



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:22 AM UTC

PDB ID : 1G1U / pdb_00001g1u
Title : THE 2.5 ANGSTROM RESOLUTION CRYSTAL STRUCTURE OF THE
RXRALPHA LIGAND BINDING DOMAIN IN TETRAMER IN THE AB-
SENCE OF LIGAND
Authors : Gampe Jr., R.T.; Montana, V.G.; Lambert, M.H.; Wisely, G.B.; Milburn,
M.V.; Xu, H.E.
Deposited on : 2000-10-13
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

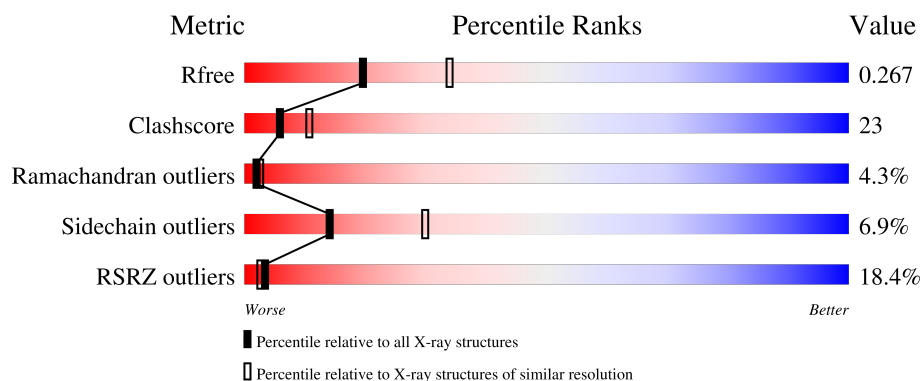
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 $\leq 5\%$. 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	238	
1	B	238	
1	C	238	
1	D	238	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7208 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
1	A	228	Total	C	N	O	S	0	0	0
			1724	1104	301	310	9			
1	B	229	Total	C	N	O	S	0	0	0
			1739	1115	303	312	9			
1	C	226	Total	C	N	O	S	0	0	0
			1704	1093	293	309	9			
1	D	229	Total	C	N	O	S	0	0	0
			1731	1110	301	311	9			

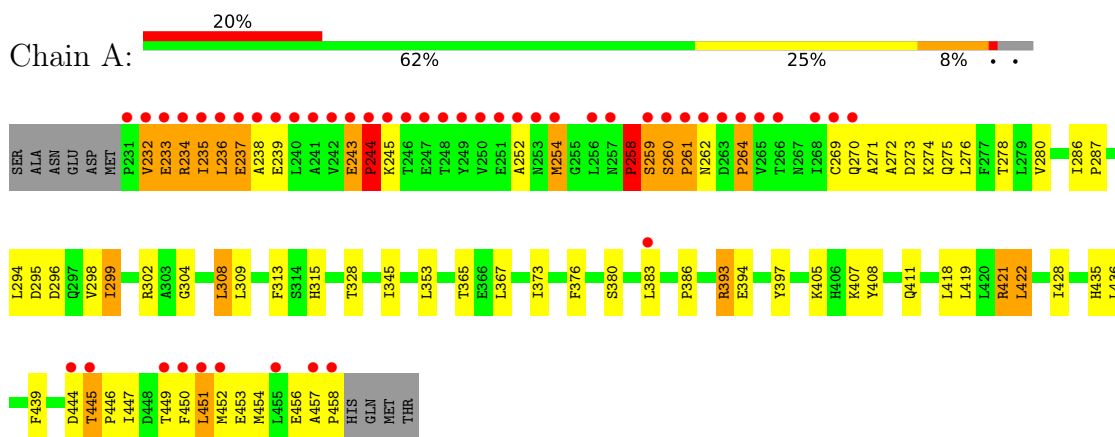
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	85	Total	O	0	0
			85	85		
2	B	98	Total	O	0	0
			98	98		
2	C	59	Total	O	0	0
			59	59		
2	D	68	Total	O	0	0
			68	68		

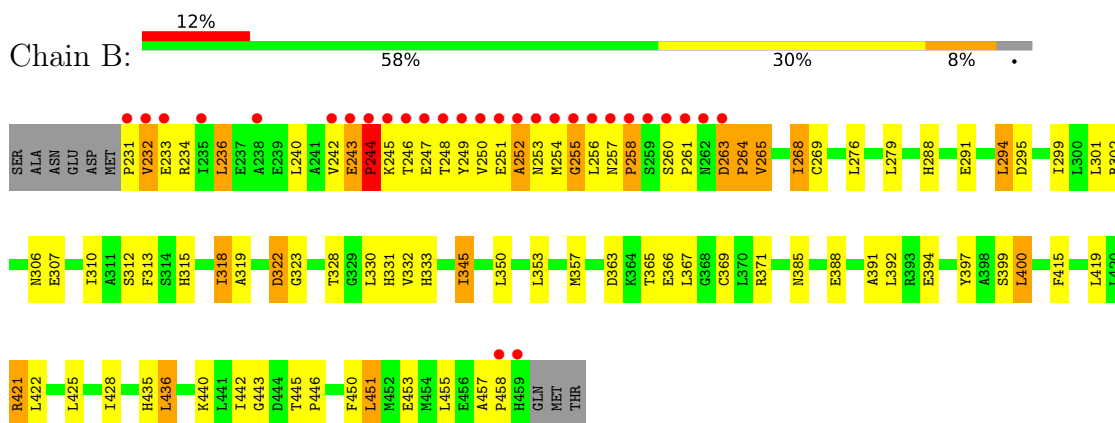
3 Residue-property plots [i](#)

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.

