Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 03:39 AM EST

PDB ID	:	4J5W
Title	:	Crystal Structure of the apo-PXR/RXRalpha LBD Heterotetramer Complex
Authors	:	Wallace, B.D.; Betts, L.; Redinbo, M.R.
Deposited on	:	2013-02-10
Resolution	:	2.80 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 (i)) were used in the production of this report:

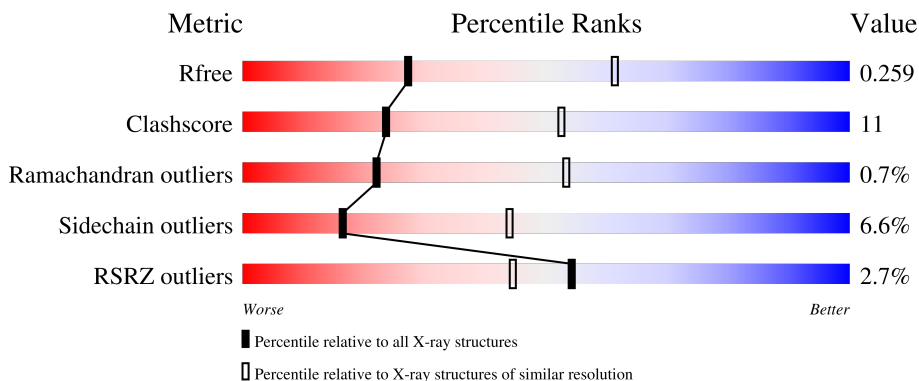|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	Percentile Ranks	Value
Rfree		0.259
Clashscore		11
Ramachandran outliers		0.7%
Sidechain outliers		6.6%
RSRZ outliers		2.7%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	336	2% 61% 25% •• 12%
1	B	336	3% 64% 20% • 13%
2	C	264	% 57% 25% • 14%
2	D	264	3% 61% 23% • 14%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8580 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	1	0
			2406	1543	417	428	18			
1	B	293	Total	C	N	O	S	0	0	0
			2383	1527	413	425	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	127	SER	-	expression tag	UNP O75469
A	128	ASN	-	expression tag	UNP O75469
A	129	ALA	-	expression tag	UNP O75469
A	435	GLY	-	linker	UNP Q15788
A	436	GLY	-	linker	UNP Q15788
A	437	SER	-	linker	UNP Q15788
A	438	GLY	-	linker	UNP Q15788
A	439	GLY	-	linker	UNP Q15788
B	127	SER	-	expression tag	UNP O75469
B	128	ASN	-	expression tag	UNP O75469
B	129	ALA	-	expression tag	UNP O75469
B	435	GLY	-	linker	UNP Q15788
B	436	GLY	-	linker	UNP Q15788
B	437	SER	-	linker	UNP Q15788
B	438	GLY	-	linker	UNP Q15788
B	439	GLY	-	linker	UNP Q15788

- Molecule 2 is a protein called Retinoic acid receptor RXR-alpha, Nuclear receptor coactivator 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	226	Total	C	N	O	S	0	1	0
			1804	1157	315	322	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	227	Total 1810	C 1161	N 316	O 323	S 10	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	463	GLY	-	linker	UNP P19793
C	464	GLY	-	linker	UNP P19793
C	465	SER	-	linker	UNP P19793
C	466	GLY	-	linker	UNP Q15788
C	467	GLY	-	linker	UNP Q15788
D	463	GLY	-	linker	UNP P19793
D	464	GLY	-	linker	UNP P19793
D	465	SER	-	linker	UNP P19793
D	466	GLY	-	linker	UNP Q15788
D	467	GLY	-	linker	UNP Q15788

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	55	Total 55	O 55	0	0
4	B	44	Total 44	O 44	0	0
4	C	26	Total 26	O 26	0	0
4	D	50	Total 50	O 50	0	0

