



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:55 AM GMT

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 validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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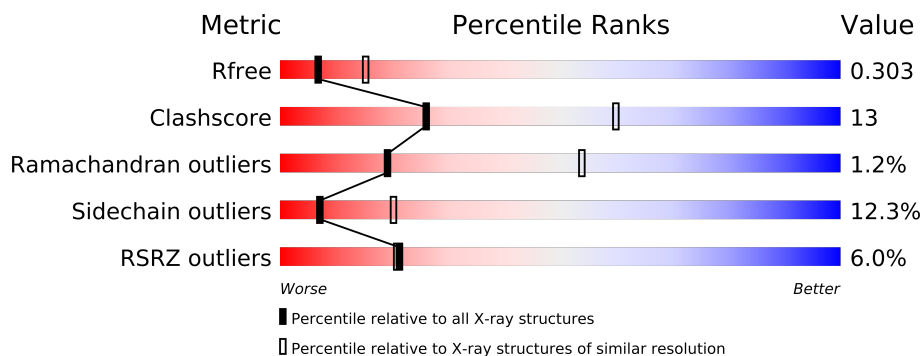
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	219	
1	B	219	
1	C	219	
1	D	219	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6196 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

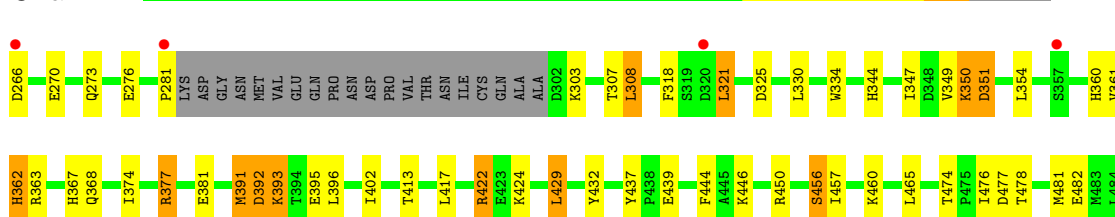
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	13	Total	O	0	0
			13	13		
2	C	10	Total	O	0	0
			10	10		
2	D	14	Total	O	0	0
			14	14		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

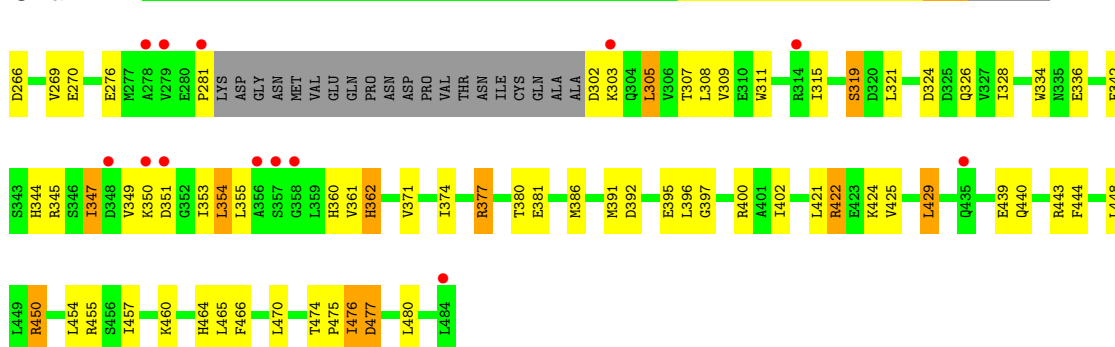
#### • Molecule 1: Nuclear hormone receptor RXR

Chain A:



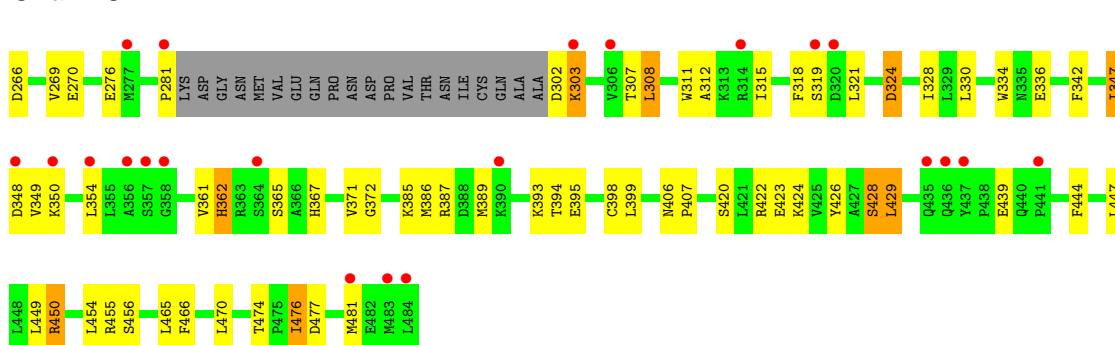
#### • Molecule 1: Nuclear hormone receptor RXR