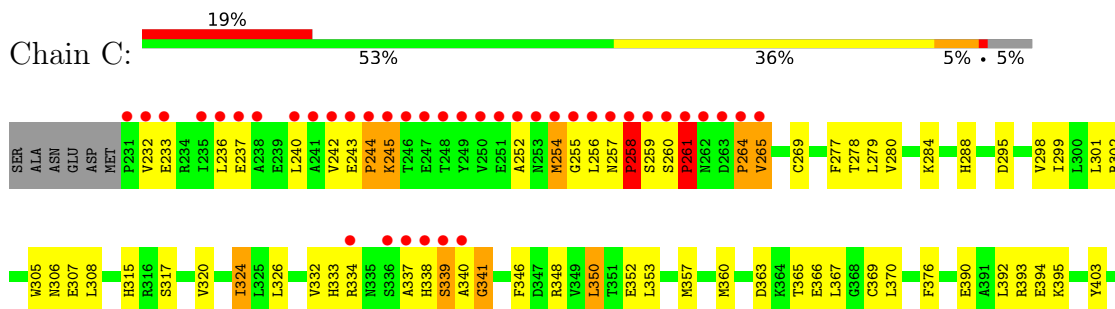
• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

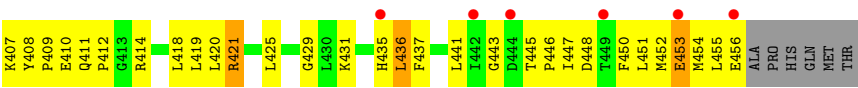


• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA

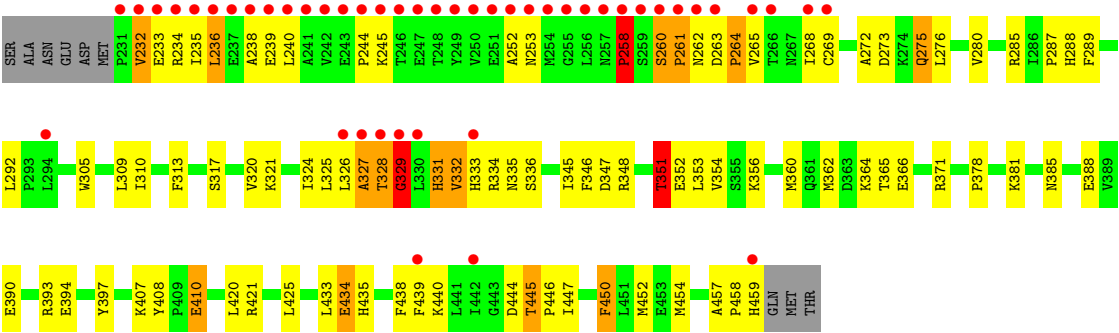


• Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA





● Molecule 1: RETINOIC ACID RECEPTOR RXR-ALPHA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.06Å 99.31Å 94.98Å 90.00° 97.38° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.50) 98.2 (20.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.50Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.220 , 0.271 0.219 , 0.267	Depositor DCC
R_{free} test set	3201 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 67.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7208	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.44	0/1756	1.10	17/2378 (0.7%)
1	B	0.47	0/1773	0.98	8/2403 (0.3%)
1	C	0.46	0/1736	0.96	4/2356 (0.2%)
1	D	0.43	0/1765	1.02	13/2394 (0.5%)
All	All	0.45	0/7030	1.02	42/9531 (0.4%)

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ARG	N-CA-C	-11.15	98.62	114.12
1	A	233	GLU	N-CA-C	-8.71	103.18	112.93
1	A	235	ILE	N-CA-C	-8.68	104.28	112.96
1	A	236	LEU	N-CA-C	-8.67	102.14	112.89
1	D	331	HIS	N-CA-C	7.76	127.34	110.80
1	D	244	PRO	N-CA-CB	7.63	110.11	103.31
1	B	263	ASP	CA-C-N	7.63	129.37	119.84
1	B	263	ASP	C-N-CA	7.63	129.37	119.84
1	A	270	GLN	N-CA-C	-7.61	102.93	111.07
1	A	237	GLU	N-CA-C	-7.11	104.41	113.23
1	B	421	ARG	N-CA-C	-7.07	104.69	113.38
1	B	258	PRO	N-CA-CB	6.79	110.38	103.25
1	B	244	PRO	N-CA-CB	6.71	110.30	103.25
1	C	258	PRO	N-CA-CB	6.70	110.28	103.25
1	A	451	LEU	N-CA-C	-6.67	103.49	111.69
1	D	332	VAL	N-CA-C	6.52	117.99	109.58
1	D	258	PRO	N-CA-CB	6.48	110.05	103.25
1	D	261	PRO	N-CA-CB	6.44	110.01	103.25
1	A	258	PRO	N-CA-CB	6.42	110.00	103.25
1	A	264	PRO	N-CA-CB	6.36	109.93	103.25
1	C	244	PRO	N-CA-CB	6.32	109.88	103.25
1	A	261	PRO	N-CA-CB	6.31	109.87	103.25
1	A	244	PRO	N-CA-CB	6.30	109.87	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	458	PRO	N-CA-CB	6.25	109.88	103.00
1	B	265	VAL	N-CA-C	6.14	117.62	110.62
1	B	261	PRO	N-CA-CB	6.08	109.63	103.25
1	D	351	THR	N-CA-C	5.91	117.39	111.07
1	C	261	PRO	N-CA-CB	5.84	109.38	103.25
1	D	235	ILE	N-CA-C	-5.68	106.17	111.45
1	D	354	VAL	N-CA-C	5.55	115.68	110.30
1	A	421	ARG	N-CA-C	-5.53	106.38	113.23
1	A	411	GLN	CA-C-N	5.20	125.50	119.47
1	A	411	GLN	C-N-CA	5.20	125.50	119.47
1	B	232	VAL	N-CA-C	5.20	115.81	110.36
1	D	385	ASN	CA-C-N	5.17	125.22	119.32
1	D	385	ASN	C-N-CA	5.17	125.22	119.32
1	C	421	ARG	N-CA-C	-5.15	107.17	113.50
1	D	328	THR	N-CA-C	5.14	117.08	108.23
1	A	373	ILE	N-CA-C	-5.12	105.50	110.42
1	D	329	GLY	N-CA-C	5.12	125.31	113.18
1	D	346	PHE	N-CA-C	-5.09	105.81	111.36
1	A	238	ALA	N-CA-C	-5.02	106.66	112.89

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	1724	0	1692	83	0
1	B	1739	0	1719	74	0
1	C	1704	0	1672	98	0
1	D	1731	0	1702	77	0
2	A	85	0	0	1	0
2	B	98	0	0	1	0
2	C	59	0	0	1	0
2	D	68	0	0	1	0
All	All	7208	0	6785	312	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 23.

