Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2024 – 04:28 AM EST

PDB ID	:	4JAZ
Title	:	Crystal structure of the complex between PPARgamma LBD and trans-resveratrol
Authors	:	Pochetti, G.; Capelli, D.; Montanari, R.; Calleri, E.; Moaddel, R.; Temporini, C.
Deposited on	:	2013-02-19
Resolution	:	2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

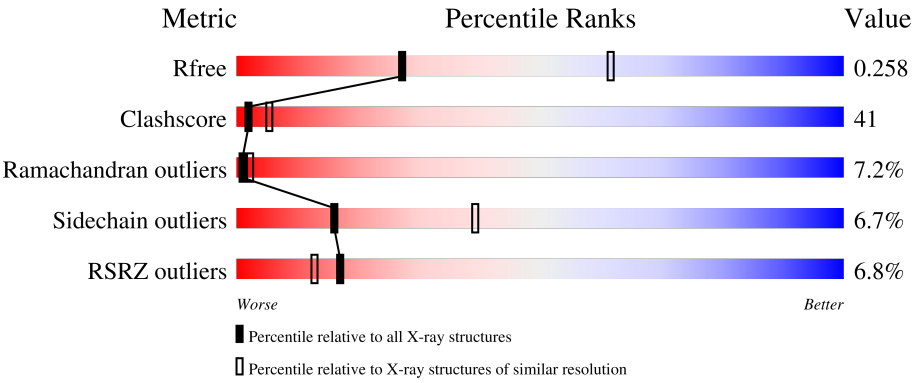
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	287	5% 41% 44% 8% · 7%
1	B	287	8% 40% 43% 9% · 7%

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	STL	A	501	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4438 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.

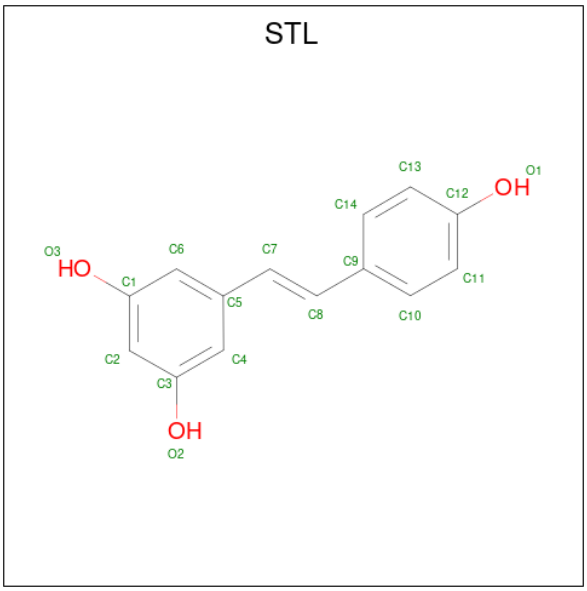
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2149	1387	352	400	10			
1	B	267	Total	C	N	O	S	33	0	0
			2140	1381	350	399	10			

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 RESVERATROL (three-letter code: STL) (formula: $C_{14}H_{12}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 17 14 3	0	0

- Molecule 3 is water.

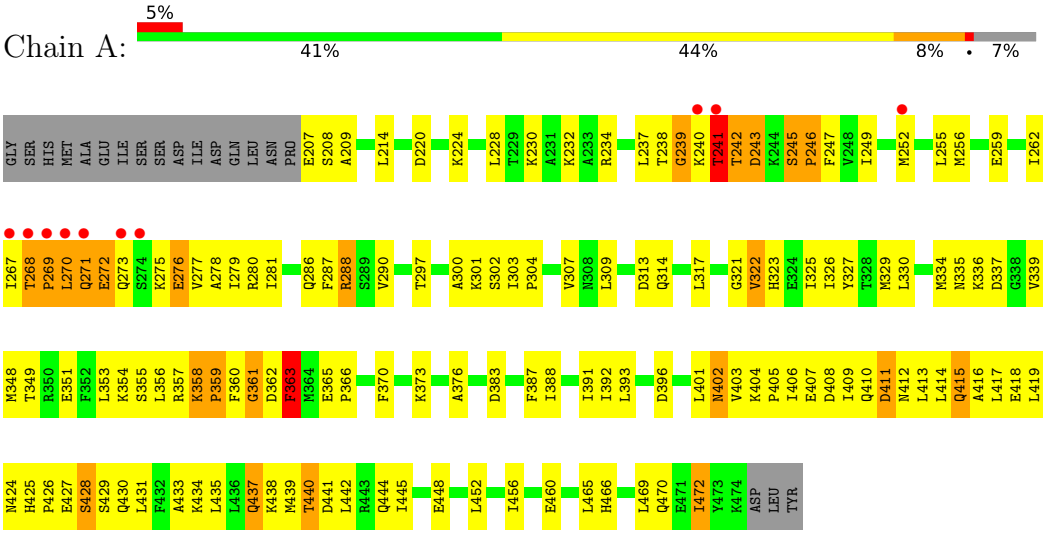
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	65	Total O 65 65	0	0
3	B	67	Total O 67 67	0	0