3 Residue-property plots ⓘ

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: Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1
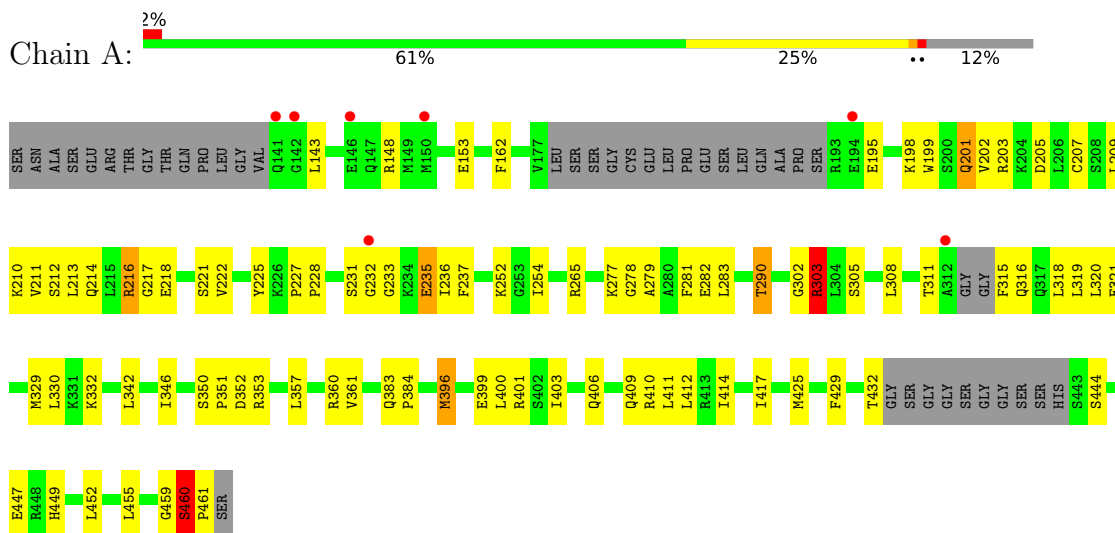
Chain A:

• Molecule 1: Nuclear receptor subfamily 1 group I member 2, Nuclear receptor coactivator 1
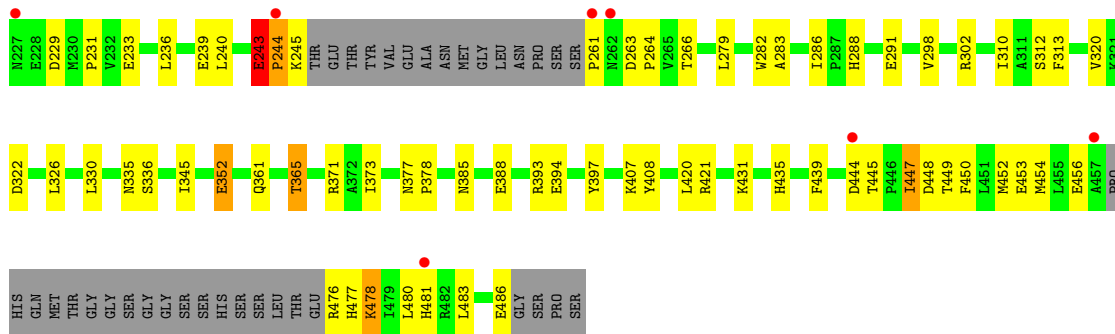
Chain B:

