Full wwPDB X-ray Structure Validation Report (i)

Sep 2, 2023 – 01:27 PM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

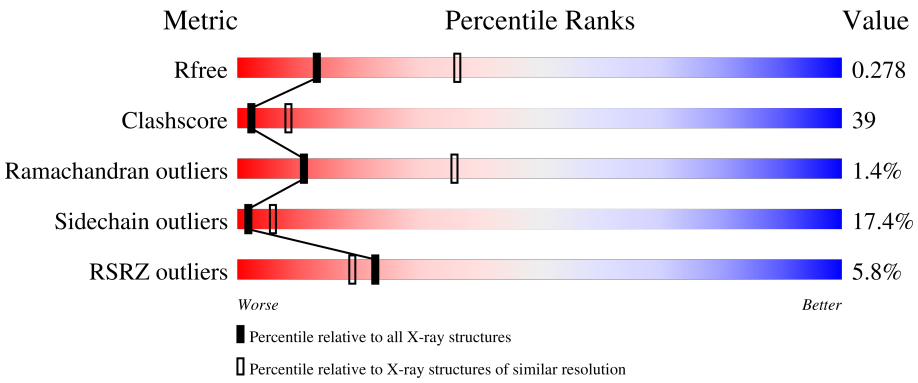
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	5%, 52%, 29%, 7%, 12%
1	B	240	4%, 35%, 43%, 10%, 12%
2	C	16	12%, 31%, 31%, 31%, 6%
2	D	16	19%, 38%, 25%, 6%, 31%

2 Entry composition (i)

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

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

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

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

- Molecule 3 is water.

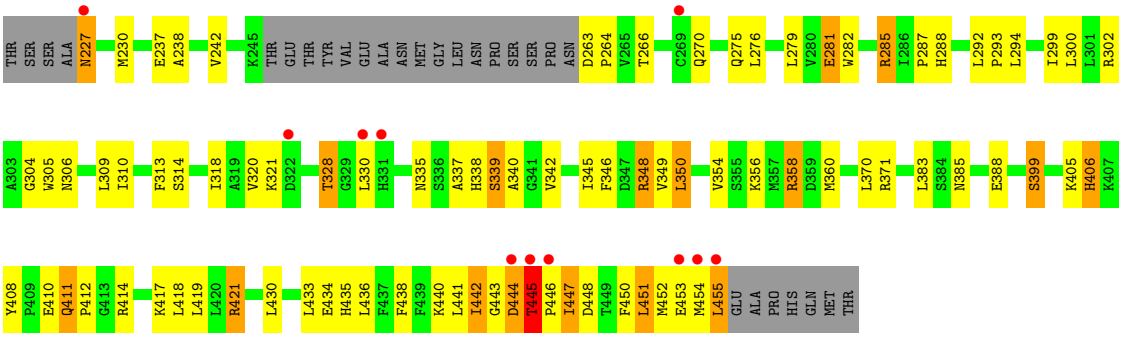
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	19	19	19	0	0
3	B	16	16	16	0	0
3	C	2	2	2	0	0
3	D	2	2	2	0	0

3 Residue-property plots (i)

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

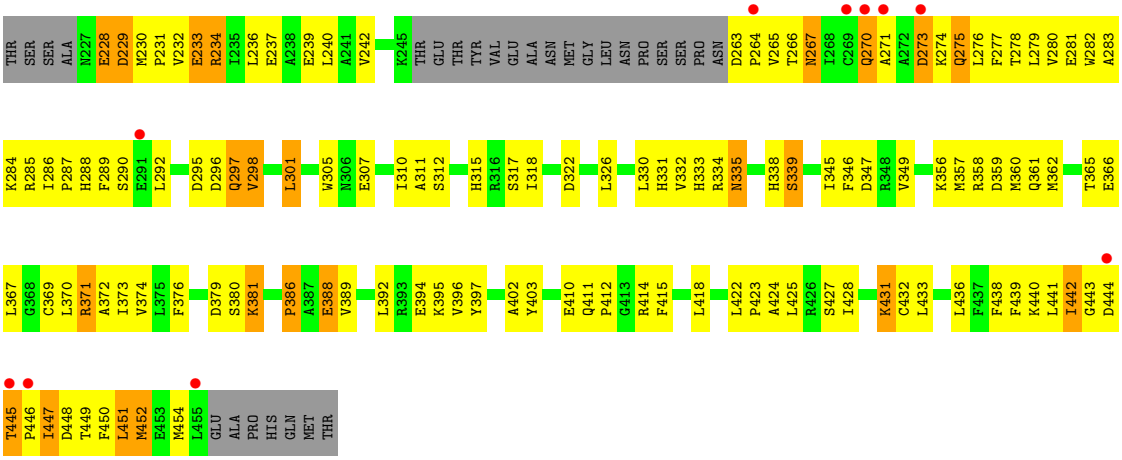
• Molecule 1: Retinoic acid receptor RXR-alpha

