Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 05:15 PM EDT

PDB ID	:	3D24
Title	:	Crystal structure of ligand-binding domain of estrogen-related receptor alpha (ERRalpha) in complex with the peroxisome proliferators-activated receptor coactivator-1alpha box3 peptide (PGC-1alpha)
Authors	:	Moras, D.; Greschik, H.; Flaig, R.; Sato, Y.; Rochel, N.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2008-05-07
Resolution	:	2.11 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:

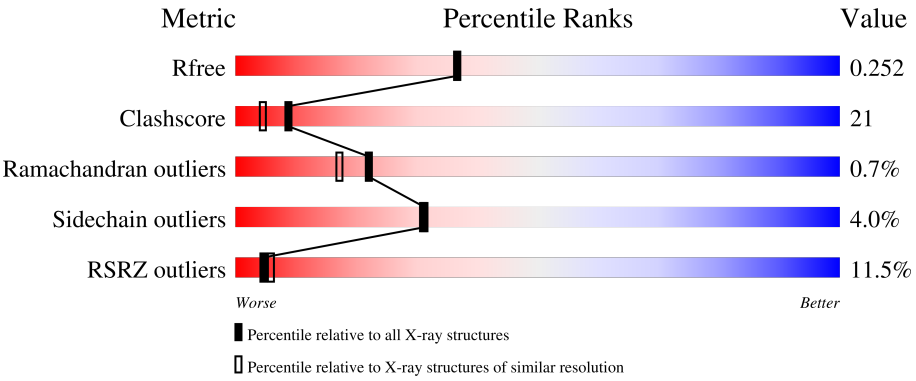
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	253	9% 53% 28% · 17%
1	C	253	8% 61% 23% · 15%
2	B	22	23% 18% 36% 5% 41%
2	D	22	18% 32% 32% 36%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3794 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 Steroid hormone receptor ERR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1624	1040	277	301	6			
1	C	216	Total	C	N	O	S	0	1	0
			1678	1072	287	311	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	MET	-	expression tag	UNP P11474
A	172	ARG	-	expression tag	UNP P11474
A	173	SER	-	expression tag	UNP P11474
A	174	HIS	-	expression tag	UNP P11474
A	175	HIS	-	expression tag	UNP P11474
A	176	HIS	-	expression tag	UNP P11474
A	177	HIS	-	expression tag	UNP P11474
A	178	HIS	-	expression tag	UNP P11474
A	179	HIS	-	expression tag	UNP P11474
A	180	GLY	-	expression tag	UNP P11474
A	181	PRO	-	expression tag	UNP P11474
A	182	GLY	-	expression tag	UNP P11474
A	183	LEU	-	expression tag	UNP P11474
A	184	VAL	-	expression tag	UNP P11474
A	185	PRO	-	expression tag	UNP P11474
A	186	ARG	-	expression tag	UNP P11474
A	187	GLY	-	expression tag	UNP P11474
A	188	SER	-	expression tag	UNP P11474
A	189	LYS	-	expression tag	UNP P11474
A	190	THR	-	expression tag	UNP P11474
A	191	ALA	-	expression tag	UNP P11474
C	171	MET	-	expression tag	UNP P11474
C	172	ARG	-	expression tag	UNP P11474
C	173	SER	-	expression tag	UNP P11474
C	174	HIS	-	expression tag	UNP P11474

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Chain	Residue	Modelled	Actual	Comment	Reference
C	175	HIS	-	expression tag	UNP P11474
C	176	HIS	-	expression tag	UNP P11474
C	177	HIS	-	expression tag	UNP P11474
C	178	HIS	-	expression tag	UNP P11474
C	179	HIS	-	expression tag	UNP P11474
C	180	GLY	-	expression tag	UNP P11474
C	181	PRO	-	expression tag	UNP P11474
C	182	GLY	-	expression tag	UNP P11474
C	183	LEU	-	expression tag	UNP P11474
C	184	VAL	-	expression tag	UNP P11474
C	185	PRO	-	expression tag	UNP P11474
C	186	ARG	-	expression tag	UNP P11474
C	187	GLY	-	expression tag	UNP P11474
C	188	SER	-	expression tag	UNP P11474
C	189	LYS	-	expression tag	UNP P11474
C	190	THR	-	expression tag	UNP P11474
C	191	ALA	-	expression tag	UNP P11474

