



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:19 PM GMT

PDB ID : 3R29  
Title : Crystal structure of RXRalpha ligand-binding domain complexed with corepressor SMRT2  
Authors : Zhang, H.; Chen, L.; Chen, J.; Jiang, H.; Shen, X.  
Deposited on : 2011-03-14  
Resolution : 2.90 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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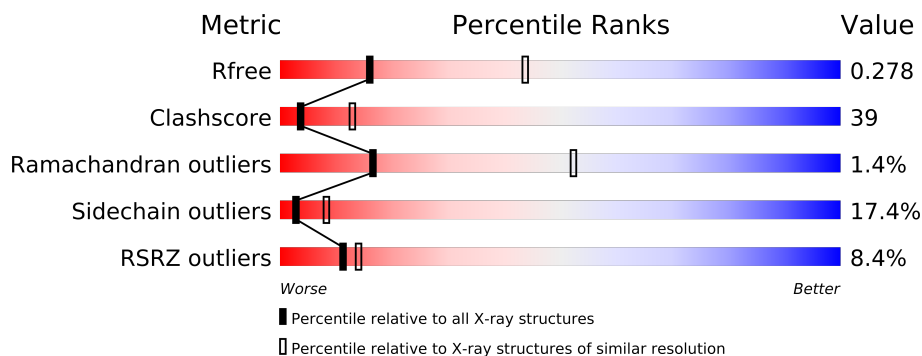
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	240	
1	B	240	
2	C	16	
2	D	16	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3595 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 Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1677	1077	288	302	10			
1	B	212	Total	C	N	O	S	0	0	0
			1677	1077	288	302	10			

- Molecule 2 is a protein called Nuclear receptor corepressor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	16	Total	C	N	O	S	0	0	0
			119	75	22	20	2			
2	D	11	Total	C	N	O	S	0	0	0
			83	54	15	13	1			

- Molecule 3 is water.

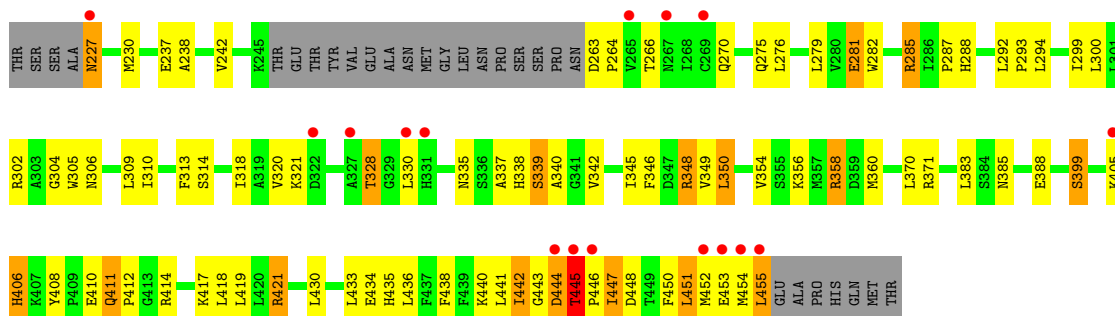
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	16	Total	O	0	0
			16	16		
3	C	2	Total	O	0	0
			2	2		
3	D	2	Total	O	0	0
			2	2		

### 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.

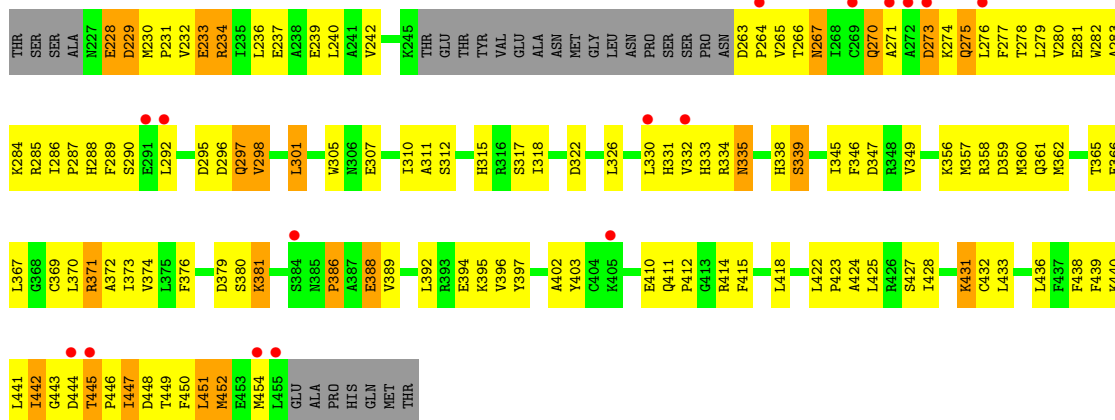
- Molecule 1: Retinoic acid receptor RXR-alpha

