98	0.63
1:D:392:ASP:HB2	1:D:395:GLU:H	1.64	0.62
1:A:391:MET:HE3	1:A:396:LEU:HA	1.82	0.62
1:C:407:PRO:HD3	1:C:422:ARG:HH11	1.63	0.62
1:D:349:VAL:HG12	1:D:350:LYS:O	1.99	0.61
1:A:361:VAL:O	1:A:362:HIS:CB	2.43	0.61
1:D:318:PHE:O	1:D:321:LEU:HB2	2.00	0.61
1:B:374:ILE:CD1	1:B:464:HIS:CD2	2.84	0.61
1:B:391:MET:HE3	1:B:396:LEU:HD13	1.84	0.60
1:B:381:GLU:O	1:B:450:ARG:NH1	2.35	0.60
1:C:406:ASN:HA	1:C:422:ARG:HH12	1.67	0.60
1:C:361:VAL:O	1:C:362:HIS:CB	2.44	0.59
1:C:347:ILE:HG22	1:C:348:ASP:OD2	2.01	0.59
1:C:311:TRP:CE2	1:C:315:ILE:HD11	2.38	0.59
1:C:349:VAL:HG12	1:C:350:LYS:O	2.03	0.59
1:B:424:LYS:NZ	2:B:10:HOH:O	2.35	0.58
1:D:405:PHE:O	1:D:422:ARG:NH1	2.36	0.58
1:C:349:VAL:HG21	1:C:354:LEU:HB2	1.85	0.58
1:C:308:LEU:HD12	1:C:330:LEU:HD22	1.85	0.58
1:A:377:ARG:HG2	1:A:377:ARG:NH1	2.08	0.57
1:B:450:ARG:HH11	1:B:450:ARG:CG	2.07	0.57
1:C:406:ASN:HA	1:C:422:ARG:NH1	2.20	0.57
1:D:392:ASP:HB2	1:D:395:GLU:HG3	1.86	0.56
1:B:429:LEU:HD13	1:B:444:PHE:CE1	2.40	0.56
1:D:392:ASP:OD1	1:D:437:TYR:OH	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HD13	1:A:330:LEU:HD22	1.88	0.56
1:B:421:LEU:HD23	1:B:421:LEU:N	2.21	0.55
1:A:363:ARG:O	1:A:367:HIS:HD2	1.89	0.55
1:A:308:LEU:HD13	1:A:330:LEU:CD2	2.37	0.55
1:A:377:ARG:HH11	1:A:377:ARG:CG	2.16	0.55
1:B:349:VAL:HG12	1:B:350:LYS:O	2.07	0.55
1:C:449:LEU:HA	2:C:9:HOH:O	2.05	0.55
1:C:476:ILE:CD1	1:C:476:ILE:N	2.56	0.55
1:A:349:VAL:HG12	1:A:350:LYS:O	2.06	0.54
1:D:360:HIS:CE1	1:D:362:HIS:CE1	2.95	0.54
1:B:353:ILE:C	1:B:353:ILE:HD12	2.28	0.54
1:D:347:ILE:CD1	1:D:386:MET:HB3	2.30	0.53
1:B:324:ASP:O	1:B:328:ILE:HG13	2.09	0.52
1:D:303:LYS:O	1:D:307:THR:HG23	2.09	0.52
1:A:349:VAL:HG21	1:A:354:LEU:HB2	1.92	0.52
1:A:413:THR:HG23	2:A:60:HOH:O	2.10	0.52
1:C:399:LEU:HD11	1:C:447:LEU:HB3	1.91	0.51
1:C:269:VAL:HG23	1:C:428:SER:OG	2.10	0.51
1:C:385:LYS:O	1:C:389:MET:HG2	2.11	0.51
1:B:361:VAL:O	1:B:362:HIS:HB2	2.11	0.51
1:B:422:ARG:HH11	1:B:422:ARG:CG	2.04	0.51
1:D:361:VAL:O	1:D:362:HIS:CB	2.47	0.50
1:B:440:GLN:OE1	1:B:443:ARG:HD2	2.11	0.50
1:D:381:GLU:O	1:D:450:ARG:NH1	2.44	0.50
1:C:311:TRP:O	1:C:315:ILE:HD12	2.12	0.50
1:D:438:PRO:HD2	1:D:439:GLU:OE1	2.11	0.50
1:A:391:MET:HE3	1:A:396:LEU:CA	2.41	0.50
1:A:325:ASP:OD2	2:A:57:HOH:O	2.18	0.50
1:B:361:VAL:O	1:B:362:HIS:CB	2.59	0.49
1:C:308:LEU:CD1	1:C:330:LEU:HD22	2.42	0.49
1:A:360:HIS:CE1	1:A:362:HIS:CE1	3.00	0.49
1:B:392:ASP:HB2	1:B:395:GLU:H	1.76	0.49
1:A:318:PHE:O	1:A:321:LEU:HB2	2.12	0.49
1:B:374:ILE:HD11	1:B:464:HIS:CD2	2.46	0.49
1:B:476:ILE:CD1	1:B:476:ILE:N	2.63	0.49
1:C:347:ILE:O	1:C:387:ARG:NE	2.46	0.48
1:D:398:CYS:CB	1:D:429:LEU:HG	2.43	0.48
1:B:305:LEU:O	1:B:309:VAL:HG23	2.13	0.48
1:B:421:LEU:O	1:B:425:VAL:HG23	2.13	0.48
1:B:347:ILE:HD11	1:B:386:MET:C	2.34	0.48
1:C:276:GLU:HB3	1:C:393:LYS:HE3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:GLU:HG3	1:D:426:TYR:OH	2.14	0.48
1:B:429:LEU:HD13	1:B:444:PHE:HD1	1.79	0.47
1:B:276:GLU:OE1	1:B:400:ARG:HD3	2.14	0.47
