



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:02 AM GMT

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

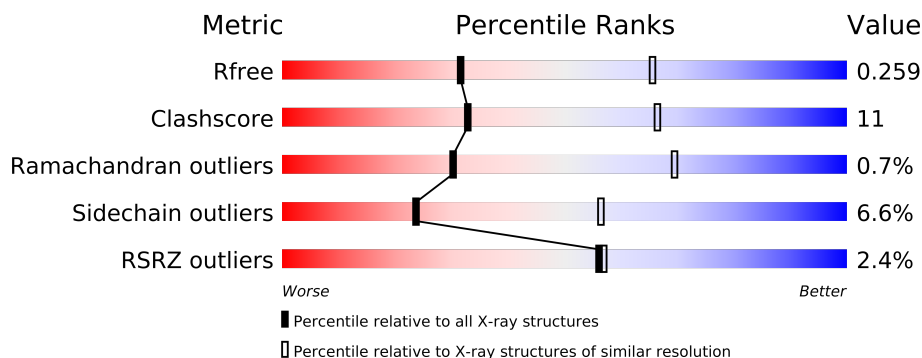
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	336	
1	B	336	
2	C	264	
2	D	264	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	D	501	-	X

2 Entry composition

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

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

- Molecule 1 is a protein called Nuclear 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			

Continued on next page...

Continued from previous page...

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

There are 10 discrepancies between the modelled and reference sequences:

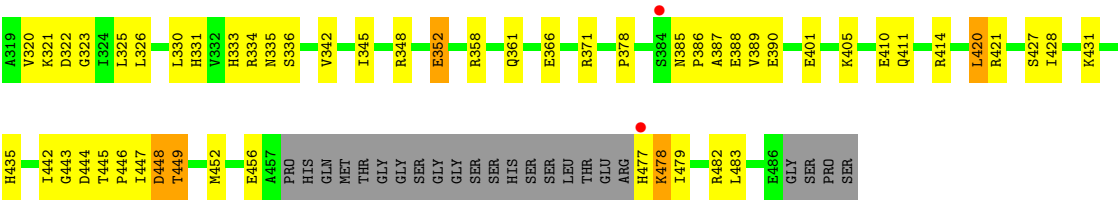
Chain	Residue	Modelled	Actual	Comment	Reference
C	463	GLY	-	LINKER	UNP P19793
C	464	GLY	-	LINKER	UNP P19793
C	465	SER	-	LINKER	UNP P19793
C	466	GLY	-	LINKER	UNP Q15788
C	467	GLY	-	LINKER	UNP Q15788
D	463	GLY	-	LINKER	UNP P19793
D	464	GLY	-	LINKER	UNP P19793
D	465	SER	-	LINKER	UNP P19793
D	466	GLY	-	LINKER	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	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

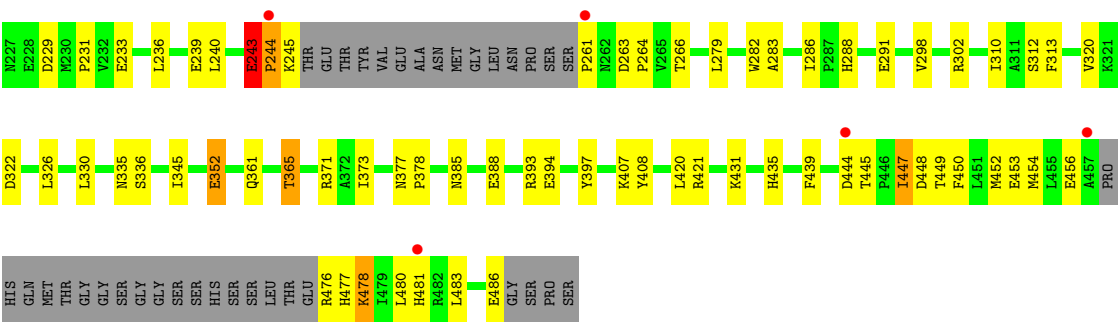
- Molecule 4 is water.

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



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

Chain D:



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
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1061)	Depositor
R, R_{free}	0.250 , 0.298 0.254 , 0.259	Depositor DCC
R_{free} test set	1608 reflections (5.07%)	DCC
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 , 11.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 31748 reflections (0.006%)	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.*

¹Intensities estimated from amplitudes.