Chain A: 



- Molecule 1: Retinoic acid receptor RXR-alpha

Chain B: 



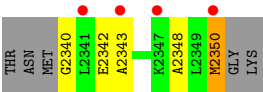
- Molecule 2: Nuclear receptor corepressor 2

Chain C: 



- Molecule 2: Nuclear receptor corepressor 2

Chain D: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.22Å 118.22Å 84.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.77 – 2.90 44.75 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.77-2.90) 96.6 (44.75-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.98 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.326 0.254 , 0.278	Depositor DCC
$R_{free}$ test set	664 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.8	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 13628 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	3595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.47% 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	0.88	1/1710 (0.1%)	0.89	1/2311 (0.0%)
1	B	0.81	0/1710	0.92	1/2311 (0.0%)
2	C	0.89	0/118	1.58	2/154 (1.3%)
2	D	0.53	0/82	0.82	0/107
All	All	0.84	1/3620 (0.0%)	0.93	4/4883 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	GLU	CG-CD	5.12	1.59	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2349	LEU	N-CA-C	-7.68	90.28	111.00
1	A	445	THR	N-CA-C	-7.57	90.56	111.00
1	B	270	GLN	N-CA-C	-6.99	92.13	111.00
2	C	2339	MET	N-CA-C	6.05	127.33	111.00

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	1677	0	1716	88	2
1	B	1677	0	1716	168	2
2	C	119	0	135	25	1
2	D	83	0	97	3	1
3	A	19	0	0	0	0
3	B	16	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
All	All	3595	0	3664	279	4

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 39.

All (279) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:283:ALA:HB1	1:B:289:PHE:CE1	1.20	1.68
1:B:283:ALA:CB	1:B:289:PHE:CE1	1.76	1.67
1:B:283:ALA:HB1	1:B:289:PHE:CZ	1.46	1.50
1:B:444:ASP:HB3	1:B:446:PRO:CD	1.57	1.35
1:B:444:ASP:CB	1:B:446:PRO:HD2	1.59	1.32
1:A:441:LEU:O	1:A:444:ASP:OD2	1.53	1.26
1:B:444:ASP:C	1:B:446:PRO:HD2	1.58	1.24
1:B:451:LEU:H	1:B:451:LEU:CD2	1.51	1.22
1:A:447:ILE:O	1:A:447:ILE:HD12	1.39	1.20
1:B:438:PHE:O	1:B:442:ILE:CD1	1.91	1.18
1:A:445:THR:HB	1:A:446:PRO:CD	1.74	1.16
1:B:442:ILE:H	1:B:442:ILE:HD13	1.01	1.14
1:B:234:ARG:HH11	1:B:234:ARG:HG3	1.07	1.12
1:A:445:THR:HB	1:A:446:PRO:HD3	1.32	1.10
1:B:295:ASP:O	1:B:298:VAL:HG23	1.52	1.10
1:B:439:PHE:HA	1:B:442:ILE:HD11	1.30	1.09
1:A:444:ASP:HA	1:A:447:ILE:HB	1.17	1.08
1:B:449:THR:HA	1:B:451:LEU:HD21	1.30	1.08
1:A:444:ASP:HA	1:A:447:ILE:CB	1.85	1.07
1:B:334:ARG:NH1	1:B:347:ASP:OD2	1.89	1.05
1:B:444:ASP:HB3	1:B:446:PRO:HD2	1.05	1.04
1:B:444:ASP:CA	1:B:446:PRO:HD2	1.88	1.03
1:B:451:LEU:HD23	1:B:451:LEU:N	1.61	1.02
1:B:451:LEU:HD23	1:B:451:LEU:H	0.86	1.02
1:B:438:PHE:O	1:B:442:ILE:HD12	1.58	1.02
2:C:2346:ARG:HG3	2:C:2346:ARG:HH21	1.19	1.02
1:B:283:ALA:CA	1:B:289:PHE:CE1	2.26	1.01
1:A:455:LEU:HD13	1:A:455:LEU:O	1.58	1.01