1:D:270:GLU:H	1:D:270:GLU:CD	2.18	0.47
1:D:273:GLN:CB	2:D:14:HOH:O	2.63	0.47
1:B:276:GLU:OE1	1:B:397:GLY:HA2	2.15	0.47
1:C:429:LEU:HD13	1:C:444:PHE:CD1	2.49	0.46
1:D:339:ILE:HA	1:D:342:PHE:CE2	2.50	0.46
1:A:477:ASP:O	1:A:478:THR:C	2.54	0.46
1:B:374:ILE:HD12	1:B:464:HIS:CD2	2.51	0.46
1:C:395:GLU:HG2	1:C:447:LEU:HD11	1.96	0.46
1:D:269:VAL:HG13	1:D:428:SER:OG	2.16	0.46
1:A:266:ASP:N	1:A:424:LYS:HZ1	2.14	0.46
1:C:318:PHE:O	1:C:321:LEU:HB2	2.16	0.46
1:B:377:ARG:HG2	1:B:381:GLU:OE2	2.15	0.45
1:A:392:ASP:OD1	1:A:437:TYR:OH	2.30	0.45
1:B:319:SER:HA	1:B:326:GLN:NE2	2.31	0.45
1:C:399:LEU:HD23	1:C:399:LEU:HA	1.79	0.45
1:C:424:LYS:O	1:C:428:SER:HB3	2.17	0.45
1:A:377:ARG:HG2	1:A:381:GLU:OE2	2.16	0.45
1:B:311:TRP:CE2	1:B:315:ILE:HD11	2.51	0.45
1:A:344:HIS:CG	1:A:396:LEU:HD22	2.53	0.44
1:C:429:LEU:HD13	1:C:444:PHE:HD1	1.82	0.44
1:A:456:SER:HG	1:B:455:ARG:HH11	1.64	0.44
1:C:398:CYS:CB	1:C:429:LEU:HG	2.47	0.44
1:C:324:ASP:O	1:C:328:ILE:HG13	2.18	0.44
1:B:319:SER:HA	1:B:326:GLN:HE22	1.83	0.43
1:D:276:GLU:HB3	1:D:393:LYS:HE2	2.00	0.43
1:B:344:HIS:CG	1:B:396:LEU:HD22	2.53	0.43
1:B:371:VAL:HG21	1:B:466:PHE:CD2	2.53	0.43
1:C:266:ASP:N	1:C:424:LYS:HZ1	2.16	0.43
1:C:423:GLU:HG2	1:C:426:TYR:OH	2.19	0.43
1:A:374:ILE:HG12	1:A:460:LYS:HB3	2.00	0.43
1:D:423:GLU:CG	1:D:426:TYR:OH	2.66	0.43
1:A:417:LEU:HD12	1:A:417:LEU:O	2.18	0.43
1:D:351:ASP:HB3	2:D:59:HOH:O	2.19	0.43
1:B:270:GLU:H	1:B:270:GLU:CD	2.21	0.42
1:A:351:ASP:OD2	1:A:363:ARG:N	2.40	0.42
1:C:347:ILE:HD11	1:C:386:MET:C	2.39	0.42
1:D:371:VAL:HG21	1:D:466:PHE:CD2	2.54	0.42
1:D:420:SER:O	1:D:424:LYS:HG3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:303:LYS:O	1:C:307:THR:HG23	2.20	0.42
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.89	0.42
1:D:353:ILE:C	1:D:353:ILE:HD12	2.40	0.42
1:D:392:ASP:OD2	1:D:432:TYR:OH	2.16	0.42
1:D:474:THR:HA	1:D:475:PRO:HD3	1.97	0.42
1:A:391:MET:HE1	1:A:396:LEU:HD13	2.02	0.41
1:A:392:ASP:OD2	1:A:432:TYR:CZ	2.71	0.41
1:C:302:ASP:HB3	2:C:19:HOH:O	2.19	0.41
1:D:363:ARG:O	1:D:367:HIS:HD2	2.04	0.41
1:A:276:GLU:HB3	1:A:393:LYS:HE2	2.02	0.41
1:C:367:HIS:CE1	1:C:372:GLY:HA3	2.55	0.41
1:A:392:ASP:CB	1:A:395:GLU:H	2.32	0.41
1:C:336:GLU:HG2	1:C:454:LEU:HG	2.02	0.41
1:C:371:VAL:HG21	1:C:466:PHE:CD2	2.55	0.41
1:D:402:ILE:O	1:D:422:ARG:NH1	2.53	0.41
1:B:355:LEU:HD11	1:B:470:LEU:HD22	2.02	0.41
1:A:429:LEU:HD13	1:A:444:PHE:HD1	1.85	0.41
1:C:398:CYS:HB3	1:C:429:LEU:HG	2.03	0.41
1:D:392:ASP:HB3	1:D:394:THR:H	1.86	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	195/219 (89%)	181 (93%)	12 (6%)	2 (1%)	15	44
1	B	195/219 (89%)	181 (93%)	11 (6%)	3 (2%)	10	33
1	C	195/219 (89%)	180 (92%)	12 (6%)	3 (2%)	10	33
1	D	195/219 (89%)	175 (90%)	19 (10%)	1 (0%)	29	61
All	All	780/876 (89%)	717 (92%)	54 (7%)	9 (1%)	13	39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	C	362	HIS
1	C	477	ASP
1	D	362	HIS
1	B	351	ASP
1	B	362	HIS
1	B	477	ASP
1	A	351	ASP
1	C	481	MET