All (312) 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:C:411:GLN:NE2	1:C:414:ARG:HD2	1.60	1.17
1:C:324:ILE:HD11	1:C:441:LEU:HD21	1.50	0.92
1:C:411:GLN:HE22	1:C:414:ARG:HD2	1.22	0.92
1:A:232:VAL:HG23	1:A:235:ILE:HD12	1.53	0.88
1:D:327:ALA:H	1:D:331:HIS:CE1	1.91	0.87
1:A:233:GLU:HA	1:A:236:LEU:HB3	1.56	0.86
1:C:348:ARG:HD2	1:C:352:GLU:OE2	1.77	0.84
1:A:299:ILE:HD11	1:A:380:SER:HB3	1.59	0.83
1:D:327:ALA:N	1:D:331:HIS:NE2	2.29	0.80
1:A:269:CYS:HG	1:C:269:CYS:HG	1.17	0.79
1:A:235:ILE:HD11	1:A:287:PRO:HD2	1.66	0.77
1:A:273:ASP:CG	1:C:265:VAL:HG22	2.11	0.76
1:A:232:VAL:O	1:A:236:LEU:N	2.19	0.75
1:B:269:CYS:HG	1:D:269:CYS:HG	0.79	0.74
1:D:263:ASP:O	1:D:265:VAL:N	2.21	0.73
1:D:328:THR:N	1:D:331:HIS:NE2	2.38	0.71
1:A:446:PRO:O	1:A:449:THR:HG22	1.90	0.71
1:A:449:THR:HG23	1:A:450:PHE:N	2.07	0.70
1:C:307:GLU:HG2	1:C:425:LEU:HG	1.73	0.70
1:A:273:ASP:OD2	1:C:265:VAL:HG22	1.91	0.70
1:D:435:HIS:O	1:D:440:LYS:HE2	1.92	0.70
1:A:444:ASP:HB2	1:C:302:ARG:HH12	1.57	0.69
1:D:232:VAL:HG12	1:D:233:GLU:OE2	1.93	0.69
1:B:445:THR:HB	1:B:446:PRO:HD3	1.73	0.69
1:C:280:VAL:O	1:C:284:LYS:HG3	1.93	0.68
1:C:332:VAL:HG22	1:C:337:ALA:HB2	1.74	0.68
1:D:325:LEU:O	1:D:326:LEU:HD23	1.93	0.67
1:A:447:ILE:O	1:A:451:LEU:HB2	1.94	0.67
1:C:259:SER:C	1:C:261:PRO:N	2.52	0.67
1:A:295:ASP:O	1:A:299:ILE:HG22	1.94	0.67
1:B:254:MET:O	1:B:256:LEU:N	2.28	0.67
1:A:235:ILE:O	1:A:239:GLU:HG3	1.95	0.66
1:C:243:GLU:O	1:C:245:LYS:N	2.28	0.66
1:A:302:ARG:NH1	1:C:448:ASP:OD1	2.27	0.66
1:B:302:ARG:HH12	1:D:444:ASP:HB2	1.60	0.66
1:B:310:ILE:HG23	1:B:425:LEU:HD11	1.78	0.66
1:D:310:ILE:HA	1:D:313:PHE:CE2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:C	1:B:250:VAL:H	2.04	0.66
1:C:411:GLN:HE21	1:C:414:ARG:HD2	1.55	0.66
1:C:451:LEU:O	1:C:455:LEU:HD23	1.95	0.65
1:C:243:GLU:C	1:C:245:LYS:H	2.04	0.65
1:B:254:MET:O	1:B:257:ASN:N	2.29	0.65
1:A:280:VAL:HG11	1:C:454:MET:HB3	1.78	0.64
1:A:274:LYS:O	1:A:278:THR:HG23	1.97	0.64
1:A:233:GLU:O	1:A:237:GLU:HB2	1.98	0.64
1:A:449:THR:HG23	1:A:450:PHE:H	1.60	0.64
1:C:445:THR:HB	1:C:446:PRO:HD3	1.80	0.64
1:D:252:ALA:O	1:D:328:THR:HG23	1.98	0.63
1:A:235:ILE:HG12	1:A:286:ILE:HD13	1.80	0.63
1:D:268:ILE:HD12	1:D:268:ILE:H	1.64	0.62
1:D:351:THR:HG22	1:D:352:GLU:HG3	1.81	0.62
1:C:252:ALA:C	1:C:254:MET:H	2.08	0.62
1:C:435:HIS:C	1:C:436:LEU:HD12	2.24	0.62
1:A:450:PHE:O	1:A:454:MET:HG3	2.00	0.62
1:C:411:GLN:NE2	1:C:414:ARG:CD	2.52	0.61
1:B:457:ALA:HB1	1:B:458:PRO:HD2	1.83	0.61
1:B:295:ASP:O	1:B:299:ILE:HG12	2.01	0.61
1:D:360:MET:CE	1:D:362:MET:HE3	2.29	0.61
1:B:323:GLY:H	1:B:331:HIS:HE1	1.48	0.61
1:D:239:GLU:OE2	1:D:371:ARG:HD3	2.01	0.61
1:D:390:GLU:O	1:D:394:GLU:HG3	2.00	0.60
1:B:345:ILE:HD13	1:B:345:ILE:O	2.01	0.60
1:C:353:LEU:O	1:C:357:MET:HG3	2.01	0.60
1:C:255:GLY:C	1:C:257:ASN:H	2.09	0.60
1:C:346:PHE:O	1:C:350:LEU:HD22	2.01	0.60
1:C:233:GLU:O	1:C:237:GLU:HG3	2.01	0.59
1:C:288:HIS:CE1	1:C:395:LYS:NZ	2.70	0.59
1:A:299:ILE:CD1	1:A:380:SER:HB3	2.32	0.59
1:A:271:ALA:O	1:A:273:ASP:N	2.35	0.59
1:A:273:ASP:OD1	1:C:264:PRO:HG2	2.03	0.59
1:D:333:HIS:HB2	1:D:335:ASN:OD1	2.03	0.59
1:A:232:VAL:CG2	1:A:235:ILE:HD12	2.27	0.59
1:C:376:PHE:CE1	1:C:392:LEU:HD23	2.38	0.58
1:C:306:ASN:HD21	1:C:429:GLY:C	2.12	0.58
1:D:334:ARG:HG2	1:D:334:ARG:HH11	1.67	0.58
1:D:458:PRO:O	1:D:459:HIS:C	2.46	0.58
1:A:376:PHE:O	1:A:393:ARG:HD3	2.03	0.58
1:C:232:VAL:HG23	1:C:369:CYS:SG	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:VAL:O	1:A:232:VAL:HG13	2.04	0.57
1:A:296:ASP:HA	1:A:299:ILE:CG2	2.33	0.57
1:B:315:HIS:O	1:B:318:ILE:HD12	2.03	0.57
1:D:305:TRP:O	1:D:309:LEU:HD23	2.05	0.57
1:B:391:ALA:O	1:B:394:GLU:HG3	2.06	0.56
1:B:345:ILE:HD11	1:B:428:ILE:HG23	1.88	0.56
1:C:279:LEU:HD21	1:C:305:TRP:HA	1.88	0.56
1:A:243:GLU:O	1:A:244:PRO:C	2.47	0.56
1:D:407:LYS:HG2	1:D:408:TYR:CE1	2.40	0.56
1:B:369:CYS:CB	1:B:400:LEU:HG	2.35	0.55
1:C:393:ARG:HD3	1:D:420:LEU:HD13	1.88	0.55
1:D:253:ASN:HA	1:D:329:GLY:N	2.21	0.55
1:D:328:THR:N	1:D:331:HIS:CE1	2.75	0.55
1:D:332:VAL:HG13	1:D:336:SER:HB2	1.89	0.55
1:A:445:THR:OG1	1:A:446:PRO:HD3	2.06	0.55
1:A:446:PRO:C	1:A:449:THR:HG22	2.30	0.55
1:D:234:ARG:HE	1:D:287:PRO:HG3	1.71	0.54
1:A:383:LEU:HD11	1:A:386:PRO:HG3	1.89	0.54
1:D:234:ARG:NE	1:D:287:PRO:HG3	2.22	0.54
1:C:407:LYS:C	1:C:409:PRO:HD3	2.32	0.54
1:A:252:ALA:HB3	1:A:328:THR:O	2.07	0.54
1:C:324:ILE:HG23	1:C:346:PHE:CZ	2.43	0.54
1:B:310:ILE:HA	1:B:313:PHE:CE2	2.43	0.54
1:D:240:LEU:HD21	1:D:364:LYS:HD2	1.89	0.54
1:D:258:PRO:C	1:D:260:SER:H	2.15	0.54
1:B:315:HIS:O	1:B:318:ILE:HG23	2.07	0.54
1:B:236:LEU:O	1:B:240:LEU:HG	2.08	0.53