• Molecule 2: Retinoic acid receptor RXR-alpha, Nuclear receptor coactivator 1

Chain C:
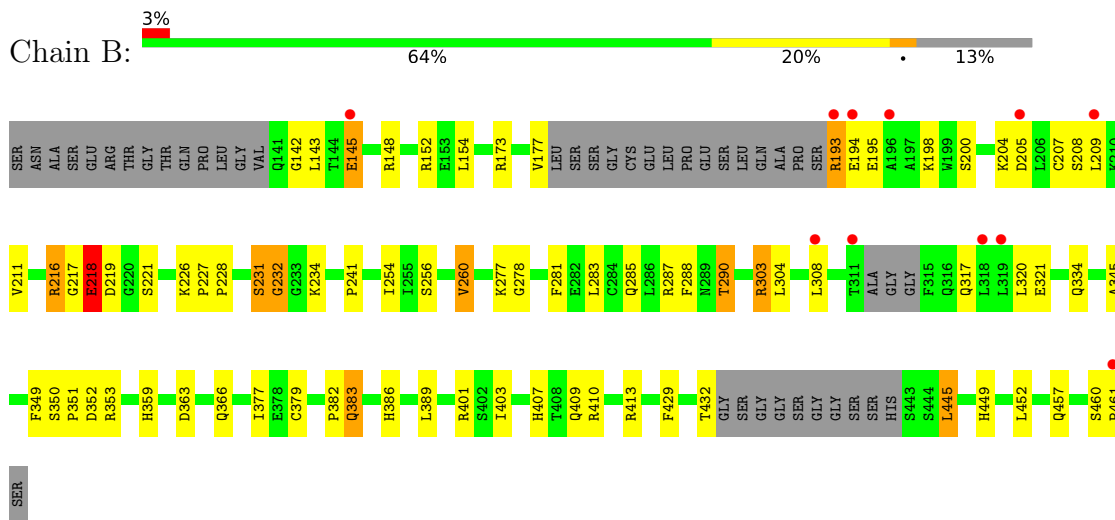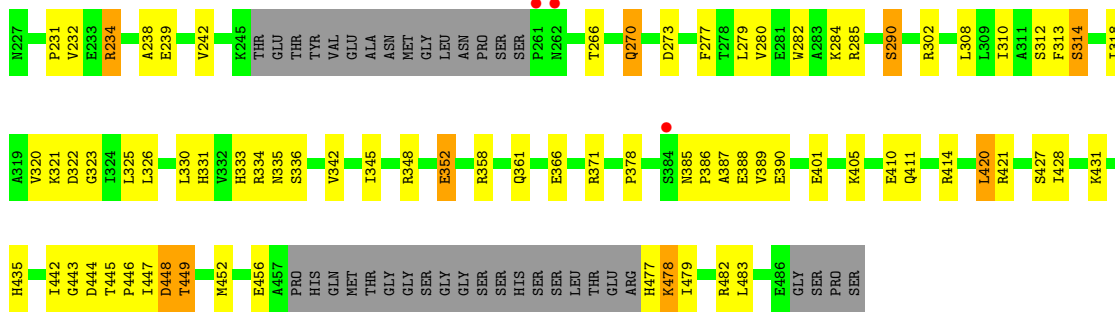
• Molecule 2: Retinoic acid receptor RXR-alpha, Nuclear receptor coactivator 1

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.26Å 109.55Å 169.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.80 48.54 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.54-2.80) 96.1 (48.54-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.8_1061	Depositor
R, R_{free}	0.250 , 0.298 0.254 , 0.259	Depositor DCC
R_{free} test set	1610 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.7	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 38.8	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	8580	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1729e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.30	0/2460	0.50	2/3309 (0.1%)
1	B	0.29	0/2433	0.46	1/3274 (0.0%)
2	C	0.28	0/1842	0.48	0/2486
2	D	0.24	0/1848	0.43	0/2494
All	All	0.28	0/8583	0.47	3/11563 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	303[A]	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	303[B]	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	B	232	GLY	N-CA-C	5.19	126.08	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	216	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	B	218	GLU	Peptide
2	D	243	GLU	Peptide