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:LEU:HD22	1:A:455:LEU:O	1.59	1.01
1:B:442:ILE:H	1:B:442:ILE:CD1	1.72	1.01
1:B:283:ALA:HB3	1:B:289:PHE:CE1	1.96	1.01
1:B:283:ALA:HB3	1:B:289:PHE:HE1	1.26	1.00
1:B:444:ASP:C	1:B:446:PRO:CD	2.29	1.00
2:C:2349:LEU:C	2:C:2350:MET:HG3	1.83	0.98
1:B:445:THR:N	1:B:446:PRO:HD2	1.77	0.97
1:B:284:LYS:HG2	1:B:290:SER:OG	1.64	0.97
1:B:334:ARG:HA	1:B:346:PHE:CE2	2.00	0.97
1:B:270:GLN:O	1:B:271:ALA:HB3	1.64	0.96
1:B:283:ALA:CB	1:B:289:PHE:HE1	1.36	0.94
1:B:442:ILE:HD13	1:B:442:ILE:N	1.83	0.94
2:C:2345:ILE:O	2:C:2349:LEU:HD12	1.66	0.93
1:B:445:THR:N	1:B:446:PRO:CD	2.30	0.93
1:B:287:PRO:O	1:B:288:HIS:HB2	1.66	0.92
1:A:447:ILE:C	1:A:447:ILE:HD12	1.85	0.91
1:B:444:ASP:CB	1:B:446:PRO:CD	2.30	0.91
1:B:439:PHE:CA	1:B:442:ILE:HD11	2.01	0.90
2:C:2347:LYS:O	2:C:2349:LEU:O	1.91	0.88
1:A:444:ASP:HA	1:A:447:ILE:CG2	2.04	0.87
1:B:292:LEU:O	1:B:297:GLN:NE2	2.07	0.86
1:B:335:ASN:O	1:B:339:SER:OG	1.94	0.86
1:B:449:THR:C	1:B:451:LEU:HD23	1.96	0.86
1:B:449:THR:CA	1:B:451:LEU:HD21	2.05	0.86
1:A:453:GLU:O	1:A:454:MET:HB2	1.76	0.85
2:C:2349:LEU:O	2:C:2350:MET:SD	2.36	0.83
1:B:283:ALA:CB	1:B:289:PHE:CZ	2.30	0.82
1:A:444:ASP:CA	1:A:447:ILE:HB	2.06	0.81
2:C:2345:ILE:O	2:C:2349:LEU:CD1	2.28	0.81
1:B:444:ASP:O	1:B:447:ILE:HG22	1.81	0.81
2:C:2346:ARG:HH21	2:C:2346:ARG:CG	1.94	0.81
1:A:445:THR:CB	1:A:446:PRO:CD	2.55	0.81
1:B:369:CYS:O	1:B:373:ILE:HG12	1.81	0.80
1:A:455:LEU:CD1	1:A:455:LEU:O	2.30	0.80
2:C:2349:LEU:O	2:C:2350:MET:CG	2.29	0.80
1:B:288:HIS:HB3	1:B:392:LEU:HD21	1.63	0.79
1:A:455:LEU:HD22	1:A:455:LEU:C	1.99	0.79
1:B:297:GLN:O	1:B:301:LEU:HD23	1.83	0.79
1:A:455:LEU:CD2	1:A:455:LEU:O	2.30	0.79
1:B:449:THR:HA	1:B:451:LEU:CD2	2.12	0.79
1:B:270:GLN:O	1:B:271:ALA:CB	2.30	0.78
1:B:444:ASP:CB	1:B:446:PRO:CG	2.62	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:410:GLU:O	1:A:412:PRO:HD3	1.83	0.77
1:B:234:ARG:NH1	1:B:234:ARG:HG3	1.83	0.77
1:B:295:ASP:C	1:B:298:VAL:HG23	2.06	0.76
1:A:360:MET:HE1	1:A:417:LYS:HB3	1.67	0.75
1:B:357:MET:HG2	1:B:362:MET:CE	2.17	0.75
2:C:2349:LEU:H	2:C:2349:LEU:HD12	1.52	0.75
1:B:451:LEU:N	1:B:451:LEU:CD2	2.30	0.73
1:B:449:THR:CA	1:B:451:LEU:CD2	2.66	0.73
1:A:345:ILE:O	1:A:349:VAL:HG23	1.88	0.73
1:B:438:PHE:O	1:B:442:ILE:HD13	1.89	0.72
1:B:307:GLU:HG2	1:B:425:LEU:HG	1.69	0.72
1:B:444:ASP:HB2	1:B:446:PRO:CG	2.18	0.71
1:A:447:ILE:HG13	1:A:448:ASP:N	2.05	0.71
2:C:2346:ARG:NH2	2:C:2346:ARG:HG3	1.97	0.71
2:C:2349:LEU:HD12	2:C:2349:LEU:N	2.06	0.70
1:B:315:HIS:O	1:B:318:ILE:CG1	2.38	0.70
1:B:444:ASP:HB3	1:B:446:PRO:HD3	1.71	0.69
1:B:239:GLU:OE1	1:B:282:TRP:NE1	2.26	0.69
1:A:444:ASP:O	1:A:445:THR:C	2.30	0.69
1:A:443:GLY:O	1:A:444:ASP:C	2.30	0.69
1:B:442:ILE:N	1:B:442:ILE:CD1	2.49	0.69