1:D:445:THR:N	1:D:446:PRO:CD	2.72	0.53
1:A:302:ARG:HH12	1:C:448:ASP:CG	2.16	0.53
1:B:268:ILE:HD13	1:B:268:ILE:C	2.34	0.53
1:C:324:ILE:HG12	1:C:332:VAL:CG1	2.38	0.53
1:D:275:GLN:HG3	1:D:309:LEU:HD11	1.90	0.53
1:C:298:VAL:O	1:C:302:ARG:HG3	2.09	0.53
1:D:238:ALA:HA	1:D:285:ARG:HE	1.73	0.53
1:D:327:ALA:C	1:D:331:HIS:CE1	2.87	0.53
1:A:436:LEU:N	1:A:436:LEU:HD22	2.24	0.52
1:A:271:ALA:O	1:A:272:ALA:HB3	2.08	0.52
1:D:348:ARG:HD3	1:D:352:GLU:OE2	2.09	0.52
1:B:231:PRO:N	1:B:234:ARG:HD3	2.25	0.52
1:B:233:GLU:CD	1:B:233:GLU:H	2.18	0.52
1:D:236:LEU:C	1:D:236:LEU:HD13	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:HG3	1:A:397:TYR:CZ	2.45	0.52
1:B:385:ASN:O	1:B:388:GLU:HG2	2.10	0.52
1:D:356:LYS:O	1:D:360:MET:HG2	2.09	0.52
1:C:348:ARG:HH21	1:C:431:LYS:HD3	1.75	0.52
1:B:232:VAL:HG23	1:B:399:SER:HB3	1.92	0.52
1:A:269:CYS:O	1:A:271:ALA:O	2.28	0.51
1:B:231:PRO:CD	1:B:234:ARG:HH11	2.22	0.51
1:C:363:ASP:OD1	1:C:366:GLU:HG3	2.09	0.51
1:B:245:LYS:O	1:B:247:GLU:N	2.43	0.51
1:A:232:VAL:HG22	1:A:235:ILE:HB	1.93	0.51
1:A:233:GLU:O	1:A:237:GLU:CB	2.58	0.51
1:A:260:SER:C	1:A:262:ASN:H	2.18	0.51
1:B:268:ILE:HG12	1:B:442:ILE:CD1	2.41	0.51
1:B:330:LEU:HD13	1:B:331:HIS:N	2.26	0.51
1:C:437:PHE:O	1:C:441:LEU:HB2	2.09	0.51
1:C:436:LEU:HD12	1:C:436:LEU:N	2.26	0.51
1:C:255:GLY:C	1:C:257:ASN:N	2.68	0.51
1:C:411:GLN:HE22	1:C:414:ARG:CD	2.07	0.51
1:A:449:THR:CG2	1:A:450:PHE:N	2.73	0.51
1:C:403:TYR:CZ	1:C:407:LYS:HD3	2.45	0.51
1:C:411:GLN:HE22	1:C:414:ARG:HH11	1.60	0.50
1:C:454:MET:HE2	1:C:454:MET:HA	1.93	0.50
1:B:254:MET:O	1:B:255:GLY:C	2.54	0.50
1:B:232:VAL:HG13	1:B:365:THR:HG23	1.93	0.50
1:B:269:CYS:CB	1:D:269:CYS:HG	2.23	0.50
1:B:367:LEU:O	1:B:371:ARG:HG3	2.12	0.50
1:C:257:ASN:O	1:C:259:SER:N	2.44	0.50
1:D:347:ASP:O	1:D:351:THR:HB	2.12	0.50
1:B:276:LEU:O	1:B:279:LEU:HB3	2.10	0.50
1:D:268:ILE:HD12	1:D:268:ILE:N	2.27	0.50
1:B:369:CYS:HB3	1:B:400:LEU:HG	1.94	0.50
1:A:259:SER:O	1:A:260:SER:O	2.30	0.50
1:B:264:PRO:HG3	1:B:450:PHE:CG	2.47	0.49
1:C:324:ILE:HD11	1:C:326:LEU:HD21	1.93	0.49
1:B:363:ASP:OD1	1:B:366:GLU:HG3	2.13	0.49
1:D:360:MET:HE3	1:D:362:MET:HB2	1.94	0.49
1:D:444:ASP:HA	1:D:447:ILE:HD12	1.95	0.49
1:D:450:PHE:CE2	1:D:454:MET:HE3	2.48	0.49
1:A:232:VAL:C	1:A:234:ARG:H	2.20	0.49
1:A:436:LEU:HD12	1:A:439:PHE:CD2	2.47	0.49
1:C:255:GLY:HA2	1:C:259:SER:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD13	1:B:330:LEU:C	2.38	0.48
1:C:259:SER:O	1:C:261:PRO:N	2.46	0.48
1:C:288:HIS:CE1	1:C:395:LYS:HZ3	2.30	0.48
1:A:383:LEU:HD12	1:A:383:LEU:O	2.13	0.48
1:D:326:LEU:HB2	1:D:331:HIS:CD2	2.49	0.48
1:A:280:VAL:HG11	1:C:454:MET:CB	2.44	0.48
1:C:332:VAL:CG2	1:C:337:ALA:HB2	2.43	0.48
1:A:449:THR:CG2	1:A:450:PHE:H	2.24	0.48
1:D:292:LEU:HD12	1:D:388:GLU:OE2	2.12	0.48
1:A:258:PRO:C	1:A:260:SER:H	2.22	0.48
1:B:242:VAL:O	1:B:243:GLU:CB	2.62	0.48
1:C:236:LEU:HD13	1:C:236:LEU:O	2.14	0.48
1:A:234:ARG:HG3	2:A:515:HOH:O	2.13	0.48
1:A:304:GLY:O	1:A:308:LEU:HD22	2.14	0.48
1:A:234:ARG:HA	1:A:237:GLU:HB3	1.96	0.48
1:A:394:GLU:HA	1:A:397:TYR:CE2	2.48	0.48
1:A:452:MET:O	1:A:456:GLU:HB3	2.14	0.48
1:B:248:THR:C	1:B:250:VAL:N	2.69	0.47
1:C:257:ASN:O	1:C:258:PRO:C	2.57	0.47
1:C:338:HIS:O	1:C:340:ALA:N	2.47	0.47
1:B:394:GLU:HA	1:B:397:TYR:CE2	2.48	0.47
1:C:337:ALA:O	1:C:338:HIS:C	2.57	0.47
1:C:411:GLN:HB3	1:C:414:ARG:HB2	1.96	0.47
1:D:287:PRO:O	1:D:288:HIS:HB2	2.14	0.47
1:B:236:LEU:O	1:B:236:LEU:HD22	2.15	0.47
1:B:232:VAL:HG13	1:B:365:THR:CG2	2.45	0.47
1:C:410:GLU:O	1:C:412:PRO:HD3	2.15	0.47
1:A:252:ALA:C	1:A:254:MET:H	2.22	0.47
1:A:259:SER:O	1:A:260:SER:C	2.58	0.47
1:C:333:HIS:O	1:C:337:ALA:HB2	2.14	0.47
1:C:236:LEU:HD13	1:C:236:LEU:C	2.40	0.46
1:B:264:PRO:O	1:B:268:ILE:HG22	2.15	0.46
1:A:380:SER:HB2	1:A:383:LEU:HD23	1.96	0.46
1:D:439:PHE:CE1	1:D:447:ILE:HD11	2.50	0.46
1:B:263:ASP:HA	1:B:264:PRO:HD3	1.74	0.46
1:B:322:ASP:OD2	1:B:333:HIS:HD2	1.99	0.46
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.74	0.46
1:C:236:LEU:HD23	1:C:365:THR:HA	1.98	0.46
1:D:325:LEU:HD12	1:D:331:HIS:CE1	2.51	0.46
1:A:260:SER:O	1:A:262:ASN:N	2.42	0.46
1:B:313:PHE:CD1	1:B:313:PHE:C	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:SER:OG	1:D:324:ILE:HA	2.16	0.46
1:A:436:LEU:HD12	1:A:439:PHE:HD2	1.81	0.45
1:C:242:VAL:O	1:C:243:GLU:C	2.59	0.45
1:B:421:ARG:HA	1:B:421:ARG:NE	2.31	0.45
1:A:422:LEU:HD12	1:A:422:LEU:HA	1.78	0.45
1:B:245:LYS:C	1:B:247:GLU:H	2.24	0.45
1:D:263:ASP:N	1:D:264:PRO:CD	2.80	0.45
1:D:394:GLU:HA	1:D:397:TYR:CE2	2.52	0.45
1:A:232:VAL:HG11	1:A:365:THR:HG23	1.99	0.45
1:A:299:ILE:HD11	1:A:380:SER:CB	2.41	0.45
