



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:06 AM GMT

PDB ID : 2ZK4
Title : Human peroxisome proliferator-activated receptor gamma ligand binding domain complexed with 15-oxo-eicosatetraenoic acid
Authors : Waku, T.; Shiraki, T.; Oyama, T.; Fujimoto, Y.; Morikawa, K.
Deposited on : 2008-03-12
Resolution : 2.57 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

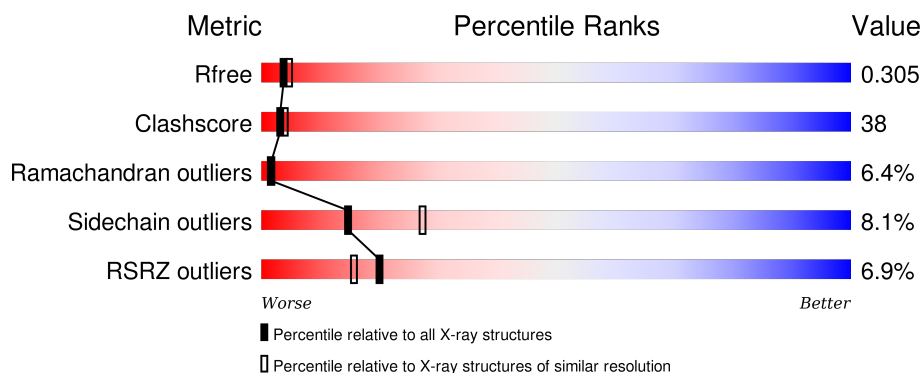
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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. 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	286	
1	B	286	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	OCR	B	2	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4370 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.

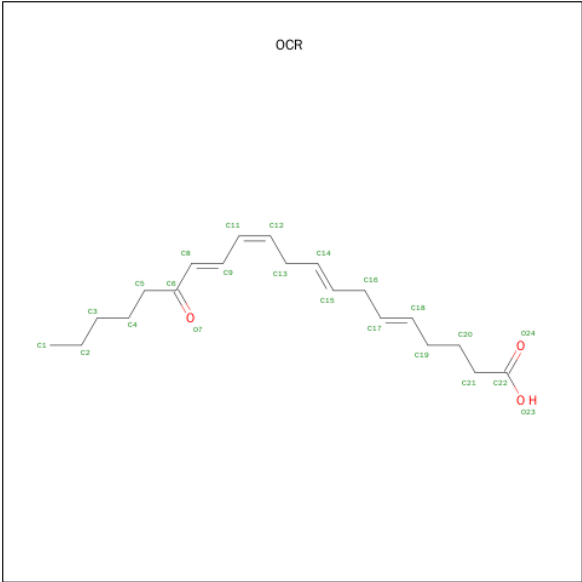
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	0
			2186	1409	358	409	10			
1	B	263	Total	C	N	O	S	0	0	0
			2110	1363	346	392	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	EXPRESSION TAG	UNP P37231
A	192	SER	-	EXPRESSION TAG	UNP P37231
A	193	HIS	-	EXPRESSION TAG	UNP P37231
A	194	MET	-	EXPRESSION TAG	UNP P37231
B	191	GLY	-	EXPRESSION TAG	UNP P37231
B	192	SER	-	EXPRESSION TAG	UNP P37231
B	193	HIS	-	EXPRESSION TAG	UNP P37231
B	194	MET	-	EXPRESSION TAG	UNP P37231

- Molecule 2 is (5E,8E,11Z,13E)-15-OXOICOSA-5,8,11,13-TETRAENOIC ACID (three-letter code: OCR) (formula: C₂₀H₃₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	20	3		
2	B	1	Total	C	O	0	0
			23	20	3		

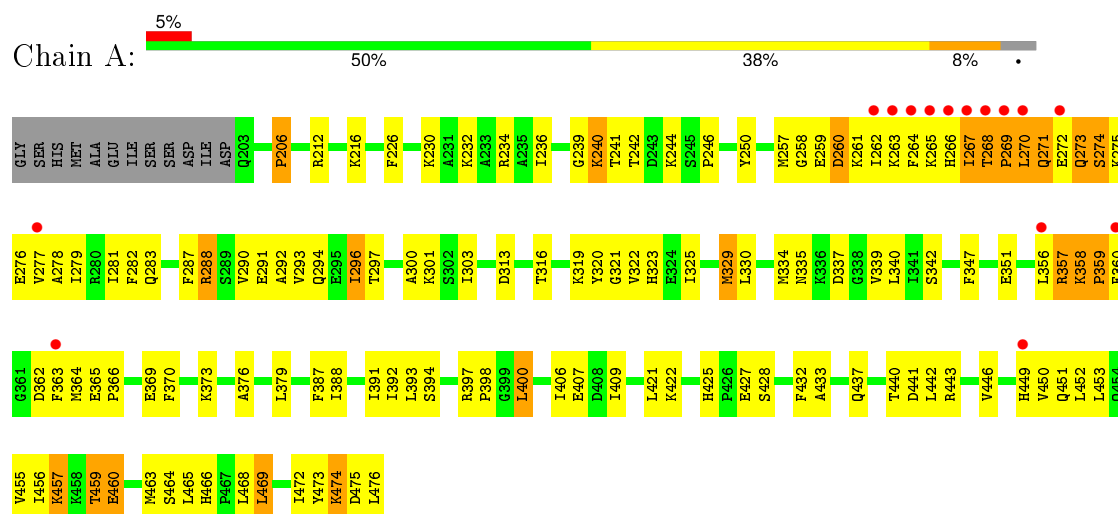
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	11	Total	O	0	0
			11	11		

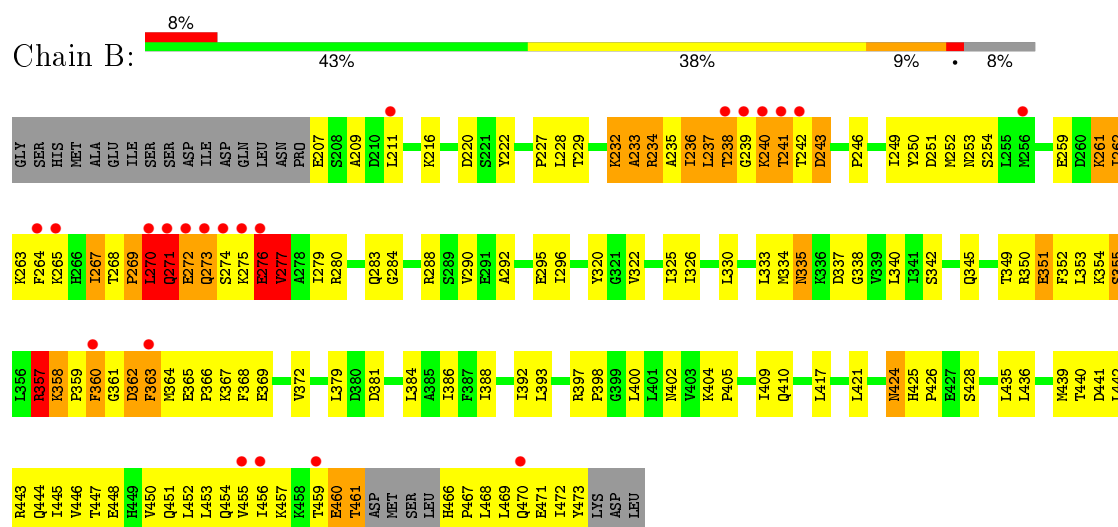
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.35Å 61.17Å 118.60Å 90.00° 102.85° 90.00°	Depositor
Resolution (Å)	32.72 – 2.57 45.97 – 2.57	Depositor EDS
% Data completeness (in resolution range)	93.6 (32.72-2.57) 93.6 (45.97-2.57)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.306 0.245 , 0.305	Depositor DCC
R_{free} test set	947 reflections (4.81%)	DCC
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 54.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 20541 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4370	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: OCR

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	0.47	0/2223	0.68	1/2995 (0.0%)
1	B	0.48	0/2146	0.72	1/2891 (0.0%)
All	All	0.48	0/4369	0.70	2/5886 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	LEU	CA-CB-CG	7.18	131.81	115.30
1	A	206	PRO	N-CA-CB	5.26	109.61	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2186	0	2238	136	0