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(°)	Ideal(°)
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

Continued on next page...

Continued from previous page...

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

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	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

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 11.

All (190) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:HB2	1:A:216:ARG:HH11	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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:B:352:ASP:OD2	4:B:508:HOH:O	2.15	0.65
1:A:203:ARG:NH1	1:A:232:GLY:HA2	2.12	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:OE1	2:D:486:GLU:N	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:444:ASP:OD1	2:D:445:THR:N	2.37	0.57
2:D:393:ARG:NH2	4:D:610:HOH:O	2.36	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
2:C:442:ILE:HG13	2:C:443:GLY:N	2.24	0.52
1:A:410:ARG:NH1	4:A:550:HOH:O	2.33	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:345:ILE:HD13	2:C:431:LYS:HB3	1.91	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:B:401:ARG:HG2	2:C:427:SER:HB2	1.92	0.51
1:A:211:VAL:HG12	1:A:308:LEU:HD23	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:B:200:SER:O	1:B:204:LYS:HG3	2.11	0.51
1:A:383:GLN:HB2	1:A:384:PRO:HD3	1.92	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:N	1:A:218:GLU:OE1	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
2:C:445:THR:HB	2:C:446:PRO:HD2	1.95	0.49
1:A:316:GLN:HA	1:A:319:LEU:HD12	1.93	0.49
1:A:143:LEU:HB2	1:A:148:ARG:HG3	1.94	0.49
1:A:360:ARG:HG3	1:A:361:VAL:H	1.76	0.49
1:A:216:ARG:NH2	1:A:302:GLY:O	2.46	0.49
2:C:447:ILE:HD12	2:C:449:THR:H	1.77	0.49
2:C:242:VAL:HG21	2:C:282:TRP:HB2	1.95	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
1:A:279:ALA:HB2	1:A:353:ARG:HH12	1.79	0.47
2:D:345:ILE:HD13	2:D:431:LYS:HD3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:213:LEU:HB3	1:A:225:TYR:HB3	1.97	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:D:431:LYS:O	2:D:435:HIS:HD2	1.99	0.46
2:C:410:GLU:HG2	2:C:411:GLN:HG2	1.98	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:B:154:LEU:HD21	1:B:345:ALA:HB2	1.97	0.46
1:A:252:LYS:HE2	1:A:455:LEU:HD22	1.96	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
2:D:240:LEU:O	2:D:244:PRO:HD3	2.16	0.45
1:B:382:PRO:HD2	1:B:386:HIS:CD2	2.51	0.45
2:C:366:GLU:OE2	2:C:414:ARG:NH2	2.48	0.45
1:A:202:VAL:HG13	1:A:414:ILE:HG12	1.98	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
2:C:318:ILE:HD11	2:C:358[A]:ARG:HA	1.99	0.44
1:A:412:LEU:HA	1:A:412:LEU:HD23	1.79	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:406:GLN:HA	1:A:409:GLN:HG2	2.00	0.43
2:D:373:ILE:O	4:D:616:HOH:O	2.21	0.43
2:D:261:PRO:HA	2:D:264:PRO:HD3	2.00	0.43
1:A:282:GLU:HB3	1:A:400:LEU:HD21	1.99	0.43
1:A:217:GLY:N	1:A:221:SER:O	2.50	0.43
1:A:198:LYS:HB3	1:A:198:LYS:HE2	1.58	0.43
1:A:279:ALA:HB1	1:A:283:LEU:HD13	2.00	0.43
1:A:222:VAL:HG13	1:B:226:LYS:HB3	2.01	0.43
1:A:199:TRP:CE3	1:A:417:ILE:HD12	2.53	0.43
1:B:350:SER:HA	1:B:351:PRO:HD3	1.87	0.43
2:C:284:LYS:HD2	2:C:284:LYS:HA	1.90	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:277:PHE:CD1	2:C:483:LEU:HD21	2.53	0.43
1:B:349:PHE:O	1:B:366:GLN:HB2	2.19	0.42
1:B:195:GLU:HA	1:B:198:LYS:HD3	2.00	0.42
1:A:330:LEU:HD13	1:A:396:MET:HG2	2.00	0.42
2:C:345:ILE:HD11	2:C:428:ILE:HG23	2.01	0.42
1:B:460:SER:OG	1:B:461:PRO:HD3	2.19	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:D:477:HIS:NE2	2:D:481:HIS:HB2	2.34	0.42
2:C:326:LEU:HD12	2:C:330:LEU:HB2	2.02	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
2:D:445:THR:HG23	2:D:447:ILE:HD12	2.02	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: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
1:A:201:GLN:NE2	1:A:205:ASP:OD1	2.53	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
2:C:310:ILE:O	2:C:314:SER:HB2	2.20	0.41
2:D:444:ASP:OD1	2:D:445:THR:HG22	2.21	0.41
1:B:317:GLN:HA	1:B:320:LEU:HD13	2.02	0.41
2:C:378:PRO:HG3	2:C:390:GLU:HG3	2.02	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
1:A:236:ILE:HG13	1:A:237:PHE:CD1	2.56	0.41
1:B:254:ILE:HG23	1:B:283:LEU:HD23	2.02	0.41
1:B:145:GLU:OE1	1:B:152:ARG:NH2	2.53	0.41
1:A:329:MET:O	1:A:332:LYS:HG2	2.20	0.41
2:D:229:ASP:O	2:D:231:PRO:HD3	2.20	0.41
2:C:239:GLU:OE2	2:C:282:TRP:NE1	2.54	0.41
2:C:318:ILE:HD12	2:C:318:ILE:HA	1.76	0.41
1:B:407:HIS:CE1	1:B:429:PHE:HE2	2.39	0.41
2:C:477:HIS:HB3	2:C:478:LYS:H	1.64	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:315:PHE:HA	1:A:318:LEU:HG	2.03	0.41
2:D:385:ASN:ND2	2:D:388:GLU:OE1	2.53	0.41
1:A:342:LEU:O	1:A:346:ILE:HG13	2.21	0.41
2:D:394:GLU:HA	2:D:397:TYR:HB3	2.03	0.41
2:D:330:LEU:HA	2:D:330:LEU:HD12	1.85	0.40
1:B:211:VAL:HG12	1:B:308:LEU:HD23	2.02	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