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.

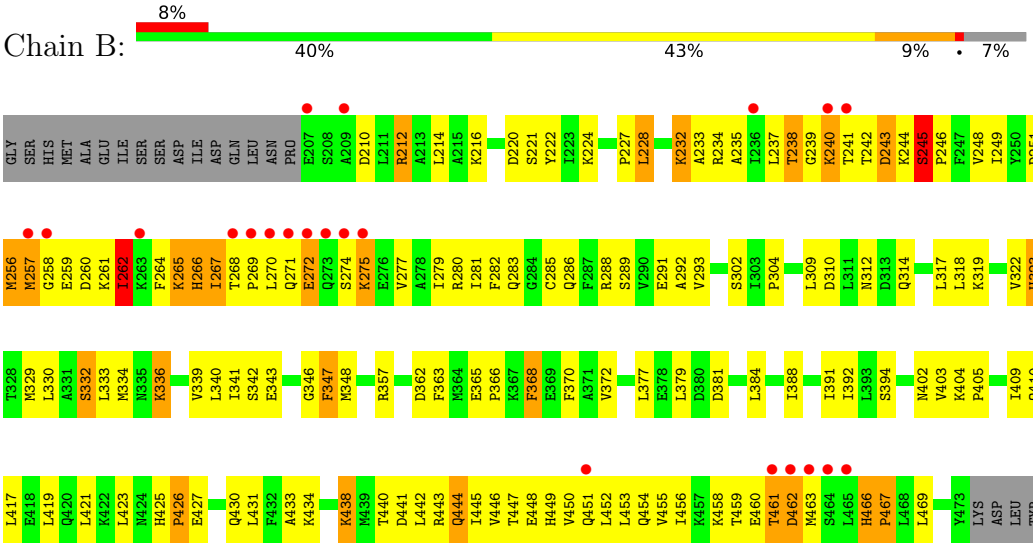
• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain A:



• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.72Å 63.38Å 119.76Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	10.00 – 2.85 26.13 – 2.85	Depositor EDS
% Data completeness (in resolution range)	85.0 (10.00-2.85) 85.1 (26.13-2.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.85Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.264 0.229 , 0.258	Depositor DCC
R_{free} test set	695 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 80.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4438	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0/2186	0.74	4/2945 (0.1%)
1	B	0.63	3/2177 (0.1%)	0.75	2/2934 (0.1%)
All	All	0.55	3/4363 (0.1%)	0.74	6/5879 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	368	PHE	CE2-CZ	-5.54	1.26	1.37
1	B	368	PHE	CA-C	-5.38	1.39	1.52
1	B	368	PHE	C-O	-5.36	1.13	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	245	SER	N-CA-CB	-5.86	101.71	110.50
1	A	241	THR	CA-C-N	-5.75	104.56	117.20
1	A	437	GLN	O-C-N	-5.54	113.84	122.70
1	A	243	ASP	CA-C-N	-5.48	105.15	117.20
1	B	245	SER	CB-CA-C	5.46	120.48	110.10
1	A	440	THR	CA-CB-OG1	-5.31	97.84	109.00

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	2149	0	2217	166	0
1	B	2140	0	2204	193	0
2	A	17	0	11	3	0
3	A	65	0	0	5	0
3	B	67	0	0	13	0
All	All	4438	0	4432	358	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 41.