Chain A:



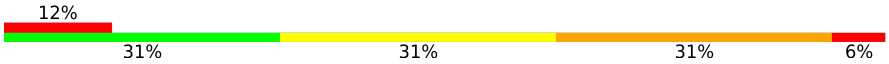
• Molecule 1: Retinoic acid receptor RXR-alpha

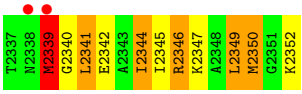
Chain B:



• Molecule 2: Nuclear receptor corepressor 2

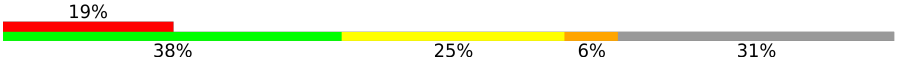
Chain C:

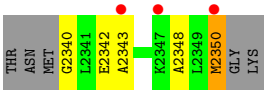




• Molecule 2: Nuclear receptor corepressor 2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	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) 96.5 (44.75-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.52 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.326 0.253 , 0.278	Depositor DCC
R_{free} test set	683 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	68.7	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.6	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	0.91	EDS
Total number of atoms	3595	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[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 (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	1677	0	1716	88	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 39.

All (279) 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: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:HD12	1:A:447:ILE:O	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:HD13	1:B:442:ILE:H	1.01	1.14
1:B:234:ARG:HG3	1:B:234:ARG:HH11	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:438:PHE:O	1:B:442:ILE:HD12	1.58	1.02
1:B:451:LEU:H	1:B:451:LEU:HD23	0.86	1.02
1:B:451:LEU:HD23	1:B:451:LEU:N	1.61	1.02
2:C:2346:ARG:HH21	2:C:2346:ARG:HG3	1.19	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:455:LEU:O	1:A:455:LEU:HD22	1.59	1.01
1:B:442:ILE:CD1	1:B:442:ILE:H	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:HD12	1:A:447:ILE:C	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:O	1:A:455:LEU:CD1	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:A:455:LEU:O	1:A:455:LEU:CD2	2.30	0.79
1:B:297:GLN:O	1:B:301:LEU:HD23	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:410:GLU:O	1:A:412:PRO:HD3	1.83	0.77
1:B:234:ARG:HG3	1:B:234:ARG:NH1	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:HD12	2:C:2349:LEU:H	1.52	0.75
1:B:451:LEU:CD2	1:B:451:LEU:N	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:HG3	2:C:2346:ARG:NH2	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:CD1	1:B:442:ILE:N	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:CG	1:B:448:ASP:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:312:SER:OG	1:B:371:ARG:NH2	2.31	0.63
1:B:392:LEU:O	1:B:396:VAL:HG23	1.98	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
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: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:286:ILE:HG21	1:B:376:PHE:HZ	1.65	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:A:281:GLU:OE1	2:C:2352:LYS:NZ	2.34	0.60
1:B:315:HIS:O	1:B:318:ILE:HG13	2.00	0.60
1:A:452:MET:H	1:A:455:LEU:HB3	1.67	0.60
1:A:227:ASN:N	1:A:227:ASN:HD22	1.99	0.60
1:A:238:ALA:HB2	1:A:285:ARG:HB3	1.84	0.59
1:A:338:HIS:C	1:A:340:ALA:H	2.04	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:229:ASP:HB2	1:B:395:LYS:HD3	1.86	0.58
1:B:287:PRO:O	1:B:288:HIS:CB	2.44	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:HA	1:A:275:GLN:NE2	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:A:350:LEU:HA	1:A:354:VAL:HB	1.88	0.54
1:B:361:GLN:CG	1:B:361:GLN:O	2.55	0.54
1:B:345:ILE:HD11	1:B:432:CYS:SG	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:360:MET:O	1:B:361:GLN:HG2	2.08	0.54
1:B:371:ARG:O	1:B:372:ALA:C	2.46	0.54
2:D:2348:ALA:C	2:D:2350:MET:H	2.10	0.53
1:B:276:LEU:O	1:B:280:VAL:HG22	2.08	0.53
1:A:430:LEU:O	1:A:434:GLU:HG3	2.08	0.53
1:B:402:ALA:O	1:B:403:TYR:C	2.45	0.53
1:A:263:ASP:HA	1:A:266:THR:HB	1.90	0.53
1:B:326:LEU:HD11	1:B:332:VAL:HG23	1.91	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:275:GLN:HG3	1:A:309:LEU:HD22	1.93	0.50
1:A:443:GLY:O	1:A:445:THR:OG1	2.29	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:A:356:LYS:HE3	1:B:379:ASP:OD1	2.13	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:B:441:LEU:HD12	1:B:447:ILE:CD1	2.42	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:267:ASN:N	1:B:267:ASN:OD1	2.46	0.48
1:B:450:PHE:C	1:B:452:MET:H	2.16	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:334:ARG:CA	1:B:346:PHE:HE2	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:PHE:C	1:B:442:ILE:CD1	2.78	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:292:LEU:O	1:A:293:PRO:C	2.49	0.47
1:A:410:GLU:HG2	1:A:411:GLN:N	2.30	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:A:294:LEU:HD21	2:C:2346:ARG:HD3	1.96	0.47
1:B:440:LYS:HB3	1:B:440:LYS:HE3	1.67	0.47
1:B:441:LEU:HD12	1:B:447:ILE:HD12	1.97	0.47
1:B:444:ASP:HB2	1:B:446:PRO:HG2	1.94	0.47
1:B:334:ARG:CZ	1:B:347:ASP:OD2	2.59	0.46
1:B:388:GLU:OE2	1:B:392:LEU:HD13	2.15	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:439:PHE:CA	1:B:442:ILE:CD1	2.87	0.45
1:B:448:ASP:O	1:B:451:LEU:HD22	2.16	0.45
1:A:227:ASN:N	1:A:227:ASN:ND2	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:C	1:B:381:LYS:CD	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:O	1:A:328:THR:OG1	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:A:337:ALA:HB1	1:A:342:VAL:HG23	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2339:MET:CG	2:C:2339:MET:O	2.65	0.44
2:C:2341:LEU:C	2:C:2341:LEU:CD2	2.84	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
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:A:450:PHE:C	1:A:451:LEU:O	2.52	0.43
1:B:283:ALA:CA	1:B:289:PHE:HE1	1.80	0.43
1:B:289:PHE:CD2	1:B:289:PHE:C	2.91	0.43
1:A:287:PRO:CB	1:A:288:HIS:HD2	2.31	0.43
1:A:383:LEU:HD23	1:A:383:LEU:HA	1.81	0.43
1:A:418:LEU:O	1:A:419:LEU:C	2.57	0.43
1:B:448:ASP:OD2	1:B:448:ASP:C	2.52	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
1:B:263:ASP:O	1:B:267:ASN:OD1	2.37	0.43
2:C:2349:LEU:CD1	2:C:2349:LEU:H	2.26	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:346:PHE:CE2	1:A:350:LEU:CD1	3.02	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: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
1:B:315:HIS:O	1:B:315:HIS:ND1	2.44	0.42
2:C:2346:ARG:CG	2:C:2346:ARG:NH2	2.63	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:A:282:TRP:CE2	1:A:371:ARG:NH1	2.89	0.41
1:B:410:GLU:HG2	1:B:411:GLN:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:LEU:HD23	1:A:433:LEU:HA	1.80	0.41
1:B:273:ASP:O	1:B:276:LEU:HB3	2.21	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:A:299:ILE:O	1:A:300:LEU:C	2.59	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