- Molecule 2 is a protein called Peroxisome proliferator-activated receptor gamma coactivator 1-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	13	Total	C	N	O	S	0	0	0
			106	67	18	20	1			
2	D	14	Total	C	N	O	S	0	0	0
			114	71	19	23	1			

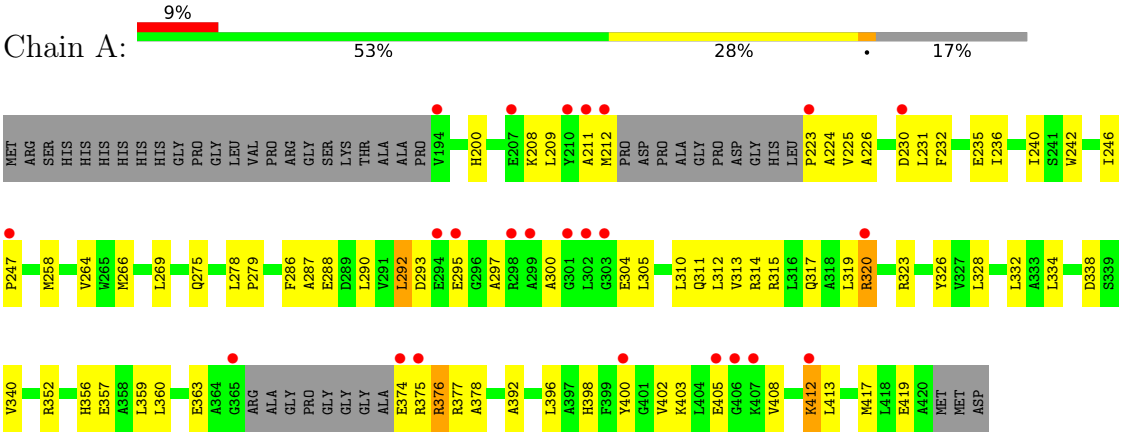
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	2	Total	O	0	0
			2	2		
3	C	163	Total	O	0	0
			163	163		
3	D	7	Total	O	0	0
			7	7		

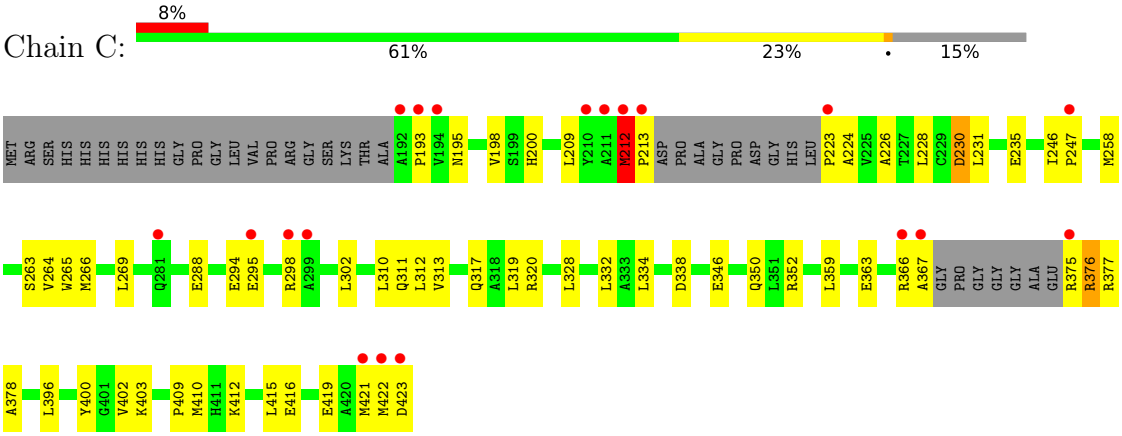
3 Residue-property plots (i)

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.