Chain B:



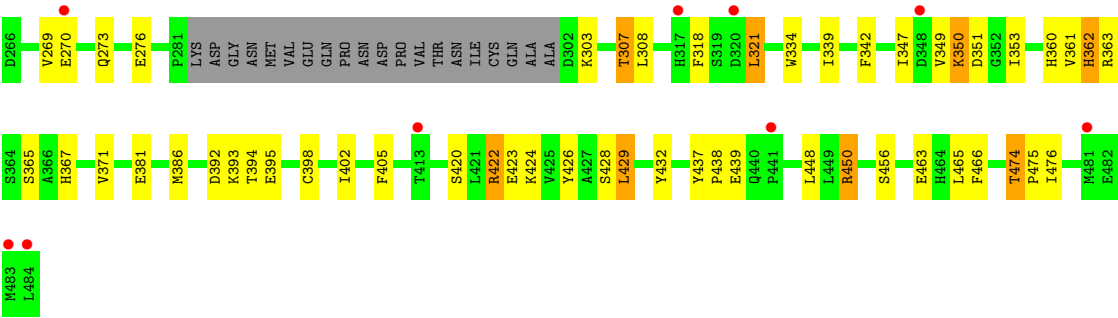
#### • Molecule 1: Nuclear hormone receptor RXR

Chain C:



#### • Molecule 1: Nuclear hormone receptor RXR

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.56 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.202 , 0.257 0.252 , 0.303	Depositor DCC
$R_{free}$ test set	1165 reflections (5.11%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	1.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 23274 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	6196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (165) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HD13	1:B:476:ILE:H	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:HG3	1:A:422:ARG:HH11	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:N	1:C:476:ILE:HD13	1.87	0.88
1:C:407:PRO:CD	1:C:422:ARG:HH11	1.92	0.82
1:B:476:ILE:CD1	1:B:476:ILE:H	1.93	0.81
1:A:377:ARG:HH11	1:A:377:ARG:HG2	1.44	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:B:450:ARG:HG3	1:B:450:ARG:NH1	1.97	0.76
1:A:273:GLN:CB	2:A:48:HOH:O	2.34	0.76
1:B:402:ILE:O	1:B:422:ARG:NH1	2.17	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:312:ALA:HA	1:C:315:ILE:HD13	1.79	0.63
1:B:345:ARG:HG2	1:B:354:LEU:HD23	1.81	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:NH1	1:A:377:ARG:HG2	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
1:A:308:LEU:HD13	1:A:330:LEU:HD22	1.88	0.56
1:B:421:LEU:N	1:B:421:LEU:HD23	2.21	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:N	1:C:476:ILE:CD1	2.56	0.55
1:D:360:HIS:CE1	1:D:362:HIS:CE1	2.95	0.54
1:A:349:VAL:HG12	1:A:350:LYS:O	2.06	0.54
1:B:353:ILE:HD12	1:B:353:ILE:C	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:385:LYS:O	1:C:389:MET:HG2	2.11	0.51
1:C:269:VAL:HG23	1:C:428:SER:OG	2.10	0.51
1:B:361:VAL:O	1:B:362:HIS:HB2	2.11	0.51
1:B:422:ARG:CG	1:B:422:ARG:HH11	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:476:ILE:CD1	1:B:476:ILE:N	2.63	0.49
1:B:374:ILE:HD11	1:B:464:HIS:CD2	2.46	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:C:276:GLU:HB3	1:C:393:LYS:HE3	1.96	0.48
1:B:347:ILE:HD11	1:B:386:MET:C	2.34	0.48
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:A:477:ASP:O	1:A:478:THR:C	2.54	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:HA	1:C:399:LEU:HD23	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:C:266:ASP:N	1:C:424:LYS:HZ1	2.16	0.43
1:B:371:VAL:HG21	1:B:466:PHE:CD2	2.53	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:D:351:ASP:HB3	2:D:59:HOH:O	2.19	0.43
1:A:417:LEU:O	1:A:417:LEU:HD12	2.18	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
1:C:303:LYS:O	1:C:307:THR:HG23	2.20	0.42
1:D:353:ILE:C	1:D:353:ILE:HD12	2.40	0.42
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.89	0.42
1:D:392:ASP:OD2	1:D:432:TYR:OH	2.16	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:C:367:HIS:CE1	1:C:372:GLY:HA3	2.55	0.41
1:A:276:GLU:HB3	1:A:393:LYS:HE2	2.02	0.41
1:A:392:ASP:CB	1:A:395:GLU:H	2.32	0.41
1:D:402:ILE:O	1:D:422:ARG:NH1	2.53	0.41
1:C:371:VAL:HG21	1:C:466:PHE:CD2	2.55	0.41
1:C:336:GLU:HG2	1:C:454:LEU:HG	2.02	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