1:A:345:ILE:HD11	1:A:428:ILE:HG23	1.99	0.45
1:C:288:HIS:CE1	1:C:395:LYS:HZ1	2.33	0.45
1:D:240:LEU:CD2	1:D:364:LYS:HD2	2.47	0.45
1:D:408:TYR:HA	1:D:410:GLU:OE2	2.17	0.45
1:B:265:VAL:HG21	1:D:272:ALA:HB1	1.99	0.45
1:C:447:ILE:O	1:C:451:LEU:HG	2.16	0.45
1:B:236:LEU:C	1:B:236:LEU:HD13	2.41	0.45
1:B:288:HIS:HD2	1:B:291:GLU:OE1	2.00	0.45
1:B:353:LEU:O	1:B:357:MET:HG3	2.17	0.45
1:B:415:PHE:CZ	1:B:419:LEU:HD11	2.52	0.45
1:C:317:SER:O	1:C:320:VAL:HG22	2.17	0.44
1:C:348:ARG:HD3	1:D:381:LYS:NZ	2.32	0.44
1:C:421:ARG:NE	1:C:421:ARG:HA	2.32	0.44
1:A:276:LEU:HG	1:C:450:PHE:HE2	1.82	0.44
1:B:252:ALA:C	1:B:254:MET:N	2.73	0.44
1:B:394:GLU:HA	1:B:397:TYR:CD2	2.53	0.44
1:D:325:LEU:HD12	1:D:331:HIS:ND1	2.32	0.44
1:A:421:ARG:HA	1:A:421:ARG:NE	2.32	0.44
1:C:338:HIS:O	1:C:339:SER:C	2.60	0.44
1:D:236:LEU:HG	1:D:365:THR:OG1	2.18	0.44
1:C:346:PHE:O	1:C:350:LEU:CD2	2.66	0.43
1:C:403:TYR:OH	1:C:407:LYS:HD3	2.18	0.43
1:B:307:GLU:HG2	1:B:425:LEU:HG	2.00	0.43
1:C:338:HIS:C	1:C:340:ALA:N	2.75	0.43
1:C:360:MET:CE	1:C:418:LEU:HD12	2.48	0.43
1:C:408:TYR:N	1:C:409:PRO:HD3	2.33	0.43
1:C:411:GLN:NE2	1:C:414:ARG:HH11	2.15	0.43
1:D:457:ALA:O	1:D:458:PRO:C	2.60	0.43
1:A:232:VAL:C	1:A:235:ILE:H	2.27	0.43
1:A:235:ILE:HD11	1:A:287:PRO:CD	2.41	0.43
1:B:435:HIS:O	1:B:440:LYS:HE2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:LEU:O	1:D:280:VAL:HG23	2.18	0.43
1:C:360:MET:HE1	1:C:418:LEU:HD12	1.99	0.43
1:D:331:HIS:ND1	1:D:331:HIS:N	2.66	0.43
1:D:434:GLU:HG2	1:D:435:HIS:CD2	2.54	0.43
1:A:454:MET:HE2	1:C:277:PHE:CD1	2.54	0.43
1:B:323:GLY:HA3	1:B:332:VAL:O	2.18	0.43
1:C:242:VAL:HG21	1:C:278:THR:O	2.19	0.43
1:C:252:ALA:C	1:C:254:MET:N	2.74	0.43
1:A:296:ASP:O	1:A:299:ILE:HG23	2.19	0.42
1:A:274:LYS:NZ	1:A:275:GLN:HE22	2.18	0.42
1:B:310:ILE:HG23	1:B:425:LEU:CD1	2.48	0.42
1:B:318:ILE:HD13	1:B:319:ALA:N	2.35	0.42
1:A:232:VAL:CG1	1:A:365:THR:HG23	2.49	0.42
1:A:452:MET:O	1:A:456:GLU:CB	2.67	0.42
1:B:318:ILE:HD13	1:B:319:ALA:H	1.84	0.42
1:B:451:LEU:O	1:B:455:LEU:HG	2.19	0.42
1:D:421:ARG:HD2	2:D:524:HOH:O	2.18	0.42
1:C:390:GLU:O	1:C:394:GLU:HG3	2.18	0.42
1:D:439:PHE:HE1	1:D:447:ILE:HD11	1.83	0.42
1:D:457:ALA:HB1	1:D:458:PRO:HD2	2.02	0.42
1:A:258:PRO:C	1:A:260:SER:N	2.76	0.42
1:C:452:MET:O	1:C:456:GLU:HA	2.18	0.42
1:B:245:LYS:C	1:B:247:GLU:N	2.76	0.42
1:A:435:HIS:O	1:A:436:LEU:C	2.63	0.42
1:C:236:LEU:O	1:C:240:LEU:HG	2.19	0.42
1:C:295:ASP:O	1:C:299:ILE:HG13	2.19	0.42
1:B:243:GLU:O	1:B:244:PRO:CB	2.68	0.42
1:C:315:HIS:CG	1:C:367:LEU:HD22	2.55	0.42
1:C:443:GLY:C	1:C:446:PRO:HD2	2.45	0.42
1:D:233:GLU:CD	1:D:233:GLU:H	2.28	0.42
1:D:407:LYS:HB3	1:D:408:TYR:CD1	2.54	0.42
1:B:294:LEU:HD23	1:D:452:MET:SD	2.60	0.42
1:D:328:THR:C	1:D:331:HIS:CE1	2.98	0.42
1:B:252:ALA:O	1:B:254:MET:N	2.53	0.41
1:B:443:GLY:C	1:B:446:PRO:HD2	2.45	0.41
1:C:279:LEU:HD11	1:C:308:LEU:HB3	2.02	0.41
1:C:348:ARG:O	1:C:352:GLU:HB2	2.20	0.41
1:A:407:LYS:HG2	1:A:408:TYR:CE1	2.54	0.41
1:B:306:ASN:O	1:B:310:ILE:HG22	2.20	0.41
1:A:232:VAL:HA	1:A:235:ILE:HB	2.02	0.41
1:B:330:LEU:HD22	2:B:480:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:HIS:O	1:C:341:GLY:N	2.44	0.41
1:C:420:LEU:HD13	1:D:393:ARG:HD3	2.02	0.41
1:D:262:ASN:C	1:D:264:PRO:HD2	2.45	0.41
1:D:233:GLU:CD	1:D:233:GLU:N	2.79	0.41
1:D:236:LEU:O	1:D:236:LEU:HD22	2.20	0.41
1:D:289:PHE:O	1:D:292:LEU:HB2	2.19	0.41
1:D:334:ARG:HG2	1:D:334:ARG:NH1	2.33	0.41
1:A:313:PHE:CD1	1:A:313:PHE:C	2.98	0.41
1:D:324:ILE:O	1:D:331:HIS:HB2	2.20	0.41
1:C:232:VAL:O	1:C:232:VAL:HG22	2.20	0.41
1:C:255:GLY:O	1:C:257:ASN:N	2.54	0.41
1:C:333:HIS:O	1:C:337:ALA:CB	2.68	0.41
1:C:411:GLN:HE22	1:C:414:ARG:NH1	2.18	0.41
1:D:313:PHE:CE2	1:D:438:PHE:HZ	2.39	0.41
1:B:264:PRO:HB2	1:D:273:ASP:OD1	2.21	0.41
1:A:315:HIS:CG	1:A:367:LEU:HD22	2.55	0.41
1:A:450:PHE:HA	1:A:453:GLU:CB	2.51	0.41
1:B:301:LEU:HD23	1:B:301:LEU:HA	1.90	0.41
1:A:299:ILE:HD12	1:A:383:LEU:HB3	2.04	0.40
1:A:383:LEU:CD1	1:A:386:PRO:HG3	2.50	0.40
1:B:310:ILE:HD11	1:B:428:ILE:HG21	2.02	0.40
1:C:453:GLU:O	1:C:456:GLU:HB3	2.21	0.40
1:D:378:PRO:HG3	1:D:390:GLU:OE1	2.22	0.40
1:A:236:LEU:O	1:A:236:LEU:HD13	2.22	0.40
1:A:258:PRO:O	1:A:260:SER:N	2.54	0.40
1:B:249:TYR:HA	1:B:328:THR:C	2.47	0.40
1:C:257:ASN:C	1:C:259:SER:N	2.79	0.40
1:B:435:HIS:O	1:B:436:LEU:HB2	2.21	0.40
1:C:340:ALA:HB1	2:C:496:HOH:O	2.22	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	226/238 (95%)	202 (89%)	14 (6%)	10 (4%)	2	2
1	B	227/238 (95%)	200 (88%)	16 (7%)	11 (5%)	2	2
1	C	224/238 (94%)	193 (86%)	20 (9%)	11 (5%)	1	2
1	D	227/238 (95%)	207 (91%)	13 (6%)	7 (3%)	3	5
All	All	904/952 (95%)	802 (89%)	63 (7%)	39 (4%)	2	2