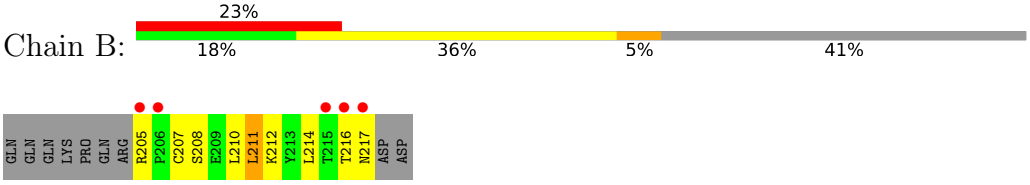
• Molecule 1: Steroid hormone receptor ERR1



• Molecule 1: Steroid hormone receptor ERR1

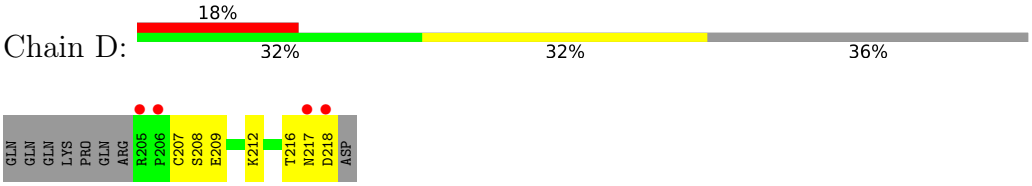


• Molecule 2: Peroxisome proliferator-activated receptor gamma coactivator 1-alpha



• Molecule 2: Peroxisome proliferator-activated receptor gamma coactivator 1-alpha

Chain D:


18%
32%
32%
36%
GLN
GLN
GLN
LYS
PRO
GLN
ARG
R205
P206
C207
S208
E209
K212
T216
N217
D218
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.40Å 56.00Å 96.20Å 90.00° 106.40° 90.00°	Depositor
Resolution (Å)	50.00 – 2.11 17.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.4 (50.00-2.11) 88.9 (17.17-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	5.68 (at 2.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.212 , 0.255 0.212 , 0.252	Depositor DCC
R_{free} test set	1584 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	3794	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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	0.27	0/1645	0.49	0/2224
1	C	0.32	0/1706	0.54	0/2305
2	B	0.34	0/107	0.49	0/144
2	D	0.35	0/115	0.59	0/155
All	All	0.30	0/3573	0.52	0/4828

There are no bond length outliers.

There are no bond angle outliers.

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	1624	0	1680	85	0
1	C	1678	0	1731	71	0
2	B	106	0	110	12	0
2	D	114	0	114	7	0
3	A	100	0	0	2	0
3	B	2	0	0	0	0
3	C	163	0	0	9	1
3	D	7	0	0	0	0
All	All	3794	0	3635	147	1

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 21.