1:A:421:ARG:HA	1:A:421:ARG:NE	2.08	0.69
1:B:449:THR:C	1:B:451:LEU:CD2	2.62	0.68
1:A:411:GLN:NE2	1:A:414:ARG:HD2	2.08	0.68
1:A:447:ILE:O	1:A:447:ILE:CD1	2.29	0.67
1:B:410:GLU:HG2	1:B:411:GLN:HG3	1.75	0.67
1:B:448:ASP:O	1:B:448:ASP:CG	2.30	0.67
1:B:237:GLU:HA	1:B:240:LEU:HD12	1.77	0.67
1:B:345:ILE:O	1:B:349:VAL:HG23	1.95	0.66
1:B:365:THR:O	1:B:369:CYS:SG	2.52	0.66
1:B:289:PHE:O	1:B:292:LEU:HB2	1.96	0.66
1:B:315:HIS:O	1:B:318:ILE:HG12	1.94	0.65
1:A:451:LEU:O	1:A:452:MET:HB3	1.97	0.65
1:A:337:ALA:O	1:A:340:ALA:N	2.30	0.65
1:B:358:ARG:O	1:B:361:GLN:N	2.28	0.65
2:C:2349:LEU:C	2:C:2350:MET:CG	2.54	0.65
1:A:445:THR:HB	1:A:446:PRO:HD2	1.72	0.64
1:B:445:THR:O	1:B:447:ILE:N	2.30	0.64
1:B:392:LEU:O	1:B:396:VAL:HG23	1.98	0.63
1:B:312:SER:OG	1:B:371:ARG:NH2	2.31	0.63
1:A:287:PRO:O	1:A:288:HIS:HB2	1.97	0.63
1:B:334:ARG:CA	1:B:346:PHE:CE2	2.79	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:455:LEU:O	1:A:455:LEU:CG	2.47	0.63
1:A:447:ILE:C	1:A:447:ILE:CD1	2.45	0.63
1:B:286:ILE:HG21	1:B:376:PHE:CZ	2.33	0.62
1:A:410:GLU:O	1:A:412:PRO:CD	2.47	0.62
1:B:381:LYS:HD2	1:B:381:LYS:C	2.19	0.62
1:B:286:ILE:HG21	1:B:376:PHE:HZ	1.65	0.62
1:A:445:THR:O	1:A:447:ILE:HG22	2.00	0.62
1:A:451:LEU:O	1:A:452:MET:CB	2.48	0.62
1:B:410:GLU:OE1	1:B:410:GLU:N	2.30	0.61
1:A:370:LEU:HD21	1:A:418:LEU:HB3	1.81	0.61
1:B:444:ASP:C	1:B:446:PRO:N	2.46	0.61
1:B:315:HIS:O	1:B:318:ILE:HG13	2.00	0.60
1:A:281:GLU:OE1	2:C:2352:LYS:NZ	2.34	0.60
1:A:452:MET:H	1:A:455:LEU:HB3	1.67	0.60
1:A:227:ASN:HD22	1:A:227:ASN:N	1.99	0.60
1:A:338:HIS:C	1:A:340:ALA:H	2.04	0.59
1:A:238:ALA:HB2	1:A:285:ARG:HB3	1.84	0.59
1:B:233:GLU:CD	1:B:233:GLU:H	2.05	0.59
1:B:450:PHE:N	1:B:451:LEU:HD23	2.17	0.59
1:B:284:LYS:HG2	1:B:290:SER:HG	1.68	0.59
1:B:287:PRO:O	1:B:288:HIS:CB	2.44	0.58
1:B:229:ASP:HB2	1:B:395:LYS:HD3	1.86	0.58
1:B:450:PHE:C	1:B:452:MET:N	2.57	0.58
1:B:448:ASP:O	1:B:451:LEU:CD2	2.50	0.58
1:B:448:ASP:O	1:B:451:LEU:HD21	2.04	0.58
1:A:444:ASP:CA	1:A:447:ILE:CG2	2.81	0.57
1:B:444:ASP:O	1:B:445:THR:C	2.41	0.57
1:B:445:THR:C	1:B:447:ILE:H	2.08	0.57
1:A:275:GLN:NE2	1:A:275:GLN:HA	2.18	0.57
1:B:444:ASP:HB3	1:B:446:PRO:CG	2.24	0.56
1:B:334:ARG:HA	1:B:346:PHE:HE2	1.63	0.56
1:A:452:MET:H	1:A:455:LEU:CB	2.18	0.56
1:A:445:THR:CB	1:A:446:PRO:HD2	2.34	0.55
1:A:242:VAL:HG11	1:A:282:TRP:HB2	1.87	0.55
1:B:361:GLN:O	1:B:361:GLN:CG	2.55	0.54
1:A:350:LEU:HA	1:A:354:VAL:HB	1.88	0.54
1:B:345:ILE:HD11	1:B:432:CYS:SG	2.47	0.54
1:A:287:PRO:O	1:A:288:HIS:CB	2.55	0.54
1:B:315:HIS:HD2	1:B:367:LEU:HB2	1.72	0.54
1:B:371:ARG:O	1:B:372:ALA:C	2.46	0.54
1:B:360:MET:O	1:B:361:GLN:HG2	2.08	0.54
2:D:2348:ALA:C	2:D:2350:MET:H	2.10	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:276:LEU:O	1:B:280:VAL:HG22	2.08	0.53
1:B:402:ALA:O	1:B:403:TYR:C	2.45	0.53