1	B	2110	0	2173	202	0
2	A	23	0	28	3	0
2	B	23	0	28	0	0
3	A	17	0	0	2	0
3	B	11	0	0	0	0
All	All	4370	0	4467	334	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 38.

All (334) 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:357:ARG:HG2	1:B:358:LYS:H	1.00	1.14
1:A:473:TYR:HA	1:A:476:LEU:HD12	1.37	1.07
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.38	1.05
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.39	1.04
1:B:357:ARG:HH11	1:B:357:ARG:HG3	1.21	1.04
1:A:240:LYS:O	1:A:241:THR:HG23	1.55	1.03
1:A:241:THR:HG21	1:A:244:LYS:HD2	1.40	1.01
1:A:267:ILE:O	1:A:269:PRO:HD3	1.58	1.01
1:A:457:LYS:HA	1:A:457:LYS:NZ	1.78	0.98
1:A:457:LYS:HE3	1:A:465:LEU:HD21	1.43	0.95
1:A:457:LYS:HD2	1:A:465:LEU:HD11	1.49	0.95
1:A:323:HIS:HE1	1:A:472:ILE:HG21	1.29	0.94
1:B:469:LEU:HD23	1:B:472:ILE:HD12	1.50	0.93
1:B:358:LYS:CB	1:B:359:PRO:HD3	1.99	0.93
1:A:271:GLN:HG2	1:A:273:GLN:O	1.69	0.92
1:A:271:GLN:HE21	1:A:274:SER:HB2	1.33	0.91
1:B:357:ARG:NH1	1:B:358:LYS:HG3	1.86	0.90
1:B:357:ARG:HG2	1:B:358:LYS:N	1.82	0.90
1:B:330:LEU:HG	1:B:334:MET:CE	2.02	0.89
1:A:291:GLU:HA	1:A:294:GLN:OE1	1.74	0.87
1:A:363:PHE:HE2	1:A:452:LEU:HB3	1.40	0.87
1:B:357:ARG:HH11	1:B:357:ARG:CG	1.88	0.86
1:B:363:PHE:HD2	1:B:452:LEU:HD22	1.39	0.85
1:B:357:ARG:CG	1:B:358:LYS:H	1.87	0.85
1:A:323:HIS:CE1	1:A:472:ILE:HG21	2.12	0.84
1:B:259:GLU:O	1:B:263:LYS:HA	1.78	0.82
1:B:446:VAL:O	1:B:450:VAL:HG23	1.79	0.82
1:B:274:SER:CA	1:B:280:ARG:HD3	2.10	0.81
1:B:265:LYS:HA	1:B:268:THR:OG1	1.80	0.81
1:A:241:THR:HG21	1:A:244:LYS:CD	2.10	0.81
1:A:283:GLN:HE21	1:A:283:GLN:HA	1.46	0.81
1:B:267:ILE:HG13	1:B:284:GLY:HA2	1.63	0.81
1:A:263:LYS:NZ	1:A:265:LYS:HE3	1.95	0.80
1:B:216:LYS:HE3	1:B:220:ASP:OD1	1.82	0.79
1:B:442:LEU:O	1:B:445:ILE:HG22	1.81	0.79
1:B:274:SER:HA	1:B:280:ARG:HD3	1.65	0.79
1:B:335:ASN:HD22	1:B:335:ASN:C	1.86	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:LYS:HA	1:A:457:LYS:HZ3	1.47	0.78
1:A:268:THR:HG23	1:A:283:GLN:HB2	1.64	0.78
1:B:363:PHE:CD2	1:B:452:LEU:HD22	2.18	0.78
1:A:263:LYS:HZ3	1:A:265:LYS:HE3	1.46	0.77
1:B:330:LEU:HG	1:B:334:MET:HE3	1.66	0.76
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.68	0.76
1:B:280:ARG:HA	1:B:283:GLN:HE21	1.50	0.76
1:B:451:GLN:NE2	1:B:451:GLN:HA	2.01	0.75
1:B:469:LEU:O	1:B:473:TYR:HD2	1.69	0.75
1:B:259:GLU:HB3	1:B:265:LYS:HE2	1.70	0.74
1:B:436:LEU:HA	1:B:439:MET:HE3	1.67	0.74
1:B:452:LEU:O	1:B:456:ILE:HG22	1.87	0.74
1:A:268:THR:HG23	1:A:283:GLN:CB	2.18	0.73
1:B:460:GLU:CD	1:B:460:GLU:H	1.91	0.73
1:B:249:ILE:O	1:B:349:THR:HG22	1.89	0.73