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	245	LYS
1	A	260	SER
1	A	457	ALA
1	B	243	GLU
1	B	244	PRO
1	B	255	GLY
1	B	264	PRO
1	C	258	PRO
1	C	260	SER
1	C	261	PRO
1	A	244	PRO
1	A	258	PRO
1	B	246	THR
1	B	251	GLU
1	C	244	PRO
1	C	245	LYS
1	C	339	SER
1	D	264	PRO
1	D	327	ALA
1	D	329	GLY
1	A	259	SER
1	B	252	ALA
1	B	258	PRO
1	D	245	LYS
1	A	243	GLU
1	A	254	MET
1	A	264	PRO
1	B	253	ASN
1	B	322	ASP
1	C	256	LEU
1	C	341	GLY
1	D	258	PRO
1	B	260	SER

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Mol	Chain	Res	Type
1	C	334	ARG
1	D	260	SER
1	D	261	PRO
1	C	254	MET
1	C	264	PRO
1	A	261	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/205 (84%)	159 (92%)	13 (8%)	12	26
1	B	176/205 (86%)	164 (93%)	12 (7%)	14	31
1	C	172/205 (84%)	164 (95%)	8 (5%)	23	47
1	D	174/205 (85%)	159 (91%)	15 (9%)	10	21
All	All	694/820 (85%)	646 (93%)	48 (7%)	14	30