All (147) 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)
2:B:216:THR:HG22	2:B:217:ASN:H	1.17	1.04
1:A:375:ARG:HE	1:C:376:ARG:HG3	1.31	0.94
1:C:212:MET:HB3	1:C:213:PRO:CA	2.05	0.87
1:A:376:ARG:H	1:A:376:ARG:HD3	1.40	0.86
1:C:195:ASN:HD22	1:C:198:VAL:H	1.25	0.83
1:C:258:MET:HE2	2:D:207:CYS:HB2	1.62	0.82
1:A:375:ARG:NE	1:C:376:ARG:HG3	1.95	0.81
1:A:412:LYS:HD3	1:A:413:LEU:H	1.48	0.79
1:A:264:VAL:HG21	1:A:334:LEU:HD12	1.65	0.77
2:B:216:THR:HG22	2:B:217:ASN:N	1.98	0.76
1:A:287:ALA:HB3	1:A:290:LEU:HB3	1.70	0.73
1:A:258:MET:HE1	2:B:211:LEU:HD22	1.71	0.73
1:A:340:VAL:HG22	1:C:311:GLN:NE2	2.03	0.73
1:A:376:ARG:NH2	1:A:376:ARG:HB2	2.03	0.72
1:C:412:LYS:O	1:C:416[A]:GLU:HG3	1.91	0.71
1:C:264:VAL:HG21	1:C:334:LEU:HD12	1.72	0.71
1:C:212:MET:HB3	1:C:213:PRO:HA	1.74	0.69
1:C:212:MET:HB3	1:C:213:PRO:C	2.13	0.69
1:A:275:GLN:HB2	1:A:326:TYR:CE1	2.28	0.68
1:C:195:ASN:ND2	1:C:198:VAL:H	1.92	0.68
1:A:412:LYS:CD	1:A:413:LEU:H	2.07	0.67
1:C:223:PRO:HG2	1:C:226:ALA:HB3	1.75	0.67
1:C:258:MET:CE	2:D:207:CYS:HB2	2.25	0.67
1:A:340:VAL:HG22	1:C:311:GLN:CD	2.14	0.67
1:C:230:ASP:HB3	3:C:535:HOH:O	1.94	0.67
1:C:363:GLU:OE1	1:C:377:ARG:HG2	1.97	0.65
1:A:356:HIS:ND1	1:C:375:ARG:HA	2.12	0.64
1:C:195:ASN:ND2	1:C:198:VAL:HG23	2.14	0.62
1:A:374:GLU:HG3	1:A:375:ARG:H	1.65	0.61
1:A:269:LEU:HD12	3:A:501:HOH:O	2.00	0.61
1:A:360:LEU:HD12	1:C:375:ARG:N	2.16	0.60
2:B:216:THR:CG2	2:B:217:ASN:H	2.01	0.60
1:A:412:LYS:HD3	1:A:412:LYS:N	2.17	0.60
1:C:193:PRO:HB2	3:C:573:HOH:O	2.02	0.59
1:A:376:ARG:HB2	1:A:376:ARG:HH21	1.68	0.59
1:A:402:VAL:O	1:A:405:GLU:HG2	2.02	0.59
1:C:403:LYS:HA	1:C:410:MET:CE	2.32	0.59
2:B:208:SER:O	2:B:212:LYS:HG2	2.03	0.59
1:A:405:GLU:OE2	1:A:408:VAL:HG23	2.02	0.58
1:C:346:GLU:O	1:C:350:GLN:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:GLU:HG3	1:A:375:ARG:N	2.18	0.58
1:A:360:LEU:HD21	1:C:376:ARG:NH1	2.19	0.58
1:C:235:GLU:HB3	1:C:269:LEU:HD22	1.86	0.58
1:A:258:MET:HE2	2:B:210:LEU:HD23	1.86	0.57
1:A:224:ALA:HB1	1:A:300:ALA:HB1	1.87	0.56
1:A:258:MET:CE	2:B:207:CYS:HB2	2.36	0.56
1:C:228:LEU:HD12	1:C:302:LEU:HD21	1.87	0.56
1:A:212:MET:CE	1:A:230:ASP:HB3	2.35	0.56