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	287/336 (85%)	270 (94%)	16 (6%)	1 (0%)	50	84
1	B	285/336 (85%)	272 (95%)	12 (4%)	1 (0%)	43	80
2	C	221/264 (84%)	206 (93%)	14 (6%)	1 (0%)	38	76
2	D	222/264 (84%)	209 (94%)	9 (4%)	4 (2%)	13	39
All	All	1015/1200 (85%)	957 (94%)	51 (5%)	7 (1%)	30	69

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%)	21	50
1	B	262/295 (89%)	246 (94%)	16 (6%)	26	61
2	C	197/227 (87%)	184 (93%)	13 (7%)	24	56
2	D	197/227 (87%)	183 (93%)	14 (7%)	21	51
All	All	921/1044 (88%)	859 (93%)	62 (7%)	24	55

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
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

Continued on next page...

Continued from previous page...

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

Some 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	485	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 ⓘ

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.

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, 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%)	0.10	5 (1%) 67 68	12, 29, 65, 86	0
1	B	293/336 (87%)	0.23	11 (3%) 38 38	15, 31, 68, 97	0
2	C	226/264 (85%)	0.13	4 (1%) 65 66	18, 38, 61, 80	0
2	D	227/264 (85%)	0.00	5 (2%) 59 60	17, 31, 58, 76	0
All	All	1040/1200 (86%)	0.12	25 (2%) 56 57	12, 32, 64, 97	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	312	ALA	4.8
1	B	209	LEU	4.2
1	B	311	THR	3.8
2	D	261	PRO	3.8
1	B	319	LEU	3.5
1	A	142	GLY	3.4
1	B	308	LEU	3.3
1	B	207	CYS	3.3
1	B	461	PRO	2.9
1	A	141	GLN	2.9
2	C	261	PRO	2.9
2	C	262	ASN	2.8
2	C	384	SER	2.7
1	A	194	GLU	2.5
2	D	457	ALA	2.5
2	D	244	PRO	2.4
1	B	196	ALA	2.4
2	C	477	HIS	2.3
2	D	481	HIS	2.2
1	A	232	GLY	2.2
1	B	193	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	444	ASP	2.1
1	B	208	SER	2.1
1	B	159	MET	2.0
1	B	210	LYS	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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	D	501	1/1	0.28	5.39	13,13,13,13	0
3	MG	C	501	1/1	0.19	0.65	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.