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	2406	0	2423	55	0
1	B	2383	0	2394	57	0
2	C	1804	0	1851	49	0
2	D	1810	0	1855	37	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	55	0	0	2	0
4	B	44	0	0	7	0
4	C	26	0	0	2	0
4	D	50	0	0	2	0
All	All	8580	0	8523	190	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (190) 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:218:GLU:OE2	4:B:544:HOH:O	1.58	1.18
1:B:219:ASP:OD1	1:B:221:SER:OG	1.85	0.93
1:A:216:ARG:HH11	1:A:216:ARG:HB2	1.42	0.83
1:A:278:GLY:HA3	1:A:353:ARG:HD2	1.62	0.80
2:C:366:GLU:OE1	2:C:414:ARG:NH1	2.17	0.76
2:C:231:PRO:HB2	2:C:234:ARG:HB2	1.70	0.72
2:C:302:ARG:NH2	2:C:456:GLU:O	2.24	0.71
1:B:216:ARG:HB3	1:B:217:GLY:HA3	1.73	0.68
1:B:218:GLU:CD	4:B:544:HOH:O	2.19	0.68
2:C:320:VAL:HG11	2:C:325:LEU:HB2	1.74	0.68
1:A:216:ARG:HH12	1:A:303[A]:ARG:HA	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:SER:HA	1:B:232:GLY:C	2.15	0.67
1:A:209:LEU:HD11	1:A:321:GLU:HG2	1.78	0.66
1:B:148:ARG:HG3	1:B:152:ARG:HH21	1.61	0.66
2:C:447:ILE:O	2:C:452:MET:HG2	1.96	0.65
1:B:359:HIS:NE2	2:C:352:GLU:OE2	2.25	0.65
1:A:203:ARG:NH1	1:A:232:GLY:HA2	2.12	0.65
1:B:352:ASP:OD2	4:B:508:HOH:O	2.15	0.65
2:C:239:GLU:OE2	2:C:371:ARG:NH1	2.30	0.63
1:B:277:LYS:NZ	4:B:527:HOH:O	2.31	0.63
1:A:228:PRO:HB3	1:B:219:ASP:O	1.98	0.63
1:B:143:LEU:O	1:B:148:ARG:NH2	2.33	0.62
1:A:216:ARG:HH12	1:A:303[B]:ARG:HA	1.63	0.61
1:B:173:ARG:NH1	4:B:530:HOH:O	2.25	0.60
2:C:385:ASN:ND2	2:C:388:GLU:OE2	2.34	0.59
1:B:217:GLY:O	1:B:218:GLU:HB3	2.02	0.59
2:D:263:ASP:OD1	2:D:266:THR:N	2.33	0.59
2:C:290:SER:OG	4:C:601:HOH:O	2.16	0.59
1:A:352:ASP:HB3	2:D:352:GLU:HG2	1.84	0.58
1:B:226:LYS:NZ	1:B:227:PRO:O	2.26	0.58
2:D:486:GLU:N	2:D:486:GLU:OE1	2.36	0.58
1:A:207:CYS:HA	1:A:210:LYS:HE2	1.85	0.58
2:D:326:LEU:HD12	2:D:330:LEU:HB3	1.86	0.58
1:A:216:ARG:NH1	1:A:303[A]:ARG:HA	2.18	0.57
2:D:393:ARG:NH2	4:D:610:HOH:O	2.36	0.57
2:D:444:ASP:OD1	2:D:445:THR:N	2.37	0.57
1:B:173:ARG:HD2	1:B:241:PRO:HB3	1.87	0.56
2:D:239:GLU:OE2	2:D:282:TRP:NE1	2.39	0.56
1:A:353:ARG:NH1	4:A:501:HOH:O	2.39	0.55
2:D:302:ARG:HG2	2:D:454:MET:HE1	1.89	0.55
1:B:218:GLU:O	1:B:218:GLU:HG2	2.06	0.55
1:B:303:ARG:HD3	1:B:304:LEU:HD12	1.87	0.55
2:C:238:ALA:HA	2:C:285:ARG:HD2	1.89	0.55
1:B:352:ASP:HB3	2:C:352:GLU:HG2	1.89	0.54
1:A:459:GLY:O	1:A:460:SER:HB2	2.07	0.54
2:D:310:ILE:HA	2:D:313:PHE:CE2	2.42	0.54
1:A:460:SER:N	1:A:461:PRO:HD3	2.23	0.54
1:B:173:ARG:HH11	1:B:241:PRO:HB3	1.73	0.54
2:C:442:ILE:HD12	2:C:444:ASP:HB2	1.90	0.53
4:B:504:HOH:O	2:C:421:ARG:NH2	2.40	0.53
2:D:407:LYS:HG2	2:D:408:TYR:CE2	2.44	0.53
1:A:410:ARG:NH1	4:A:550:HOH:O	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:345:ILE:HD13	2:C:431:LYS:HB3	1.91	0.52
2:C:442:ILE:HG13	2:C:443:GLY:N	2.24	0.52
2:C:479:ILE:O	2:C:482:ARG:HG3	2.09	0.52
1:A:216:ARG:NH1	1:A:303[B]:ARG:HA	2.24	0.52
1:A:214:GLN:HB3	1:A:305:SER:HB2	1.92	0.52
1:B:281:PHE:HE2	1:B:403:ILE:HG22	1.75	0.52
1:A:211:VAL:HG12	1:A:308:LEU:HD23	1.92	0.51
1:B:401:ARG:HG2	2:C:427:SER:HB2	1.92	0.51