1:A:400:TYR:HE1	1:A:419:GLU:HG2	1.70	0.56
1:A:231:LEU:O	1:A:235:GLU:HG3	2.06	0.55
1:C:403:LYS:HA	1:C:410:MET:HE3	1.88	0.55
1:C:409:PRO:HG2	3:C:586:HOH:O	2.05	0.55
1:A:400:TYR:CE1	1:A:403:LYS:HE3	2.41	0.55
1:C:366:ARG:HH11	1:C:366:ARG:HG3	1.71	0.55
1:A:278:LEU:HB2	1:A:279:PRO:HD3	1.89	0.55
1:A:304:GLU:OE1	1:A:304:GLU:HA	2.08	0.54
1:A:200:HIS:CD2	1:A:247:PRO:HD3	2.44	0.53
1:A:258:MET:HE2	2:B:207:CYS:HB2	1.91	0.53
1:A:286:PHE:CD1	1:A:292:LEU:HD21	2.43	0.53
1:A:357:GLU:OE2	1:C:375:ARG:HG2	2.10	0.52
1:A:360:LEU:HD11	1:C:376:ARG:HD2	1.91	0.52
1:A:264:VAL:CG2	1:A:334:LEU:HD12	2.37	0.51
1:A:398:HIS:O	1:A:402:VAL:HG23	2.10	0.51
1:C:403:LYS:HE2	1:C:415:LEU:HD22	1.93	0.51
1:A:360:LEU:HD21	1:C:376:ARG:HH11	1.76	0.51
1:C:195:ASN:HD22	1:C:198:VAL:HG23	1.76	0.51
1:C:422:MET:SD	1:C:423:ASP:O	2.68	0.51
1:C:200:HIS:CD2	1:C:247:PRO:HD3	2.46	0.50
1:C:294:GLU:HG2	1:C:310:LEU:HD12	1.92	0.50
1:A:412:LYS:HE2	1:A:413:LEU:HB2	1.93	0.50
1:A:236:ILE:O	1:A:240:ILE:HG13	2.11	0.50
1:A:338:ASP:O	1:C:311:GLN:NE2	2.45	0.50
1:C:209:LEU:HD21	1:C:231:LEU:HD11	1.92	0.50
1:A:232:PHE:O	1:A:236:ILE:HG13	2.12	0.50
1:A:400:TYR:O	1:A:403:LYS:HG2	2.12	0.50
1:C:313:VAL:O	1:C:317:GLN:HG3	2.11	0.50
1:A:292:LEU:N	1:A:292:LEU:HD23	2.27	0.50
1:C:402:VAL:HG12	1:C:410:MET:HE1	1.94	0.49
1:A:363:GLU:OE1	1:A:377:ARG:HG2	2.11	0.49
1:A:376:ARG:HD3	1:A:376:ARG:N	2.20	0.49
1:A:375:ARG:HH11	1:C:378:ALA:H	1.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:LEU:HA	3:C:484:HOH:O	2.13	0.49
1:A:304:GLU:O	1:A:304:GLU:HG3	2.13	0.49
2:D:216:THR:O	2:D:218:ASP:N	2.45	0.49
1:A:266:MET:HB2	1:A:396:LEU:HD21	1.94	0.49
1:A:208:LYS:HB3	1:A:288:GLU:HG3	1.95	0.48
1:A:352:ARG:HD2	3:A:500:HOH:O	2.12	0.48
1:A:223:PRO:HB2	1:A:226:ALA:HB3	1.95	0.48
1:A:412:LYS:HD3	1:A:413:LEU:N	2.23	0.48
1:C:295:GLU:O	1:C:298:ARG:HB2	2.14	0.48
1:A:293:ASP:OD1	1:A:295:GLU:HB3	2.14	0.47
1:C:209:LEU:CD2	1:C:231:LEU:HD11	2.44	0.47
1:C:212:MET:CB	1:C:213:PRO:HA	2.41	0.47
1:A:313:VAL:O	1:A:317:GLN:HG3	2.14	0.47
1:C:263:SER:HA	1:C:421:MET:HG3	1.96	0.47
1:A:412:LYS:CD	1:A:412:LYS:H	2.27	0.47
1:C:212:MET:CB	1:C:213:PRO:CA	2.85	0.47