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.24	0.73
1:B:250:TYR:HA	1:B:349:THR:CG2	2.18	0.72
1:A:457:LYS:HA	1:A:457:LYS:HZ2	1.52	0.72
1:A:230:LYS:O	1:A:234:ARG:HG2	1.89	0.72
1:A:357:ARG:HH21	1:A:360:PHE:HE1	1.38	0.72
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.18	0.72
1:A:292:ALA:O	1:A:296:ILE:HD13	1.90	0.72
1:B:351:GLU:OE1	1:B:354:LYS:HE3	1.90	0.71
1:B:330:LEU:HG	1:B:334:MET:HE2	1.73	0.71
1:B:357:ARG:NH1	1:B:357:ARG:HG3	1.98	0.71
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.18	0.71
1:B:270:LEU:HD23	1:B:469:LEU:HD13	1.72	0.71
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.73	0.70
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.72	0.70
1:B:357:ARG:HH11	1:B:358:LYS:HG3	1.55	0.70
1:B:277:VAL:HG13	1:B:280:ARG:NH2	2.07	0.69
1:B:358:LYS:CB	1:B:359:PRO:CD	2.64	0.69
1:B:362:ASP:O	1:B:366:PRO:HD3	1.93	0.69
1:A:288:ARG:HD3	2:A:1:OCR:H2	1.75	0.69
1:A:271:GLN:NE2	1:A:274:SER:HB2	2.07	0.69
1:B:250:TYR:HA	1:B:349:THR:HG21	1.74	0.69
1:B:349:THR:HG23	1:B:352:PHE:HB3	1.75	0.69
1:B:352:PHE:O	1:B:355:SER:HB3	1.93	0.69
1:A:397:ARG:H	1:A:400:LEU:HD12	1.58	0.69
1:A:456:ILE:HA	1:A:459:THR:HG23	1.76	0.68
1:B:456:ILE:HG23	1:B:456:ILE:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:C	1:A:266:HIS:H	1.98	0.68
1:B:277:VAL:HG13	1:B:280:ARG:HH21	1.59	0.67
1:B:234:ARG:O	1:B:238:THR:HG22	1.94	0.67
1:B:335:ASN:ND2	1:B:337:ASP:H	1.93	0.67
1:B:288:ARG:HD2	1:B:288:ARG:O	1.93	0.67
1:A:356:LEU:O	1:A:357:ARG:HB2	1.95	0.66
1:A:400:LEU:HD22	1:A:406:ILE:CD1	2.26	0.66
1:B:330:LEU:O	1:B:334:MET:HG2	1.95	0.66
1:A:363:PHE:CD2	1:A:452:LEU:HD13	2.30	0.66
1:B:452:LEU:H	1:B:452:LEU:HD12	1.60	0.66
1:B:368:PHE:O	1:B:372:VAL:HG23	1.96	0.65
1:A:364:MET:SD	2:A:1:OCR:H11	2.36	0.65
1:B:273:GLN:HG3	1:B:274:SER:N	2.10	0.65
1:A:274:SER:O	1:A:276:GLU:N	2.30	0.65
1:B:263:LYS:C	1:B:265:LYS:H	2.00	0.65
1:B:397:ARG:O	1:B:400:LEU:HG	1.96	0.65
1:A:457:LYS:CD	1:A:465:LEU:HD11	2.24	0.65
1:B:232:LYS:O	1:B:235:ALA:N	2.30	0.65
1:B:267:ILE:HD13	1:B:268:THR:N	2.13	0.64
1:A:260:ASP:O	1:A:261:LYS:HD3	1.98	0.63
1:B:472:ILE:HG22	1:B:472:ILE:O	1.97	0.63
1:A:257:MET:O	1:A:261:LYS:HG2	1.98	0.63
1:A:283:GLN:NE2	1:A:283:GLN:HA	2.12	0.62
1:B:460:GLU:O	1:B:461:THR:HG23	2.00	0.62
1:B:273:GLN:NE2	1:B:280:ARG:HG2	2.15	0.62
1:B:359:PRO:HA	1:B:362:ASP:OD2	2.00	0.61
1:B:242:THR:O	1:B:243:ASP:HB3	2.00	0.61
1:B:436:LEU:HD23	1:B:439:MET:HE3	1.82	0.61
1:B:363:PHE:HE2	1:B:452:LEU:HB2	1.65	0.61
1:B:235:ALA:O	1:B:238:THR:HG23	2.00	0.61
1:B:363:PHE:O	1:B:366:PRO:HD2	2.01	0.61
1:B:388:ILE:O	1:B:392:ILE:HG13	2.00	0.61
1:B:436:LEU:HD23	1:B:439:MET:CE	2.31	0.60
1:B:358:LYS:HE3	1:B:359:PRO:HD3	1.83	0.60