2:C:401:GLU:HG2	2:C:405:LYS:HE2	1.91	0.51
1:A:195:GLU:O	1:A:199:TRP:HB2	2.11	0.51
1:A:383:GLN:HB2	1:A:384:PRO:HD3	1.92	0.51
1:B:200:SER:O	1:B:204:LYS:HG3	2.11	0.51
1:B:278:GLY:HA3	1:B:353:ARG:HD2	1.93	0.50
1:B:366:GLN:HG2	2:C:420:LEU:HD11	1.92	0.50
2:D:448:ASP:OD1	2:D:449:THR:N	2.44	0.50
1:A:218:GLU:OE1	1:A:218:GLU:N	2.38	0.50
2:D:236:LEU:HB2	2:D:365:THR:HB	1.93	0.50
2:D:302:ARG:NH2	2:D:456:GLU:O	2.45	0.50
1:A:233:GLY:N	1:A:235:GLU:OE2	2.27	0.49
2:C:277:PHE:HD1	2:C:483:LEU:HD21	1.77	0.49
1:A:254:ILE:HD12	1:A:283:LEU:HB3	1.95	0.49
1:A:143:LEU:HB2	1:A:148:ARG:HG3	1.94	0.49
1:A:316:GLN:HA	1:A:319:LEU:HD12	1.93	0.49
1:A:360:ARG:HG3	1:A:361:VAL:H	1.76	0.49
2:C:445:THR:HB	2:C:446:PRO:HD2	1.95	0.49
1:A:216:ARG:NH2	1:A:302:GLY:O	2.46	0.49
2:C:242:VAL:HG21	2:C:282:TRP:HB2	1.95	0.49
2:C:447:ILE:HD12	2:C:449:THR:H	1.77	0.49
2:C:279:LEU:HD11	2:C:308:LEU:HD13	1.95	0.48
2:C:318:ILE:HD11	2:C:358[B]:ARG:HA	1.96	0.48
2:D:435:HIS:HB3	2:D:439:PHE:HE2	1.78	0.48
1:A:231:SER:HB3	1:A:235:GLU:CD	2.34	0.48
2:C:386:PRO:O	2:C:389:VAL:N	2.47	0.48
2:D:283:ALA:HA	2:D:286:ILE:HD12	1.96	0.48
1:B:148:ARG:HG3	1:B:152:ARG:NH2	2.28	0.47
1:A:352:ASP:OD2	1:A:401:ARG:NH1	2.31	0.47
1:B:321:GLU:OE1	1:B:321:GLU:N	2.47	0.47
1:A:277:LYS:HD2	1:A:449:HIS:NE2	2.28	0.47
1:A:221:SER:HB3	1:B:228:PRO:HG3	1.96	0.47
1:B:142:GLY:H	1:B:379:CYS:HB3	1.79	0.47
2:C:322:ASP:OD1	2:C:323:GLY:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HB3	1:A:225:TYR:HB3	1.97	0.47
1:A:279:ALA:HB2	1:A:353:ARG:HH12	1.79	0.47
1:A:281:PHE:HE2	1:A:403:ILE:HG22	1.80	0.47
2:C:342:VAL:HG12	2:C:435:HIS:CD2	2.50	0.47
2:D:345:ILE:HD13	2:D:431:LYS:HD3	1.95	0.47
2:C:266:THR:O	2:C:270:GLN:HG2	2.15	0.47
1:B:377:ILE:HG13	1:B:389:LEU:HD23	1.97	0.47
2:C:348:ARG:O	2:C:352:GLU:HB2	2.15	0.46
2:C:410:GLU:HG2	2:C:411:GLN:HG2	1.98	0.46
2:D:431:LYS:O	2:D:435:HIS:HD2	1.99	0.46
1:B:409:GLN:HG3	1:B:413:ARG:NH1	2.31	0.46
1:B:193:ARG:HG3	1:B:194:GLU:H	1.81	0.46
2:C:331:HIS:CE1	2:C:333:HIS:HE1	2.34	0.46
1:A:252:LYS:HE2	1:A:455:LEU:HD22	1.96	0.46
1:B:154:LEU:HD21	1:B:345:ALA:HB2	1.97	0.46
2:C:335:ASN:OD1	2:C:336:SER:N	2.49	0.46
1:B:205:ASP:O	1:B:410:ARG:NH2	2.49	0.45
1:B:382:PRO:HD2	1:B:386:HIS:CD2	2.51	0.45
2:D:240:LEU:O	2:D:244:PRO:HD3	2.16	0.45
1:A:202:VAL:HG13	1:A:414:ILE:HG12	1.98	0.45
2:C:366:GLU:OE2	2:C:414:ARG:NH2	2.48	0.45
1:B:303:ARG:H	1:B:303:ARG:HG3	1.35	0.45
1:A:162:PHE:HE2	1:A:290:THR:HG21	1.82	0.44
1:B:352:ASP:OD1	1:B:352:ASP:N	2.45	0.44
2:D:335:ASN:OD1	2:D:336:SER:N	2.48	0.44
2:D:453:GLU:CG	2:D:477:HIS:HB2	2.48	0.44
1:A:412:LEU:HA	1:A:412:LEU:HD23	1.79	0.44
2:C:318:ILE:HD11	2:C:358[A]:ARG:HA	1.99	0.44
1:A:350:SER:HA	1:A:351:PRO:HD3	1.83	0.44
1:B:208:SER:OG	1:B:209:LEU:N	2.50	0.44
2:C:387:ALA:HA	2:C:390:GLU:OE1	2.18	0.44
2:C:334:ARG:NH1	4:C:608:HOH:O	2.43	0.44
1:A:425:MET:O	1:A:429:PHE:HD1	2.00	0.43
1:A:282:GLU:HB3	1:A:400:LEU:HD21	1.99	0.43
1:A:406:GLN:HA	1:A:409:GLN:HG2	2.00	0.43
2:D:261:PRO:HA	2:D:264:PRO:HD3	2.00	0.43
2:D:373:ILE:O	4:D:616:HOH:O	2.21	0.43
1:A:198:LYS:HB3	1:A:198:LYS:HE2	1.58	0.43