1:A:328:LEU:HD13	1:A:359:LEU:HA	1.97	0.47
1:C:352:ARG:NH2	3:C:571:HOH:O	2.44	0.47
1:A:258:MET:HG2	2:B:214:LEU:CD1	2.45	0.47
1:C:366:ARG:O	1:C:367:ALA:HB3	2.15	0.47
1:A:258:MET:HG2	2:B:214:LEU:HD12	1.97	0.46
1:A:292:LEU:HD12	1:A:297:ALA:HA	1.97	0.46
1:A:360:LEU:HD11	1:C:376:ARG:H	1.79	0.46
1:A:242:TRP:CZ2	1:A:246:ILE:HD11	2.50	0.45
1:A:412:LYS:HD3	1:A:412:LYS:H	1.78	0.45
1:C:264:VAL:CG2	1:C:334:LEU:HD12	2.43	0.45
1:A:319:LEU:C	1:A:320:ARG:HG2	2.37	0.45
1:A:305:LEU:HD11	1:A:398:HIS:HB3	1.99	0.45
1:A:225:VAL:HG23	1:A:300:ALA:O	2.17	0.44
1:C:403:LYS:HE3	1:C:419:GLU:OE1	2.17	0.44
1:A:376:ARG:NH2	1:A:377:ARG:H	2.15	0.44
1:A:392:ALA:O	1:A:396:LEU:HG	2.17	0.44
1:A:209:LEU:HD21	1:A:231:LEU:HD11	1.98	0.44
1:C:328:LEU:HD13	1:C:359:LEU:HA	2.00	0.44
1:A:323:ARG:HG3	1:A:323:ARG:HH11	1.82	0.43
1:C:258:MET:HE2	2:D:207:CYS:CB	2.40	0.43
1:A:212:MET:SD	1:A:230:ASP:HB3	2.58	0.43
2:D:212:LYS:NZ	2:D:212:LYS:HB2	2.33	0.43
1:C:265:TRP:HE1	1:C:421:MET:HB2	1.83	0.43
1:C:396:LEU:HD11	1:C:421:MET:SD	2.57	0.43
1:C:400:TYR:CE1	1:C:422:MET:HE3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:MET:CE	2:B:211:LEU:HD22	2.46	0.43
1:C:266:MET:HB3	1:C:421:MET:HE2	2.00	0.43
3:C:514:HOH:O	2:D:208:SER:HB3	2.17	0.43
1:C:402:VAL:HG12	1:C:410:MET:CE	2.49	0.43
1:A:236:ILE:HD13	1:A:417:MET:HG3	2.01	0.43
1:A:311:GLN:NE2	1:C:338:ASP:O	2.53	0.42
1:C:294:GLU:O	1:C:298:ARG:HG2	2.19	0.42
1:A:266:MET:CE	1:A:396:LEU:HD23	2.49	0.42
1:C:294:GLU:CG	1:C:310:LEU:HD12	2.49	0.42
1:A:412:LYS:CG	1:A:413:LEU:N	2.82	0.42
1:C:366:ARG:HG3	1:C:366:ARG:NH1	2.34	0.42
1:A:412:LYS:CD	1:A:413:LEU:N	2.80	0.42
1:A:412:LYS:CD	1:A:412:LYS:N	2.82	0.42
1:C:416[A]:GLU:OE1	2:D:209:GLU:HG2	2.19	0.42
1:A:356:HIS:CE1	1:C:376:ARG:HD3	2.55	0.41
1:C:410:MET:HE3	3:C:427:HOH:O	2.19	0.41
1:C:346:GLU:HG2	3:C:450:HOH:O	2.20	0.41
1:C:319:LEU:O	1:C:320:ARG:HB2	2.19	0.41
1:A:378:ALA:HB1	1:C:376:ARG:HH12	1.85	0.41
1:C:298:ARG:NH1	3:C:493:HOH:O	2.52	0.41
1:A:258:MET:HE1	2:B:207:CYS:O	2.21	0.40
1:A:310:LEU:O	1:A:314:ARG:HG3	2.21	0.40
1:C:246:ILE:HA	1:C:247:PRO:HD3	1.90	0.40
1:A:376:ARG:HH21	1:A:376:ARG:CB	2.34	0.40
1:A:211:ALA:HB2	1:A:290:LEU:HB2	2.02	0.40