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	232	VAL
1	A	294	LEU
1	A	298	VAL
1	A	299	ILE
1	A	308	LEU
1	A	309	LEU
1	A	353	LEU
1	A	393	ARG
1	A	405	LYS
1	A	418	LEU
1	A	419	LEU
1	A	422	LEU
1	A	445	THR
1	B	236	LEU
1	B	268	ILE

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Mol	Chain	Res	Type
1	B	294	LEU
1	B	312	SER
1	B	318	ILE
1	B	345	ILE
1	B	350	LEU
1	B	392	LEU
1	B	400	LEU
1	B	436	LEU
1	B	451	LEU
1	B	453	GLU
1	C	265	VAL
1	C	301	LEU
1	C	324	ILE
1	C	350	LEU
1	C	370	LEU
1	C	419	LEU
1	C	436	LEU
1	C	453	GLU
1	D	232	VAL
1	D	236	LEU
1	D	275	GLN
1	D	320	VAL
1	D	321	LYS
1	D	345	ILE
1	D	351	THR
1	D	353	LEU
1	D	366	GLU
1	D	410	GLU
1	D	425	LEU
1	D	433	LEU
1	D	434	GLU
1	D	445	THR
1	D	450	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	A	275	GLN
1	A	335	ASN
1	A	338	HIS
1	A	406	HIS

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Mol	Chain	Res	Type
1	B	270	GLN
1	B	288	HIS
1	B	297	GLN
1	B	331	HIS
1	B	333	HIS
1	B	335	ASN
1	B	385	ASN
1	C	267	ASN
1	C	270	GLN
1	C	275	GLN
1	C	288	HIS
1	C	297	GLN
1	C	331	HIS
1	C	333	HIS
1	C	411	GLN
1	D	267	ASN
1	D	275	GLN
1	D	333	HIS
1	D	338	HIS
1	D	385	ASN
1	D	435	HIS

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 oligosaccharides 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 ⓘ