1:B:360:PHE:CE2	1:B:456:ILE:HD11	2.37	0.60
1:B:402:ASN:O	1:B:405:PRO:HD2	2.01	0.60
1:B:325:ILE:HD11	1:B:392:ILE:HG12	1.81	0.60
1:A:277:VAL:HG13	1:A:278:ALA:N	2.16	0.60
1:B:472:ILE:HB	1:B:473:TYR:CE2	2.35	0.60
1:A:464:SER:C	1:A:465:LEU:HD23	2.23	0.60
1:A:425:HIS:HB3	1:A:428:SER:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ALA:O	1:B:296:ILE:HG12	2.03	0.59
1:B:436:LEU:HA	1:B:439:MET:CE	2.31	0.58
1:B:451:GLN:O	1:B:455:VAL:HG23	2.02	0.58
1:A:240:LYS:O	1:A:241:THR:CG2	2.41	0.58
1:B:451:GLN:HE21	1:B:451:GLN:HA	1.67	0.58
1:A:267:ILE:C	1:A:269:PRO:HD3	2.23	0.58
1:B:265:LYS:C	1:B:269:PRO:HD3	2.24	0.58
1:B:242:THR:HG23	1:B:243:ASP:N	2.18	0.58
1:A:334:MET:HG2	1:A:339:VAL:HG23	1.86	0.57
1:B:359:PRO:HD2	1:B:456:ILE:HD13	1.86	0.57
1:B:460:GLU:N	1:B:460:GLU:CD	2.56	0.57
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.34	0.57
1:A:258:GLY:O	1:A:262:ILE:HG12	2.04	0.57
1:B:279:ILE:O	1:B:283:GLN:HG3	2.05	0.57
1:A:232:LYS:O	1:A:236:ILE:HG13	2.05	0.57
1:B:384:LEU:O	1:B:388:ILE:HG12	2.03	0.57
1:A:433:ALA:O	1:A:437:GLN:HG3	2.04	0.56
1:B:335:ASN:HD22	1:B:337:ASP:H	1.52	0.56
1:B:362:ASP:O	1:B:366:PRO:CD	2.53	0.56
1:B:250:TYR:HA	1:B:349:THR:HG22	1.87	0.56
1:B:354:LYS:HD3	1:B:365:GLU:OE2	2.04	0.56
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.87	0.56
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.87	0.56
1:B:270:LEU:CD2	1:B:469:LEU:HD13	2.35	0.56
1:B:273:GLN:CG	1:B:274:SER:H	2.18	0.55
1:B:271:GLN:O	1:B:272:GLU:HG2	2.05	0.55
1:A:262:ILE:HG13	1:A:262:ILE:O	2.06	0.55
1:A:241:THR:HG21	1:A:244:LYS:CG	2.37	0.55
1:A:366:PRO:O	1:A:369:GLU:HB2	2.07	0.55
1:A:455:VAL:O	1:A:459:THR:HG22	2.06	0.55
1:A:370:PHE:CE2	1:A:442:LEU:HD21	2.42	0.55
1:A:267:ILE:CD1	1:A:287:PHE:HD2	2.20	0.54
1:A:323:HIS:HB2	3:A:1001:HOH:O	2.06	0.54
1:A:320:TYR:OH	1:A:398:PRO:HB2	2.08	0.54
1:B:273:GLN:C	1:B:275:LYS:H	2.10	0.54
1:B:459:THR:HG22	1:B:459:THR:O	2.07	0.54
1:B:349:THR:HG23	1:B:352:PHE:CB	2.37	0.54
1:B:264:PHE:O	1:B:268:THR:HG23	2.07	0.54
1:A:290:VAL:HG21	1:A:466:HIS:CD2	2.43	0.54
1:B:280:ARG:HA	1:B:283:GLN:NE2	2.21	0.54
1:A:449:HIS:NE2	1:A:453:LEU:HD11	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.43	0.53
1:B:469:LEU:O	1:B:473:TYR:CD2	2.57	0.53
1:B:358:LYS:HB2	1:B:359:PRO:CD	2.39	0.53
1:B:274:SER:HA	1:B:280:ARG:CD	2.36	0.53
1:A:279:ILE:O	1:A:283:GLN:HG2	2.08	0.53
1:B:443:ARG:O	1:B:447:THR:HG23	2.09	0.53
1:B:466:HIS:CE1	1:B:470:GLN:HG3	2.44	0.53
1:A:363:PHE:HZ	1:A:456:ILE:HG13	1.73	0.53
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.90	0.53
1:B:265:LYS:O	1:B:269:PRO:CG	2.57	0.53
1:A:323:HIS:HE1	1:A:472:ILE:CG2	2.12	0.52