1:A:430:LEU:O	1:A:434:GLU:HG3	2.08	0.53
1:B:326:LEU:HD11	1:B:332:VAL:HG23	1.91	0.53
1:A:263:ASP:HA	1:A:266:THR:HB	1.90	0.53
1:B:444:ASP:O	1:B:446:PRO:N	2.40	0.53
2:C:2341:LEU:HD23	2:C:2344:ILE:HG23	1.91	0.52
1:B:315:HIS:CD2	1:B:367:LEU:HB2	2.44	0.52
1:B:366:GLU:OE1	1:B:414:ARG:NH2	2.41	0.52
1:A:444:ASP:O	1:A:446:PRO:N	2.42	0.52
1:B:242:VAL:HG11	1:B:282:TRP:HB2	1.91	0.51
1:B:376:PHE:CZ	1:B:392:LEU:HD23	2.45	0.51
1:B:356:LYS:O	1:B:360:MET:HG2	2.10	0.51
1:A:444:ASP:O	1:A:445:THR:OG1	2.29	0.51
1:A:335:ASN:O	1:A:339:SER:OG	2.27	0.51
1:B:228:GLU:HB3	1:B:231:PRO:HA	1.92	0.51
1:B:415:PHE:O	1:B:418:LEU:HB2	2.10	0.50
1:A:443:GLY:O	1:A:445:THR:OG1	2.29	0.50
1:A:275:GLN:HG3	1:A:309:LEU:HD22	1.93	0.50
1:B:441:LEU:C	1:B:443:GLY:H	2.10	0.50
1:A:435:HIS:O	1:A:436:LEU:C	2.50	0.49
1:B:230:MET:HE3	1:B:287:PRO:HG2	1.94	0.49
1:B:386:PRO:O	1:B:389:VAL:N	2.46	0.49
1:B:441:LEU:HD12	1:B:447:ILE:CD1	2.42	0.49
1:B:234:ARG:O	1:B:237:GLU:HB2	2.13	0.49
1:B:394:GLU:HA	1:B:397:TYR:CZ	2.47	0.49
1:A:356:LYS:HE3	1:B:379:ASP:OD1	2.13	0.49
1:B:296:ASP:O	1:B:297:GLN:C	2.49	0.49
1:B:271:ALA:O	1:B:275:GLN:HG2	2.13	0.49
1:A:287:PRO:HB2	1:A:288:HIS:HD2	1.78	0.48
1:B:445:THR:C	1:B:447:ILE:N	2.64	0.48
1:B:450:PHE:C	1:B:452:MET:H	2.16	0.48
1:B:267:ASN:N	1:B:267:ASN:OD1	2.46	0.48
1:B:381:LYS:HD2	1:B:381:LYS:O	2.13	0.48
1:B:427:SER:O	1:B:431:LYS:HD3	2.14	0.48
1:B:438:PHE:C	1:B:442:ILE:CD1	2.78	0.48
1:B:334:ARG:CA	1:B:346:PHE:HE2	2.22	0.48
2:C:2349:LEU:O	2:C:2350:MET:CB	2.62	0.48
1:A:444:ASP:C	1:A:445:THR:OG1	2.53	0.48
2:C:2341:LEU:HA	2:C:2344:ILE:HG23	1.95	0.47
2:C:2341:LEU:O	2:C:2342:GLU:C	2.52	0.47
1:A:410:GLU:HG2	1:A:411:GLN:N	2.30	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:292:LEU:O	1:A:293:PRO:C	2.49	0.47
1:B:267:ASN:O	1:B:270:GLN:O	2.33	0.47
1:B:234:ARG:NH1	1:B:234:ARG:CG	2.63	0.47
1:B:440:LYS:HE3	1:B:440:LYS:HB3	1.67	0.47
1:B:441:LEU:HD12	1:B:447:ILE:HD12	1.97	0.47
1:A:294:LEU:HD21	2:C:2346:ARG:HD3	1.96	0.47
1:B:444:ASP:HB2	1:B:446:PRO:HG2	1.94	0.47
1:B:388:GLU:OE2	1:B:392:LEU:HD13	2.15	0.46
1:B:334:ARG:CZ	1:B:347:ASP:OD2	2.59	0.46
1:A:417:LYS:NZ	1:B:394:GLU:OE2	2.48	0.46
1:B:357:MET:HG2	1:B:362:MET:HE3	1.97	0.46
1:B:357:MET:HG2	1:B:362:MET:HE1	1.94	0.46
1:B:438:PHE:O	1:B:442:ILE:HD11	2.02	0.46
1:B:422:LEU:O	1:B:423:PRO:C	2.52	0.46
1:B:410:GLU:O	1:B:412:PRO:HD3	2.16	0.46
1:B:370:LEU:O	1:B:373:ILE:HB	2.16	0.46
1:B:371:ARG:O	1:B:374:VAL:N	2.49	0.46
1:B:307:GLU:O	1:B:310:ILE:N	2.49	0.45
1:B:286:ILE:O	1:B:289:PHE:HB3	2.16	0.45
1:B:448:ASP:O	1:B:451:LEU:HD22	2.16	0.45
1:B:439:PHE:CA	1:B:442:ILE:CD1	2.87	0.45
1:A:227:ASN:ND2	1:A:227:ASN:N	2.64	0.45
1:A:320:VAL:O	1:A:358:ARG:NH2	2.44	0.45
1:B:338:HIS:NE2	1:B:347:ASP:OD1	2.49	0.45
1:B:381:LYS:CD	1:B:381:LYS:C	2.85	0.45