### 5.3.1 Protein backbone ⓘ

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%)	22	60
1	B	195/219 (89%)	181 (93%)	11 (6%)	3 (2%)	15	46
1	C	195/219 (89%)	180 (92%)	12 (6%)	3 (2%)	15	46
1	D	195/219 (89%)	175 (90%)	19 (10%)	1 (0%)	38	76
All	All	780/876 (89%)	717 (92%)	54 (7%)	9 (1%)	19	54

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	362	HIS
1	C	362	HIS
1	C	477	ASP

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Mol	Chain	Res	Type
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 ⓘ

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%)	5	13
1	B	160/191 (84%)	137 (86%)	23 (14%)	5	13
1	C	160/191 (84%)	142 (89%)	18 (11%)	9	24
1	D	160/191 (84%)	145 (91%)	15 (9%)	13	34
All	All	640/764 (84%)	561 (88%)	79 (12%)	7	20

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
1	A	393	LYS
1	A	422	ARG
1	A	429	LEU
1	A	439	GLU
1	A	446	LYS

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Mol	Chain	Res	Type
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
1	C	365	SER
1	C	394	THR
1	C	420	SER
1	C	428	SER
1	C	429	LEU

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Mol	Chain	Res	Type
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

Some 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
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 chains 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 carbohydrates 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 ⓘ

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	199/219 (90%)	0.22	4 (2%) 62 63	49, 56, 62, 66	0
1	B	199/219 (90%)	0.35	13 (6%) 18 17	50, 57, 61, 65	0
1	C	199/219 (90%)	0.55	22 (11%) 6 5	50, 57, 61, 65	0
1	D	199/219 (90%)	0.31	9 (4%) 32 33	49, 57, 62, 65	0
All	All	796/876 (90%)	0.36	48 (6%) 21 21	49, 57, 61, 66	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	348	ASP	5.1
1	B	281	PRO	5.0
1	C	281	PRO	5.0
1	C	314	ARG	4.4
1	B	358	GLY	4.1
1	C	441	PRO	3.8
1	C	484	LEU	3.7
1	D	348	ASP	3.6
1	D	317	HIS	3.5
1	B	303	LYS	3.4
1	A	281	PRO	3.4
1	C	357	SER	3.3
1	C	356	ALA	3.3
1	B	435	GLN	3.3
1	B	348	ASP	3.3
1	C	435	GLN	3.2
1	C	364	SER	3.1
1	C	306	VAL	3.0
1	C	303	LYS	3.0
1	B	314	ARG	2.9
1	C	319	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	278	ALA	2.9
1	D	483	MET	2.8
1	B	484	LEU	2.8
1	C	481	MET	2.7
1	C	277	MET	2.7
1	D	270	GLU	2.5
1	D	320	ASP	2.5
1	D	484	LEU	2.4
1	B	357	SER	2.4
1	C	320	ASP	2.4
1	C	436	GLN	2.3
1	B	279	VAL	2.3
1	B	351	ASP	2.3
1	A	266	ASP	2.3
1	C	350	LYS	2.3
1	C	437	TYR	2.2
1	B	356	ALA	2.2
1	B	350	LYS	2.2
1	D	413	THR	2.2
1	D	441	PRO	2.2
1	C	358	GLY	2.2
1	C	390	LYS	2.1
1	C	354	LEU	2.1
1	D	481	MET	2.1
1	C	483	MET	2.1
1	A	320	ASP	2.0
1	A	357	SER	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 ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.