1:A:240:LYS:HG3	1:A:240:LYS:O	2.09	0.52
1:A:457:LYS:HE3	1:A:465:LEU:CD2	2.29	0.52
1:A:366:PRO:HA	1:A:369:GLU:HG3	1.91	0.52
1:A:468:LEU:C	1:A:468:LEU:HD13	2.29	0.52
1:B:246:PRO:HB3	1:B:345:GLN:O	2.09	0.52
1:B:472:ILE:HB	1:B:473:TYR:CD2	2.45	0.52
1:A:443:ARG:HH11	1:B:444:GLN:HE22	1.57	0.52
1:B:275:LYS:O	1:B:276:GLU:HB3	2.09	0.52
1:A:474:LYS:O	1:A:475:ASP:HB2	2.10	0.52
1:B:350:ARG:NH2	1:B:368:PHE:HB3	2.24	0.51
1:B:228:LEU:HD23	1:B:333:LEU:HD21	1.92	0.51
1:A:457:LYS:CE	1:A:465:LEU:HD21	2.28	0.51
1:A:456:ILE:HA	1:A:459:THR:CG2	2.40	0.51
1:A:259:GLU:HG3	1:A:264:PHE:HB2	1.92	0.51
1:B:236:ILE:O	1:B:237:LEU:C	2.49	0.51
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.41	0.51
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.26	0.51
1:A:230:LYS:NZ	1:A:379:LEU:O	2.38	0.51
1:B:273:GLN:CG	1:B:274:SER:N	2.71	0.50
1:B:350:ARG:CZ	1:B:368:PHE:HB3	2.41	0.50
1:A:474:LYS:HE3	1:A:475:ASP:OD1	2.11	0.50
1:B:425:HIS:HB3	1:B:428:SER:OG	2.11	0.50
1:A:446:VAL:O	1:A:449:HIS:HB3	2.11	0.50
1:A:264:PHE:C	1:A:266:HIS:N	2.64	0.50
1:B:261:LYS:HA	1:B:261:LYS:HE3	1.93	0.50
1:B:279:ILE:HD11	1:B:459:THR:CG2	2.42	0.50
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.47	0.50
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.41	0.49
1:B:448:GLU:O	1:B:452:LEU:HD12	2.11	0.49
1:B:335:ASN:C	1:B:335:ASN:ND2	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:HE1	1:A:296:ILE:HD12	1.77	0.49
1:A:277:VAL:CG1	1:A:278:ALA:N	2.75	0.49
1:B:471:GLU:HA	1:B:471:GLU:OE2	2.13	0.49
1:B:466:HIS:C	1:B:468:LEU:N	2.64	0.49
1:A:437:GLN:O	1:A:440:THR:HG23	2.12	0.49
1:B:436:LEU:CD2	1:B:439:MET:HE3	2.43	0.49
1:A:365:GLU:O	1:A:369:GLU:HG2	2.13	0.49
1:B:275:LYS:O	1:B:276:GLU:CB	2.61	0.48
1:B:350:ARG:NH2	1:B:365:GLU:OE1	2.38	0.48
1:A:277:VAL:O	1:A:281:ILE:HG12	2.13	0.48
1:A:357:ARG:O	1:A:359:PRO:N	2.47	0.48
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.13	0.48
1:B:259:GLU:HB3	1:B:265:LYS:CE	2.39	0.48
1:A:330:LEU:O	1:A:334:MET:HG3	2.13	0.48
1:A:443:ARG:NH1	1:B:440:THR:CG2	2.76	0.48
1:A:283:GLN:CA	1:A:283:GLN:HE21	2.14	0.48
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.40	0.48
1:B:232:LYS:O	1:B:234:ARG:N	2.46	0.48
1:A:432:PHE:HB3	3:A:1010:HOH:O	2.13	0.48
1:B:261:LYS:C	1:B:263:LYS:H	2.15	0.48
1:A:443:ARG:NH1	1:B:440:THR:HG21	2.29	0.48
1:A:373:LYS:O	1:A:376:ALA:HB3	2.14	0.48
1:B:452:LEU:O	1:B:453:LEU:C	2.52	0.48
1:B:268:THR:O	1:B:269:PRO:O	2.31	0.48
1:B:404:LYS:HB3	1:B:405:PRO:HD3	1.96	0.48
1:B:357:ARG:NH1	1:B:357:ARG:CG	2.58	0.47
1:B:357:ARG:CG	1:B:358:LYS:N	2.57	0.47
1:B:277:VAL:CG1	1:B:280:ARG:NH2	2.76	0.47
1:B:279:ILE:HG21	1:B:461:THR:HG21	1.96	0.47