1:A:320:VAL:HG12	1:A:321:LYS:N	2.32	0.45
1:A:338:HIS:C	1:A:340:ALA:N	2.70	0.45
1:A:328:THR:OG1	1:A:328:THR:O	2.35	0.44
1:A:310:ILE:O	1:A:314:SER:OG	2.31	0.44
1:A:385:ASN:HD22	1:A:388:GLU:HB2	1.83	0.44
1:B:230:MET:CE	1:B:287:PRO:HG2	2.47	0.44
1:B:263:ASP:HA	1:B:264:PRO:HD2	1.82	0.44
1:B:296:ASP:C	1:B:298:VAL:N	2.69	0.44
1:B:345:ILE:CD1	1:B:432:CYS:SG	3.05	0.44
1:A:337:ALA:HB1	1:A:342:VAL:HG23	2.00	0.44
1:A:263:ASP:HB3	1:A:264:PRO:CD	2.48	0.44
1:A:438:PHE:CZ	1:A:442:ILE:HD12	2.52	0.44
1:B:276:LEU:HB2	1:B:305:TRP:HH2	1.82	0.44
2:C:2341:LEU:C	2:C:2341:LEU:CD2	2.84	0.44
2:C:2339:MET:CG	2:C:2339:MET:O	2.65	0.44
1:A:287:PRO:C	1:A:288:HIS:CD2	2.92	0.43
1:A:230:MET:HB3	1:A:399:SER:OG	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:289:PHE:HZ	1:B:301:LEU:HD21	1.83	0.43
1:B:332:VAL:HG12	1:B:333:HIS:N	2.34	0.43
1:B:289:PHE:CD2	1:B:289:PHE:C	2.91	0.43
1:B:283:ALA:CA	1:B:289:PHE:HE1	1.80	0.43
1:A:450:PHE:C	1:A:451:LEU:O	2.52	0.43
1:B:448:ASP:OD2	1:B:448:ASP:C	2.52	0.43
1:A:287:PRO:CB	1:A:288:HIS:HD2	2.31	0.43
1:A:418:LEU:O	1:A:419:LEU:C	2.57	0.43
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.81	0.43
2:C:2341:LEU:HA	2:C:2344:ILE:CG2	2.49	0.43
1:B:274:LYS:O	1:B:275:GLN:C	2.56	0.43
1:B:282:TRP:CE2	1:B:371:ARG:NH1	2.86	0.43
2:C:2349:LEU:H	2:C:2349:LEU:CD1	2.26	0.43
1:B:263:ASP:O	1:B:267:ASN:OD1	2.37	0.43
2:D:2342:GLU:O	2:D:2343:ALA:C	2.57	0.43
1:B:286:ILE:CG2	1:B:376:PHE:HZ	2.31	0.42
1:B:424:ALA:O	1:B:428:ILE:HG13	2.19	0.42
1:A:348:ARG:O	1:A:349:VAL:C	2.57	0.42
1:B:310:ILE:O	1:B:311:ALA:C	2.58	0.42
1:A:346:PHE:CE2	1:A:350:LEU:CD1	3.02	0.42
1:B:410:GLU:HG2	1:B:411:GLN:N	2.33	0.42
1:B:286:ILE:O	1:B:287:PRO:C	2.57	0.42
1:B:440:LYS:O	1:B:443:GLY:HA3	2.19	0.42
2:C:2346:ARG:NH2	2:C:2346:ARG:CG	2.63	0.42
1:B:315:HIS:ND1	1:B:315:HIS:O	2.44	0.42
1:A:444:ASP:O	1:A:446:PRO:HD2	2.20	0.41
1:A:345:ILE:HD11	1:A:435:HIS:CD2	2.55	0.41
2:C:2349:LEU:O	2:C:2350:MET:HG3	1.95	0.41
1:A:304:GLY:O	1:A:305:TRP:C	2.58	0.41
1:B:280:VAL:HG21	2:D:2348:ALA:HB1	2.01	0.41
1:B:326:LEU:HD11	1:B:332:VAL:CG2	2.50	0.41
1:A:405:LYS:O	1:A:406:HIS:C	2.58	0.41
1:B:410:GLU:HG2	1:B:411:GLN:CG	2.46	0.41
1:A:282:TRP:CE2	1:A:371:ARG:NH1	2.89	0.41
1:B:273:ASP:O	1:B:276:LEU:HB3	2.21	0.41
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.80	0.41
1:A:411:GLN:HE22	1:A:414:ARG:HD2	1.85	0.40
1:B:242:VAL:HB	1:B:278:THR:HG23	2.03	0.40
1:B:290:SER:C	1:B:292:LEU:N	2.74	0.40
2:C:2339:MET:O	2:C:2339:MET:HG2	2.22	0.40
1:A:299:ILE:O	1:A:300:LEU:C	2.59	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:435:HIS:NE2	1:A:442:ILE:CD1[8_555]	1.42	0.78
1:B:452:MET:CE	2:C:2340:GLY:O[8_555]	1.79	0.41
1:B:234:ARG:NH1	1:B:285:ARG:NH1[8_554]	1.95	0.25
1:A:452:MET:CE	2:D:2340:GLY:O[8_555]	2.11	0.09