All (358) 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:266:HIS:CD2	1:B:267:ILE:HG22	1.37	1.55
1:B:329:MET:CE	1:B:329:MET:SD	2.05	1.44
1:B:266:HIS:HD2	1:B:267:ILE:CG2	1.51	1.24
1:B:362:ASP:OD2	1:B:452:LEU:HD11	1.44	1.16
1:B:461:THR:HG22	1:B:462:ASP:N	1.58	1.13
1:B:257:MET:HA	1:B:269:PRO:CB	1.81	1.10
1:B:461:THR:HG22	1:B:462:ASP:H	0.96	1.10
1:B:257:MET:HA	1:B:269:PRO:HB3	1.28	1.08
1:B:261:LYS:O	1:B:262:ILE:HB	1.27	1.08
1:B:265:LYS:O	1:B:266:HIS:ND1	1.85	1.07
1:B:266:HIS:CD2	1:B:267:ILE:CG2	2.28	1.06
1:B:257:MET:CA	1:B:269:PRO:HB3	1.88	1.04
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.04	1.03
1:B:466:HIS:H	1:B:467:PRO:HD2	1.21	1.03
1:B:212:ARG:HB3	1:B:212:ARG:HH11	1.27	0.97
1:B:461:THR:CG2	1:B:462:ASP:H	1.76	0.97
1:B:325:ILE:CD1	1:B:388:ILE:HG23	1.97	0.95
1:B:261:LYS:O	1:B:262:ILE:CB	2.15	0.94
1:B:466:HIS:N	1:B:467:PRO:HD2	1.80	0.92
1:B:262:ILE:HG21	1:B:264:PHE:CZ	2.03	0.91
1:B:282:PHE:CE1	1:B:363:PHE:CZ	2.58	0.91
1:A:286:GLN:NE2	1:A:465:LEU:HD12	1.86	0.90
1:B:362:ASP:CG	1:B:452:LEU:HD11	1.90	0.90
1:B:268:THR:HB	1:B:269:PRO:HD2	1.54	0.89
1:B:262:ILE:CG2	1:B:264:PHE:CZ	2.56	0.89
1:B:362:ASP:OD2	1:B:452:LEU:CD1	2.20	0.89
1:B:461:THR:O	1:B:463:MET:HG3	1.74	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:PHE:HE1	1:B:363:PHE:CZ	1.92	0.87
1:B:212:ARG:HB3	1:B:212:ARG:NH1	1.88	0.87
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.57	0.86
1:B:325:ILE:HD13	1:B:391:ILE:HD12	1.57	0.85
1:B:461:THR:CG2	1:B:462:ASP:N	2.34	0.85
1:B:363:PHE:CD2	3:B:538:HOH:O	2.30	0.84
1:B:362:ASP:CG	1:B:452:LEU:CD1	2.47	0.83
1:B:257:MET:N	1:B:269:PRO:HB3	1.93	0.83
1:B:256:MET:CE	1:B:271:GLN:HB3	2.07	0.83
1:A:439:MET:HA	1:A:442:LEU:HD12	1.59	0.83
1:A:271:GLN:C	1:A:276:GLU:HA	1.98	0.83
1:A:271:GLN:HE21	1:A:277:VAL:H	1.24	0.83
1:A:247:PHE:HB3	1:A:262:ILE:HD11	1.62	0.81
1:A:401:LEU:C	1:A:402:ASN:HD22	1.84	0.81
1:B:368:PHE:O	1:B:372:VAL:HG23	1.81	0.80
1:B:257:MET:CA	1:B:269:PRO:CB	2.54	0.80
1:B:363:PHE:CE2	3:B:538:HOH:O	2.34	0.79
1:A:325:ILE:O	1:A:329:MET:HG3	1.82	0.79
1:A:271:GLN:OE1	1:A:272:GLU:HG2	1.83	0.79
1:B:441:ASP:O	1:B:445:ILE:HG12	1.84	0.78
1:B:256:MET:HE1	1:B:271:GLN:HB3	1.64	0.77
1:A:271:GLN:HB2	1:A:277:VAL:H	1.51	0.75
1:A:363:PHE:HE2	1:A:456:ILE:HD11	1.50	0.75
1:A:370:PHE:HA	1:A:373:LYS:HE2	1.67	0.75
1:B:228:LEU:HD23	1:B:232:LYS:HD3	1.68	0.75
1:A:276:GLU:HG2	1:A:279:ILE:HG12	1.67	0.75