1:B:466:HIS:O	1:B:467:PRO:C	2.50	0.47
1:B:232:LYS:O	1:B:233:ALA:C	2.51	0.47
1:B:277:VAL:HA	1:B:280:ARG:HH21	1.79	0.47
1:B:262:ILE:O	1:B:263:LYS:C	2.52	0.47
1:B:269:PRO:O	1:B:270:LEU:HG	2.14	0.47
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.80	0.47
1:B:469:LEU:CD2	1:B:472:ILE:HD12	2.34	0.47
1:B:236:ILE:O	1:B:238:THR:N	2.47	0.46
1:A:319:LYS:HD3	1:A:320:TYR:CE1	2.49	0.46
1:A:236:ILE:HG23	1:A:244:LYS:O	2.15	0.46
1:B:466:HIS:O	1:B:469:LEU:N	2.48	0.46
1:B:251:ASP:O	1:B:254:SER:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:PHE:CE1	1:A:296:ILE:HD12	2.51	0.46
1:B:273:GLN:HG3	1:B:274:SER:H	1.75	0.46
1:B:359:PRO:CD	1:B:456:ILE:HD13	2.45	0.46
1:B:234:ARG:O	1:B:238:THR:CG2	2.61	0.46
1:B:240:LYS:O	1:B:241:THR:C	2.54	0.46
1:B:261:LYS:C	1:B:263:LYS:N	2.69	0.46
1:B:242:THR:HG23	1:B:243:ASP:H	1.81	0.46
1:B:452:LEU:O	1:B:454:GLN:N	2.49	0.46
1:B:469:LEU:HA	1:B:469:LEU:HD23	1.85	0.45
1:B:270:LEU:HD12	1:B:273:GLN:HG2	1.99	0.45
1:A:267:ILE:HD13	1:A:287:PHE:HD2	1.80	0.45
1:A:449:HIS:O	1:A:452:LEU:HB2	2.16	0.45
1:A:268:THR:HG23	1:A:283:GLN:HB3	1.95	0.45
1:B:363:PHE:CE2	1:B:452:LEU:HB2	2.49	0.45
1:B:472:ILE:O	1:B:472:ILE:CG2	2.64	0.45
1:A:313:ASP:HA	1:A:316:THR:HG22	1.99	0.45
1:B:239:GLY:O	1:B:240:LYS:C	2.55	0.45
1:B:242:THR:CG2	1:B:243:ASP:N	2.80	0.45
1:A:425:HIS:HB3	1:A:428:SER:CB	2.46	0.45
1:A:241:THR:CG2	1:A:244:LYS:HD2	2.29	0.45
1:A:250:TYR:CD2	1:A:250:TYR:N	2.84	0.45
1:B:265:LYS:HG3	1:B:268:THR:OG1	2.17	0.45
1:B:445:ILE:CG2	1:B:446:VAL:N	2.80	0.44
1:B:277:VAL:CG1	1:B:280:ARG:HH21	2.25	0.44
1:B:263:LYS:HB2	1:B:263:LYS:HE3	1.75	0.44
1:B:265:LYS:O	1:B:269:PRO:HG2	2.17	0.44
1:A:270:LEU:O	1:A:271:GLN:HB2	2.17	0.44
1:A:272:GLU:O	1:A:273:GLN:HB3	2.18	0.44
1:A:321:GLY:O	1:A:325:ILE:HG13	2.17	0.44
1:B:442:LEU:O	1:B:446:VAL:HG23	2.18	0.44
1:B:393:LEU:HG	1:B:409:ILE:HG22	2.00	0.44
1:B:270:LEU:O	1:B:272:GLU:N	2.50	0.44
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.84	0.44
1:B:259:GLU:O	1:B:265:LYS:HD3	2.17	0.44
1:B:322:VAL:O	1:B:326:ILE:HG13	2.18	0.44
1:A:216:LYS:NZ	1:A:216:LYS:CB	2.81	0.44
1:B:466:HIS:HE1	1:B:470:GLN:HG3	1.82	0.44
1:A:239:GLY:O	1:A:241:THR:N	2.50	0.43
1:B:251:ASP:OD1	1:B:251:ASP:C	2.57	0.43
1:A:363:PHE:HD2	1:A:452:LEU:HD13	1.81	0.43
1:B:350:ARG:HA	1:B:353:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PRO:O	1:B:270:LEU:CG	2.66	0.43
1:B:274:SER:N	1:B:280:ARG:HD3	2.34	0.43
1:B:252:MET:SD	1:B:277:VAL:HG11	2.59	0.43
1:B:239:GLY:O	1:B:242:THR:HG22	2.18	0.43
1:A:274:SER:C	1:A:276:GLU:N	2.72	0.43
1:B:262:ILE:CG1	1:B:264:PHE:HD1	2.32	0.43
1:A:360:PHE:C	1:A:362:ASP:H	2.21	0.42
1:B:436:LEU:O	1:B:439:MET:HB2	2.19	0.42