## 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	208/240 (87%)	183 (88%)	22 (11%)	3 (1%)	16	52
1	B	208/240 (87%)	184 (88%)	21 (10%)	3 (1%)	16	52
2	C	14/16 (88%)	11 (79%)	3 (21%)	0	100	100
2	D	9/16 (56%)	6 (67%)	3 (33%)	0	100	100
All	All	439/512 (86%)	384 (88%)	49 (11%)	6 (1%)	16	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	445	THR
1	A	411	GLN
1	A	406	HIS
1	B	277	PHE
1	B	359	ASP
1	B	386	PRO

### 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	183/207 (88%)	157 (86%)	26 (14%)	5	13
1	B	183/207 (88%)	148 (81%)	35 (19%)	2	6
2	C	12/12 (100%)	7 (58%)	5 (42%)	0	0
2	D	8/12 (67%)	7 (88%)	1 (12%)	7	19
All	All	386/438 (88%)	319 (83%)	67 (17%)	3	8

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASN
1	A	270	GLN
1	A	276	LEU
1	A	279	LEU
1	A	281	GLU
1	A	285	ARG
1	A	302	ARG
1	A	306	ASN
1	A	313	PHE
1	A	318	ILE
1	A	328	THR
1	A	330	LEU
1	A	339	SER
1	A	348	ARG
1	A	350	LEU
1	A	358	ARG
1	A	399	SER
1	A	408	TYR
1	A	421	ARG
1	A	440	LYS
1	A	442	ILE
1	A	444	ASP
1	A	445	THR
1	A	447	ILE
1	A	451	LEU
1	A	455	LEU
1	B	228	GLU
1	B	229	ASP
1	B	232	VAL
1	B	233	GLU
1	B	234	ARG
1	B	236	LEU
1	B	265	VAL