1:A:217:GLY:N	1:A:221:SER:O	2.50	0.43
1:A:199:TRP:CE3	1:A:417:ILE:HD12	2.53	0.43
1:A:222:VAL:HG13	1:B:226:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ALA:HB1	1:A:283:LEU:HD13	2.00	0.43
1:B:350:SER:HA	1:B:351:PRO:HD3	1.87	0.43
2:C:284:LYS:HA	2:C:284:LYS:HD2	1.90	0.43
2:C:277:PHE:CD1	2:C:483:LEU:HD21	2.53	0.43
1:A:330:LEU:HD13	1:A:396:MET:HG2	2.00	0.42
1:B:195:GLU:HA	1:B:198:LYS:HD3	2.00	0.42
1:B:349:PHE:O	1:B:366:GLN:HB2	2.19	0.42
1:B:460:SER:OG	1:B:461:PRO:HD3	2.19	0.42
2:C:345:ILE:HD11	2:C:428:ILE:HG23	2.01	0.42
2:D:477:HIS:HD2	2:D:478:LYS:N	2.17	0.42
1:B:350:SER:O	1:B:353:ARG:HG2	2.18	0.42
2:C:326:LEU:HD12	2:C:330:LEU:HB2	2.02	0.42
2:D:477:HIS:NE2	2:D:481:HIS:HB2	2.34	0.42
1:B:277:LYS:HD2	1:B:449:HIS:NE2	2.35	0.42
1:B:285:GLN:NE2	4:B:531:HOH:O	2.40	0.42
2:D:288:HIS:HA	2:D:291:GLU:HG2	2.01	0.42
2:D:377:ASN:HA	2:D:378:PRO:HD3	1.86	0.42
1:A:399:GLU:O	1:A:403:ILE:HG12	2.20	0.42
2:C:273:ASP:HB2	2:C:448:ASP:OD2	2.19	0.42
1:B:256:SER:O	1:B:260:VAL:HG12	2.19	0.42
1:B:234:LYS:HG2	1:B:234:LYS:O	2.19	0.42
1:B:407:HIS:CD2	1:B:407:HIS:C	2.93	0.42
2:D:298:VAL:HG13	2:D:480:LEU:HD23	2.02	0.42
2:D:445:THR:HG23	2:D:447:ILE:HD12	2.02	0.42
1:A:201:GLN:NE2	1:A:205:ASP:OD1	2.53	0.41
2:C:266:THR:HA	2:C:446:PRO:HD3	2.02	0.41
2:D:243:GLU:HG3	2:D:244:PRO:N	2.35	0.41
2:D:477:HIS:O	2:D:478:LYS:HB2	2.20	0.41
2:C:310:ILE:O	2:C:314:SER:HB2	2.20	0.41
2:D:239:GLU:OE2	2:D:371:ARG:NH1	2.53	0.41
2:D:476:ARG:HG2	2:D:477:HIS:H	1.84	0.41
1:B:317:GLN:HA	1:B:320:LEU:HD13	2.02	0.41
2:D:444:ASP:OD1	2:D:445:THR:HG22	2.21	0.41
1:A:236:ILE:HG13	1:A:237:PHE:CD1	2.56	0.41
1:B:287:ARG:O	1:B:290:THR:HG23	2.21	0.41
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.87	0.41
2:C:378:PRO:HG3	2:C:390:GLU:HG3	2.02	0.41
1:B:254:ILE:HG23	1:B:283:LEU:HD23	2.02	0.41
1:A:329:MET:O	1:A:332:LYS:HG2	2.20	0.41
1:B:145:GLU:OE1	1:B:152:ARG:NH2	2.53	0.41
2:D:229:ASP:O	2:D:231:PRO:HD3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:239:GLU:OE2	2:C:282:TRP:NE1	2.54	0.41
1:A:315:PHE:HA	1:A:318:LEU:HG	2.03	0.41
1:A:342:LEU:O	1:A:346:ILE:HG13	2.21	0.41
1:B:407:HIS:CE1	1:B:429:PHE:HE2	2.39	0.41
2:C:318:ILE:HA	2:C:318:ILE:HD12	1.76	0.41
2:C:477:HIS:HB3	2:C:478:LYS:H	1.64	0.41
2:D:385:ASN:ND2	2:D:388:GLU:OE1	2.53	0.41
2:D:394:GLU:HA	2:D:397:TYR:HB3	2.03	0.41
1:B:211:VAL:HG12	1:B:308:LEU:HD23	2.02	0.40
2:D:330:LEU:HD12	2:D:330:LEU:HA	1.85	0.40
1:B:351:PRO:HG3	1:B:363:ASP:HA	2.01	0.40
1:A:227:PRO:HA	1:A:228:PRO:HD3	1.85	0.40
2:C:310:ILE:HA	2:C:313:PHE:CE2	2.56	0.40
1:A:360:ARG:HG3	1:A:361:VAL:HG23	2.03	0.40
1:B:277:LYS:HE2	1:B:277:LYS:HB3	1.78	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/336 (85%)	270 (94%)	16 (6%)	1 (0%)	41	72
1	B	285/336 (85%)	272 (95%)	12 (4%)	1 (0%)	34	66
2	C	221/264 (84%)	206 (93%)	14 (6%)	1 (0%)	29	61
2	D	222/264 (84%)	209 (94%)	9 (4%)	4 (2%)	8	28
All	All	1015/1200 (85%)	957 (94%)	51 (5%)	7 (1%)	22	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	460	SER
2	D	244	PRO
2	C	321	LYS
2	D	478	LYS
2	D	243	GLU
1	B	383	GLN
2	D	483	LEU