1:A:252:MET:O	1:A:256:MET:HG2	1.87	0.74
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.68	0.74
1:B:362:ASP:OD2	1:B:452:LEU:HD21	1.87	0.74
1:B:257:MET:HA	1:B:269:PRO:CG	2.17	0.73
1:A:419:LEU:HA	1:A:422:LYS:HZ3	1.54	0.73
1:B:253:ASN:HA	1:B:256:MET:HB2	1.73	0.71
1:A:418:GLU:HG2	3:A:642:HOH:O	1.90	0.71
1:B:257:MET:H	1:B:269:PRO:HB3	1.52	0.70
1:B:325:ILE:HD12	1:B:388:ILE:CG2	2.01	0.70
1:B:442:LEU:O	1:B:446:VAL:HG23	1.91	0.70
1:B:410:GLN:HA	1:B:413:LEU:HD12	1.73	0.70
1:B:419:LEU:HD11	1:B:423:LEU:HD11	1.74	0.70
1:B:282:PHE:HD1	1:B:363:PHE:CE2	2.11	0.69
1:A:263:LYS:O	1:A:264:PHE:HD1	1.76	0.69
1:B:267:ILE:HG12	1:B:280:ARG:HE	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:HG23	1:B:264:PHE:CE1	2.28	0.68
1:A:437:GLN:O	1:A:440:THR:HG22	1.94	0.68
1:B:262:ILE:CG2	1:B:264:PHE:CE2	2.76	0.68
1:B:341:ILE:HG22	1:B:342:SER:N	2.08	0.68
1:A:230:LYS:O	1:A:234:ARG:HG2	1.94	0.67
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.76	0.67
1:B:282:PHE:CD1	1:B:363:PHE:CZ	2.82	0.67
1:B:252:MET:O	1:B:256:MET:HG2	1.95	0.67
1:B:430:GLN:O	1:B:434:LYS:HD3	1.95	0.66
1:A:271:GLN:O	1:A:276:GLU:HA	1.95	0.66
1:B:363:PHE:HZ	3:B:518:HOH:O	1.78	0.66
1:A:271:GLN:HB2	1:A:277:VAL:N	2.09	0.66
1:A:214:LEU:HD21	1:A:413:LEU:HD23	1.77	0.66
1:A:271:GLN:NE2	1:A:277:VAL:H	1.93	0.66
1:B:220:ASP:O	1:B:224:LYS:HG2	1.96	0.66
1:A:302:SER:O	1:A:304:PRO:HD3	1.95	0.66
1:B:463:MET:HB2	1:B:466:HIS:CD2	2.32	0.65
1:A:313:ASP:O	1:A:317:LEU:HG	1.96	0.65
1:B:451:GLN:O	1:B:454:GLN:HG2	1.95	0.65
1:A:256:MET:HE1	1:A:269:PRO:O	1.97	0.64
1:B:447:THR:O	1:B:450:VAL:HG22	1.96	0.64
1:B:438:LYS:HB2	1:B:438:LYS:NZ	2.13	0.63
1:B:277:VAL:O	1:B:281:ILE:HG13	1.99	0.63
1:A:440:THR:HB	1:B:440:THR:HG22	1.81	0.63
1:A:388:ILE:HD13	1:A:391:ILE:HD12	1.81	0.63
1:B:330:LEU:HD23	1:B:330:LEU:O	1.99	0.63
1:A:272:GLU:HA	1:A:276:GLU:HB3	1.82	0.62
1:A:262:ILE:HG22	1:A:263:LYS:N	2.15	0.62
1:A:419:LEU:HA	1:A:422:LYS:NZ	2.15	0.62
1:B:257:MET:H	1:B:269:PRO:CB	2.13	0.62
1:B:244:LYS:O	1:B:245:SER:O	2.18	0.61
1:B:212:ARG:HH11	1:B:212:ARG:CB	2.10	0.61
1:A:403:VAL:HG13	1:A:407:GLU:HG3	1.82	0.61
1:A:402:ASN:N	1:A:402:ASN:ND2	2.47	0.61
1:B:341:ILE:HD12	1:B:348:MET:HB2	1.81	0.61
1:B:237:LEU:HG	1:B:340:LEU:HD21	1.83	0.61
1:B:325:ILE:CD1	1:B:391:ILE:HD12	2.30	0.61
1:B:333:LEU:HB3	1:B:340:LEU:HB2	1.83	0.61
1:A:271:GLN:CD	1:A:272:GLU:H	2.03	0.60
1:B:282:PHE:CD1	1:B:363:PHE:CE2	2.89	0.60