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Mol	Chain	Res	Type
1	B	266	THR
1	B	267	ASN
1	B	273	ASP
1	B	275	GLN
1	B	279	LEU
1	B	281	GLU
1	B	297	GLN
1	B	298	VAL
1	B	301	LEU
1	B	317	SER
1	B	322	ASP
1	B	330	LEU
1	B	331	HIS
1	B	335	ASN
1	B	339	SER
1	B	371	ARG
1	B	380	SER
1	B	381	LYS
1	B	388	GLU
1	B	431	LYS
1	B	433	LEU
1	B	436	LEU
1	B	442	ILE
1	B	445	THR
1	B	447	ILE
1	B	451	LEU
1	B	452	MET
1	B	454	MET
2	C	2339	MET
2	C	2341	LEU
2	C	2344	ILE
2	C	2346	ARG
2	C	2350	MET
2	D	2350	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	HIS
1	A	338	HIS
1	A	385	ASN
1	A	411	GLN

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Mol	Chain	Res	Type
1	A	435	HIS
1	B	227	ASN
1	B	411	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	212/240 (88%)	0.37	16 (7%) 14 17	20, 55, 93, 105	0
1	B	212/240 (88%)	0.50	16 (7%) 14 17	25, 68, 95, 98	0
2	C	16/16 (100%)	0.87	2 (12%) 5 6	61, 69, 93, 94	0
2	D	11/16 (68%)	1.94	4 (36%) 1 1	83, 84, 86, 87	0
All	All	451/512 (88%)	0.48	38 (8%) 11 14	20, 61, 94, 105	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	LEU	5.9
1	A	454	MET	5.9
1	A	331	HIS	5.3
2	D	2343	ALA	4.6
1	A	269	CYS	4.2
1	A	444	ASP	3.7
2	D	2350	MET	3.5
1	B	455	LEU	3.5
1	A	330	LEU	3.4
1	A	327	ALA	3.4
1	B	291	GLU	3.4
1	B	264	PRO	3.4
2	D	2347	LYS	3.3
1	B	384	SER	3.2
1	B	272	ALA	3.2
1	A	445	THR	3.2
2	C	2339	MET	3.1
1	B	271	ALA	3.1
1	A	322	ASP	3.0
1	A	452	MET	2.9
2	D	2341	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	273	ASP	2.8
1	B	445	THR	2.8
1	A	405	LYS	2.8
2	C	2338	ASN	2.7
1	B	292	LEU	2.7
1	B	444	ASP	2.7
1	A	453	GLU	2.6
1	B	332	VAL	2.5
1	A	227	ASN	2.3
1	A	267	ASN	2.3
1	B	269	CYS	2.3
1	B	276	LEU	2.2
1	A	446	PRO	2.2
1	B	405	LYS	2.1
1	B	454	MET	2.1
1	B	330	LEU	2.1
1	A	265	VAL	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.