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	160/191 (84%)	137 (86%)	23 (14%)	3	10
1	B	160/191 (84%)	137 (86%)	23 (14%)	3	10
1	C	160/191 (84%)	142 (89%)	18 (11%)	6	18
1	D	160/191 (84%)	145 (91%)	15 (9%)	8	26
All	All	640/764 (84%)	561 (88%)	79 (12%)	4	15

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	GLU
1	A	303	LYS
1	A	307	THR
1	A	308	LEU
1	A	321	LEU
1	A	334	TRP
1	A	347	ILE
1	A	350	LYS
1	A	368	GLN
1	A	377	ARG
1	A	391	MET

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Mol	Chain	Res	Type
1	A	393	LYS
1	A	422	ARG
1	A	429	LEU
1	A	439	GLU
1	A	446	LYS
1	A	450	ARG
1	A	456	SER
1	A	457	ILE
1	A	465	LEU
1	A	474	THR
1	A	476	ILE
1	A	481	MET
1	B	269	VAL
1	B	303	LYS
1	B	305	LEU
1	B	307	THR
1	B	308	LEU
1	B	319	SER
1	B	321	LEU
1	B	334	TRP
1	B	342	PHE
1	B	347	ILE
1	B	354	LEU
1	B	380	THR
1	B	422	ARG
1	B	429	LEU
1	B	439	GLU
1	B	448	LEU
1	B	450	ARG
1	B	457	ILE
1	B	460	LYS
1	B	465	LEU
1	B	474	THR
1	B	476	ILE
1	B	477	ASP
1	C	270	GLU
1	C	308	LEU
1	C	319	SER
1	C	324	ASP
1	C	334	TRP
1	C	342	PHE
1	C	347	ILE

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Mol	Chain	Res	Type
1	C	365	SER
1	C	394	THR
1	C	420	SER
1	C	428	SER
1	C	429	LEU
1	C	439	GLU
1	C	450	ARG
1	C	456	SER
1	C	465	LEU
1	C	474	THR
1	C	476	ILE
1	D	307	THR
1	D	308	LEU
1	D	321	LEU
1	D	334	TRP
1	D	350	LYS
1	D	365	SER
1	D	422	ARG
1	D	429	LEU
1	D	448	LEU
1	D	450	ARG
1	D	456	SER
1	D	463	GLU
1	D	465	LEU
1	D	474	THR
1	D	476	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	GLN
1	A	317	HIS
1	A	367	HIS
1	B	304	GLN
1	B	326	GLN
1	B	436	GLN
1	B	464	HIS
1	C	317	HIS
1	C	326	GLN
1	C	344	HIS
1	C	436	GLN
1	C	464	HIS

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Mol	Chain	Res	Type
1	D	304	GLN
1	D	317	HIS
1	D	344	HIS
1	D	360	HIS
1	D	436	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.