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	208/240 (87%)	183 (88%)	22 (11%)	3 (1%)	11	36
1	B	208/240 (87%)	184 (88%)	21 (10%)	3 (1%)	11	36
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%)	11	36

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 (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	183/207 (88%)	157 (86%)	26 (14%)	3 10
1	B	183/207 (88%)	148 (81%)	35 (19%)	1 4
2	C	12/12 (100%)	7 (58%)	5 (42%)	0 0
2	D	8/12 (67%)	7 (88%)	1 (12%)	4 14
All	All	386/438 (88%)	319 (83%)	67 (17%)	2 6

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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
1	A	435	HIS
1	B	227	ASN
1	B	411	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	212/240 (88%)	0.08	11 (5%)	27	23	20, 55, 93, 105	0
1	B	212/240 (88%)	0.26	10 (4%)	31	28	25, 68, 95, 98	0
2	C	16/16 (100%)	0.61	2 (12%)	3	3	61, 69, 93, 94	0
2	D	11/16 (68%)	1.15	3 (27%)	0	0	83, 84, 86, 87	0
All	All	451/512 (88%)	0.21	26 (5%)	23	19	20, 61, 94, 105	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	455	LEU	5.8
1	A	454	MET	4.6
1	B	264	PRO	3.7
1	B	445	THR	3.7
1	A	444	ASP	3.7
2	D	2343	ALA	3.6
2	C	2338	ASN	3.2
1	B	455	LEU	3.1
1	A	331	HIS	3.0
1	B	444	ASP	3.0
1	A	445	THR	2.9
2	D	2347	LYS	2.9
1	A	330	LEU	2.9
1	A	269	CYS	2.8
1	B	269	CYS	2.6
1	B	273	ASP	2.6
1	A	227	ASN	2.5
1	B	271	ALA	2.4
1	B	446	PRO	2.3
1	B	291	GLU	2.3
2	C	2339	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	453	GLU	2.2
1	A	322	ASP	2.2
1	A	446	PRO	2.2
2	D	2350	MET	2.1
1	B	270	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.