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	228/238 (95%)	0.74	47 (20%) 2 2	14, 32, 140, 141	1 (0%)
1	B	229/238 (96%)	0.32	29 (12%) 8 6	14, 28, 121, 139	1 (0%)
1	C	226/238 (94%)	0.94	45 (19%) 3 2	21, 42, 126, 141	0
1	D	229/238 (96%)	0.77	47 (20%) 2 2	17, 39, 131, 134	1 (0%)
All	All	912/952 (95%)	0.69	168 (18%) 3 2	14, 35, 133, 141	3 (0%)

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	VAL	8.8
1	A	238	ALA	8.5
1	C	248	THR	7.6
1	A	235	ILE	7.3
1	C	257	ASN	7.3
1	B	249	TYR	7.2
1	B	262	ASN	6.8
1	B	263	ASP	6.8
1	C	256	LEU	6.7
1	B	253	ASN	6.5
1	A	244	PRO	6.4
1	D	249	TYR	6.3
1	D	248	THR	6.0
1	C	253	ASN	6.0
1	A	240	LEU	6.0
1	C	242	VAL	5.9
1	D	329	GLY	5.9
1	C	254	MET	5.8
1	D	240	LEU	5.7
1	A	246	THR	5.6
1	A	236	LEU	5.6

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Mol	Chain	Res	Type	RSRZ
1	D	234	ARG	5.4
1	B	242	VAL	5.4
1	B	259	SER	5.4
1	B	260	SER	5.3
1	D	232	VAL	5.3
1	C	249	TYR	5.2
1	A	458	PRO	5.2
1	A	260	SER	5.1
1	D	259	SER	5.1
1	D	256	LEU	5.1
1	C	250	VAL	5.0
1	D	235	ILE	5.0
1	C	258	PRO	4.9
1	A	239	GLU	4.9
1	C	243	GLU	4.9
1	B	250	VAL	4.9
1	D	243	GLU	4.7
1	B	254	MET	4.6
1	A	262	ASN	4.6
1	C	244	PRO	4.6
1	A	457	ALA	4.6
1	C	232	VAL	4.6
1	C	261	PRO	4.6
1	A	259	SER	4.5
1	A	231	PRO	4.5
1	C	337	ALA	4.5
1	D	238	ALA	4.5
1	C	260	SER	4.4
1	A	242	VAL	4.3
1	D	231	PRO	4.3
1	B	232	VAL	4.3
1	A	243	GLU	4.3
1	D	242	VAL	4.3
1	D	330	LEU	4.2
1	B	261	PRO	4.2
1	A	250	VAL	4.2
1	D	247	GLU	4.2
1	A	249	TYR	4.1
1	A	268	ILE	4.1
1	A	245	LYS	4.1
1	C	340	ALA	4.1
1	C	251	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	246	THR	4.0
1	D	250	VAL	4.0
1	A	233	GLU	4.0
1	A	252	ALA	4.0
1	C	255	GLY	4.0
1	D	236	LEU	4.0
1	D	260	SER	4.0
1	D	328	THR	4.0
1	C	247	GLU	3.9
1	D	245	LYS	3.9
1	C	252	ALA	3.8
1	C	231	PRO	3.8
1	D	246	THR	3.8
1	A	241	ALA	3.7
1	C	238	ALA	3.7
1	C	246	THR	3.7
1	C	262	ASN	3.6
1	D	251	GLU	3.6
1	B	252	ALA	3.6
1	A	263	ASP	3.6
1	B	255	GLY	3.6
1	A	261	PRO	3.5
1	C	236	LEU	3.5
1	B	251	GLU	3.4
1	A	265	VAL	3.4
1	A	264	PRO	3.4
1	A	450	PHE	3.4
1	A	247	GLU	3.3
1	C	241	ALA	3.3
1	D	254	MET	3.3
1	A	455	LEU	3.3
1	B	248	THR	3.3
1	D	241	ALA	3.3
1	B	247	GLU	3.2
1	A	234	ARG	3.2
1	B	231	PRO	3.2
1	D	239	GLU	3.2
1	A	254	MET	3.2
1	A	266	THR	3.2
1	C	259	SER	3.1
1	D	252	ALA	3.1
1	C	338	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	244	PRO	3.1
1	A	237	GLU	3.1
1	C	233	GLU	3.1
1	D	253	ASN	3.1
1	B	235	ILE	3.1
1	A	444	ASP	3.1
1	B	243	GLU	3.0
1	D	459	HIS	3.0
1	D	233	GLU	3.0
1	C	235	ILE	3.0
1	C	456	GLU	3.0
1	A	445	THR	2.9
1	B	256	LEU	2.9
1	A	270	GLN	2.9
1	A	256	LEU	2.9
1	C	240	LEU	2.9
1	D	265	VAL	2.9
1	C	237	GLU	2.8
1	D	258	PRO	2.8
1	D	266	THR	2.8
1	C	245	LYS	2.8
1	A	248	THR	2.7
1	B	244	PRO	2.7
1	B	257	ASN	2.6
1	B	245	LYS	2.6
1	D	257	ASN	2.5
1	D	262	ASN	2.5
1	C	453	GLU	2.5
1	C	336	SER	2.5
1	A	269	CYS	2.5
1	D	261	PRO	2.5
1	A	257	ASN	2.5
1	A	452	MET	2.5
1	C	444	ASP	2.5
1	B	238	ALA	2.5
1	A	383	LEU	2.4
1	C	339	SER	2.4
1	A	251	GLU	2.4
1	C	263	ASP	2.4
1	B	233	GLU	2.4
1	D	327	ALA	2.4
1	A	451	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	258	PRO	2.3
1	A	449	THR	2.3
1	B	459	HIS	2.3
1	C	265	VAL	2.3
1	D	268	ILE	2.3
1	D	237	GLU	2.3
1	C	435	HIS	2.2
1	D	263	ASP	2.2
1	B	458	PRO	2.2
1	D	255	GLY	2.2
1	D	442	ILE	2.2
1	D	294	LEU	2.2
1	A	253	ASN	2.1
1	C	264	PRO	2.1
1	D	326	LEU	2.1
1	D	333	HIS	2.1
1	D	439	PHE	2.1
1	C	442	ILE	2.1
1	D	269	CYS	2.1
1	C	334	ARG	2.0
1	C	449	THR	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 oligosaccharides 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.