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	265/295 (90%)	246 (93%)	19 (7%)	14	38
1	B	262/295 (89%)	246 (94%)	16 (6%)	18	48
2	C	197/227 (87%)	184 (93%)	13 (7%)	16	44
2	D	197/227 (87%)	183 (93%)	14 (7%)	14	39
All	All	921/1044 (88%)	859 (93%)	62 (7%)	16	43

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	GLU
1	A	201	GLN
1	A	212	SER
1	A	216	ARG
1	A	235	GLU
1	A	265	ARG
1	A	290	THR
1	A	303[A]	ARG
1	A	303[B]	ARG
1	A	311	THR
1	A	320	LEU
1	A	357	LEU
1	A	396	MET
1	A	411	LEU
1	A	432	THR

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Mol	Chain	Res	Type
1	A	444	SER
1	A	447	GLU
1	A	452	LEU
1	A	460	SER
1	B	145	GLU
1	B	177	VAL
1	B	193	ARG
1	B	207	CYS
1	B	218	GLU
1	B	231	SER
1	B	260	VAL
1	B	288	PHE
1	B	290	THR
1	B	303	ARG
1	B	334	GLN
1	B	383	GLN
1	B	432	THR
1	B	445	LEU
1	B	452	LEU
1	B	457	GLN
2	C	232	VAL
2	C	234	ARG
2	C	270	GLN
2	C	280	VAL
2	C	290	SER
2	C	312	SER
2	C	314	SER
2	C	352	GLU
2	C	361	GLN
2	C	420	LEU
2	C	448	ASP
2	C	449	THR
2	C	478	LYS
2	D	233	GLU
2	D	245	LYS
2	D	279	LEU
2	D	312	SER
2	D	320	VAL
2	D	322	ASP
2	D	352	GLU
2	D	361	GLN
2	D	365	THR