1:B:263:LYS:C	1:B:265:LYS:N	2.68	0.42
1:B:290:VAL:HG21	1:B:473:TYR:CE1	2.54	0.42
1:B:365:GLU:O	1:B:369:GLU:HG3	2.19	0.42
1:A:290:VAL:O	1:A:294:GLN:HG3	2.20	0.42
1:A:421:LEU:HD12	1:A:432:PHE:HA	2.02	0.42
1:B:359:PRO:O	1:B:361:GLY:N	2.53	0.42
1:B:229:THR:HB	1:B:381:ASP:OD2	2.19	0.42
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.54	0.42
1:B:273:GLN:HA	1:B:276:GLU:OE2	2.19	0.42
1:A:313:ASP:O	1:A:316:THR:HG22	2.20	0.42
1:B:259:GLU:C	1:B:265:LYS:HE2	2.41	0.42
1:B:262:ILE:HG22	1:B:345:GLN:HB3	2.02	0.42
1:B:335:ASN:ND2	1:B:338:GLY:H	2.18	0.41
1:B:386:ILE:HB	1:B:417:LEU:HD13	2.02	0.41
1:A:268:THR:O	1:A:268:THR:HG22	2.19	0.41
1:A:296:ILE:HG13	1:A:325:ILE:HG21	2.02	0.41
1:B:273:GLN:NE2	1:B:280:ARG:CG	2.81	0.41
1:A:300:ALA:O	1:A:303:ILE:HG13	2.19	0.41
1:A:450:VAL:O	1:A:451:GLN:C	2.59	0.41
1:A:342:SER:H	2:A:1:OCR:C22	2.33	0.41
1:B:473:TYR:N	1:B:473:TYR:CD2	2.87	0.41
1:B:242:THR:CG2	1:B:243:ASP:H	2.33	0.41
1:A:297:THR:O	1:A:301:LYS:HG3	2.20	0.41
1:A:457:LYS:CE	1:A:465:LEU:HD11	2.51	0.41
1:A:365:GLU:HB2	1:A:366:PRO:HD3	2.02	0.41
1:B:424:ASN:HB3	1:B:425:HIS:CD2	2.56	0.41
1:B:472:ILE:C	1:B:473:TYR:CD2	2.95	0.41
1:B:379:LEU:HD11	1:B:435:LEU:HD13	2.03	0.41
1:A:357:ARG:NH2	1:A:460:GLU:OE2	2.54	0.40
1:A:464:SER:O	1:A:465:LEU:HD23	2.19	0.40
1:B:274:SER:C	1:B:280:ARG:HD3	2.41	0.40
1:B:425:HIS:O	1:B:426:PRO:C	2.59	0.40
1:A:212:ARG:HA	1:A:212:ARG:HD2	1.72	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:LEU:HB3	1:B:410:GLN:HB2	2.03	0.40
1:A:282:PHE:CE2	1:A:463:MET:HE1	2.57	0.40
1:B:273:GLN:O	1:B:275:LYS:N	2.54	0.40
1:A:262:ILE:O	1:A:263:LYS:C	2.59	0.40
1:B:417:LEU:O	1:B:421:LEU:HG	2.22	0.40
1:A:335:ASN:OD1	1:A:337:ASP:N	2.54	0.40
1:A:351:GLU:HA	1:A:351:GLU:OE2	2.21	0.40
1:A:329:MET:CE	1:A:388:ILE:HG12	2.51	0.40
1:B:292:ALA:O	1:B:295:GLU:HB2	2.21	0.40
1:B:364:MET:CE	1:B:367:LYS:HG3	2.51	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	272/286 (95%)	233 (86%)	25 (9%)	14 (5%)	2	3
1	B	259/286 (91%)	209 (81%)	30 (12%)	20 (8%)	1	1
All	All	531/572 (93%)	442 (83%)	55 (10%)	34 (6%)	2	1

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	275	LYS
1	A	358	LYS
1	B	236	ILE
1	B	237	LEU
1	B	241	THR
1	B	269	PRO
1	B	276	GLU
1	B	357	ARG

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Mol	Chain	Res	Type
1	B	358	LYS
1	A	268	THR
1	A	271	GLN
1	A	357	ARG
1	A	359	PRO
1	B	209	ALA
1	B	232	LYS
1	B	233	ALA
1	B	271	GLN
1	B	272	GLU
1	B	277	VAL
1	B	342	SER
1	B	360	PHE
1	B	460	GLU
1	A	269	PRO
1	A	270	LEU
1	A	273	GLN
1	A	274	SER
1	A	394	SER
1	B	240	LYS
1	A	206	PRO
1	A	400	LEU
1	A	474	LYS
1	B	273	GLN
1	B	355	SER