All (1) 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)
3:C:529:HOH:O	3:C:529:HOH:O[2_657]	2.01	0.19

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	203/253 (80%)	192 (95%)	11 (5%)	0	100 100
1	C	211/253 (83%)	201 (95%)	8 (4%)	2 (1%)	17 12
2	B	11/22 (50%)	7 (64%)	4 (36%)	0	100 100
2	D	12/22 (54%)	10 (83%)	1 (8%)	1 (8%)	1 0
All	All	437/550 (80%)	410 (94%)	24 (6%)	3 (1%)	22 17

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	212	MET
1	C	224	ALA
2	D	217	ASN

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	172/202 (85%)	165 (96%)	7 (4%)	30 30
1	C	178/202 (88%)	172 (97%)	6 (3%)	37 38
2	B	13/22 (59%)	11 (85%)	2 (15%)	2 1
2	D	14/22 (64%)	14 (100%)	0	100 100
All	All	377/448 (84%)	362 (96%)	15 (4%)	31 31

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	LEU
1	A	312	LEU
1	A	315	ARG
1	A	320	ARG
1	A	332	LEU

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Mol	Chain	Res	Type
1	A	376	ARG
1	A	412	LYS
2	B	205	ARG
2	B	211	LEU
1	C	212	MET
1	C	230	ASP
1	C	288	GLU
1	C	312	LEU
1	C	332	LEU
1	C	376	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	311	GLN
1	C	195	ASN
1	C	275	GLN
1	C	350	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 (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	209/253 (82%)	0.60	24 (11%) 4 6	17, 45, 82, 95	0
1	C	216/253 (85%)	0.35	19 (8%) 10 12	15, 30, 72, 82	0
2	B	13/22 (59%)	2.20	5 (38%) 0 0	48, 57, 80, 83	0
2	D	14/22 (63%)	1.41	4 (28%) 0 0	19, 34, 70, 78	0
All	All	452/550 (82%)	0.55	52 (11%) 4 6	15, 38, 77, 95	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	193	PRO	9.6
1	C	213	PRO	9.2
2	B	205	ARG	7.5
1	A	365	GLY	7.1
2	D	217	ASN	7.1
1	A	212	MET	7.1
2	B	217	ASN	6.1
1	C	366	ARG	5.7
1	C	375	ARG	5.7
1	C	367	ALA	5.4
2	D	218	ASP	5.4
1	C	192	ALA	5.3
1	A	223	PRO	5.0
1	A	194	VAL	4.9
1	A	299	ALA	4.9
1	C	223	PRO	4.4
2	D	205	ARG	4.4
1	C	299	ALA	4.4
1	A	298	ARG	4.3
1	C	194	VAL	4.1
1	A	303	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	216	THR	3.9
1	A	295	GLU	3.9
1	C	421	MET	3.8
1	A	207	GLU	3.5
1	A	294	GLU	3.4
1	A	375	ARG	3.2
1	A	374	GLU	3.1
1	C	212	MET	3.1
2	D	206	PRO	3.1
1	C	295	GLU	3.0
1	C	422	MET	3.0
2	B	215	THR	3.0
1	C	423	ASP	2.9
1	A	405	GLU	2.9
1	C	247	PRO	2.8
1	C	210	TYR	2.6
1	A	302	LEU	2.6
1	A	400	TYR	2.6
2	B	206	PRO	2.6
1	C	298	ARG	2.6
1	A	320	ARG	2.4
1	C	281	GLN	2.4
1	A	301	GLY	2.4
1	A	247	PRO	2.3
1	A	406	GLY	2.2
1	A	412	LYS	2.2
1	A	210	TYR	2.2
1	A	407	LYS	2.1
1	C	211	ALA	2.1
1	A	230	ASP	2.1
1	A	211	ALA	2.1

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.