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Mol	Chain	Res	Type
2	D	420	LEU
2	D	421	ARG
2	D	447	ILE
2	D	450	PHE
2	D	452	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	333	HIS
2	C	477	HIS
2	C	485	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 ⓘ

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	294/336 (87%)	0.09	7 (2%)	59	49	12, 29, 65, 86	0
1	B	293/336 (87%)	0.22	11 (3%)	40	30	15, 31, 68, 97	0
2	C	226/264 (85%)	0.09	3 (1%)	77	72	18, 38, 61, 80	0
2	D	227/264 (85%)	-0.02	7 (3%)	49	39	17, 31, 58, 76	0
All	All	1040/1200 (86%)	0.10	28 (2%)	54	44	12, 32, 64, 97	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	LEU	3.8
1	A	232	GLY	3.6
1	B	311	THR	3.5
1	B	209	LEU	3.5
2	D	261	PRO	3.3
1	A	142	GLY	3.3
1	A	141	GLN	3.0
1	B	308	LEU	2.9
2	C	262	ASN	2.8
1	B	461	PRO	2.8
1	B	196	ALA	2.8
1	A	194	GLU	2.7
2	D	457	ALA	2.7
1	A	312	ALA	2.7
2	C	384	SER	2.6
1	B	205	ASP	2.6
2	D	481	HIS	2.6
2	C	261	PRO	2.6
2	D	262	ASN	2.5
2	D	244	PRO	2.4
1	B	194	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	444	ASP	2.4
2	D	227	ASN	2.2
1	B	145	GLU	2.2
1	B	193	ARG	2.1
1	A	146	GLU	2.1
1	B	318	LEU	2.1
1	A	150	MET	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 monosaccharides in this entry.

6.4   Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	501	1/1	0.97	0.20	10,10,10,10	0
3	MG	D	501	1/1	0.99	0.28	13,13,13,13	0

6.5   Other polymers ⓘ

There are no such residues in this entry.