1	B	227	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	243/257 (95%)	227 (93%)	16 (7%)	21	39
1	B	236/257 (92%)	213 (90%)	23 (10%)	10	18
All	All	479/514 (93%)	440 (92%)	39 (8%)	15	27

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	240	LYS
1	A	242	THR
1	A	246	PRO
1	A	260	ASP
1	A	267	ILE
1	A	288	ARG
1	A	296	ILE
1	A	329	MET
1	A	407	GLU
1	A	422	LYS
1	A	427	GLU
1	A	441	ASP
1	A	457	LYS
1	A	459	THR
1	A	460	GLU
1	A	469	LEU
1	B	207	GLU
1	B	211	LEU
1	B	234	ARG
1	B	238	THR
1	B	243	ASP
1	B	253	ASN
1	B	261	LYS
1	B	262	ILE
1	B	267	ILE
1	B	270	LEU
1	B	271	GLN
1	B	276	GLU
1	B	277	VAL
1	B	335	ASN
1	B	340	LEU
1	B	351	GLU
1	B	357	ARG
1	B	362	ASP
1	B	363	PHE
1	B	424	ASN
1	B	441	ASP
1	B	457	LYS
1	B	461	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	283	GLN
1	A	308	ASN
1	A	430	GLN
1	A	444	GLN
1	A	470	GLN
1	B	217	HIS
1	B	271	GLN
1	B	273	GLN
1	B	283	GLN
1	B	286	GLN
1	B	308	ASN
1	B	335	ASN
1	B	424	ASN
1	B	430	GLN
1	B	444	GLN
1	B	451	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OCR	A	1	1	19,22,22	1.91	1 (5%)	17,23,23	2.43	1 (5%)
2	OCR	B	2	1	19,22,22	2.13	2 (10%)	17,23,23	1.64	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OCR	A	1	1	-	0/19/21/21	0/0/0/0
2	OCR	B	2	1	-	0/19/21/21	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	OCR	C11-C9	3.51	1.54	1.44
2	A	1	OCR	C9-C8	7.72	1.54	1.34
2	B	2	OCR	C9-C8	7.90	1.55	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	OCR	C11-C9-C8	-9.56	103.42	124.66
2	B	2	OCR	C11-C9-C8	-6.33	110.61	124.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	OCR	3	0

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	274/286 (95%)	0.47	15 (5%) 29 24	33, 50, 75, 88	0
1	B	263/286 (91%)	0.59	22 (8%) 14 10	32, 50, 79, 85	0
All	All	537/572 (93%)	0.53	37 (6%) 20 16	32, 50, 78, 88	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	7.1
1	B	274	SER	5.8
1	B	241	THR	5.4
1	A	264	PHE	4.9
1	B	363	PHE	4.8
1	A	267	ILE	4.6
1	A	269	PRO	4.3
1	B	273	GLN	4.2
1	A	363	PHE	4.0
1	B	271	GLN	3.9
1	A	265	LYS	3.8
1	B	459	THR	3.7
1	B	456	ILE	3.7
1	B	276	GLU	3.6
1	B	265	LYS	3.5
1	B	360	PHE	3.2
1	B	270	LEU	3.2
1	A	272	GLU	3.0
1	B	272	GLU	2.9
1	B	239	GLY	2.8
1	B	275	LYS	2.7
1	A	268	THR	2.7
1	B	240	LYS	2.7
1	A	356	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	264	PHE	2.6
1	B	211	LEU	2.5
1	A	360	PHE	2.4
1	A	266	HIS	2.3
1	A	263	LYS	2.3
1	B	238	THR	2.2
1	A	449	HIS	2.2
1	A	262	ILE	2.2
1	B	242	THR	2.1
1	B	256	MET	2.1
1	B	455	VAL	2.1
1	B	470	GLN	2.0
1	A	277	VAL	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	OCR	B	2	23/23	0.82	0.26	2.03	60,64,68,68	0
2	OCR	A	1	23/23	0.80	0.32	1.50	69,72,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.