1:B:362:ASP:OD2	1:B:452:LEU:CD2	2.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:LEU:HD21	1:B:347:PHE:HE1	1.67	0.60
1:A:241:THR:O	1:A:243:ASP:N	2.33	0.60
1:A:276:GLU:CG	1:A:279:ILE:HG12	2.30	0.60
1:B:243:ASP:OD1	1:B:243:ASP:N	2.34	0.59
1:A:238:THR:C	1:A:240:LYS:H	2.05	0.59
1:A:252:MET:CE	1:A:271:GLN:HG2	2.32	0.59
1:A:419:LEU:O	1:A:423:LEU:HG	2.02	0.59
1:B:412:ASN:C	1:B:412:ASN:HD22	2.04	0.59
1:B:466:HIS:N	1:B:467:PRO:CD	2.62	0.59
1:A:264:PHE:C	1:A:266:HIS:H	2.06	0.59
1:A:242:THR:O	1:A:242:THR:HG22	2.02	0.59
1:B:262:ILE:HG21	1:B:264:PHE:CE2	2.37	0.59
1:A:268:THR:HB	1:A:269:PRO:CD	2.33	0.59
1:A:403:VAL:CG1	1:A:407:GLU:HG3	2.32	0.59
1:B:267:ILE:HD12	1:B:268:THR:H	1.68	0.59
1:A:277:VAL:HA	1:A:280:ARG:HD3	1.84	0.58
1:B:233:ALA:O	1:B:237:LEU:HB2	2.03	0.58
1:A:263:LYS:HD3	1:A:263:LYS:C	2.23	0.58
1:B:216:LYS:HD2	3:B:506:HOH:O	2.02	0.58
1:B:271:GLN:HA	1:B:271:GLN:HE21	1.69	0.58
1:A:271:GLN:HE21	1:A:277:VAL:N	1.99	0.58
1:B:365:GLU:N	1:B:366:PRO:HD2	2.19	0.58
1:A:262:ILE:HG22	1:A:263:LYS:H	1.68	0.58
1:A:276:GLU:OE2	1:A:357:ARG:HD2	2.04	0.58
1:A:270:LEU:HD13	1:A:271:GLN:N	2.18	0.58
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.86	0.58
1:B:257:MET:N	1:B:269:PRO:CB	2.64	0.57
1:A:268:THR:HB	1:A:269:PRO:HD3	1.86	0.57
1:A:349:THR:HG22	1:A:351:GLU:H	1.68	0.57
1:B:363:PHE:CZ	3:B:518:HOH:O	2.52	0.57
1:A:271:GLN:NE2	1:A:272:GLU:N	2.52	0.57
1:A:440:THR:O	1:A:444:GLN:HG2	2.03	0.57
1:A:307:VAL:HA	1:A:314:GLN:OE1	2.05	0.57
1:A:243:ASP:HB2	3:A:606:HOH:O	2.04	0.56
1:A:365:GLU:N	1:A:366:PRO:HD2	2.20	0.56
1:B:237:LEU:HD21	1:B:347:PHE:CE1	2.40	0.56
1:B:257:MET:HA	1:B:269:PRO:HG3	1.85	0.56
1:B:286:GLN:O	1:B:289:SER:HB2	2.06	0.56
1:B:334:MET:HG2	1:B:339:VAL:HB	1.88	0.56
1:B:237:LEU:O	1:B:239:GLY:O	2.23	0.56
1:B:362:ASP:OD1	1:B:452:LEU:HD13	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:VAL:HG12	1:A:323:HIS:N	2.21	0.56
1:A:402:ASN:HD22	1:A:402:ASN:N	1.99	0.56
1:A:326:ILE:HG22	1:A:327:TYR:CD1	2.41	0.56
1:B:256:MET:C	1:B:258:GLY:H	2.09	0.56
1:B:266:HIS:CD2	1:B:267:ILE:N	2.73	0.56
1:B:289:SER:O	1:B:293:VAL:HG23	2.06	0.56
1:B:362:ASP:O	1:B:366:PRO:CD	2.54	0.56
1:A:413:LEU:O	1:A:416:ALA:HB3	2.06	0.55
1:B:384:LEU:O	1:B:388:ILE:HG13	2.07	0.55
1:A:271:GLN:HE22	1:A:276:GLU:HB2	1.72	0.55
1:A:387:PHE:O	1:A:391:ILE:HG13	2.06	0.55
1:B:362:ASP:CG	1:B:452:LEU:HD13	2.25	0.55
1:A:278:ALA:HB2	1:A:356:LEU:HD22	1.87	0.55
1:A:326:ILE:HG22	1:A:327:TYR:HD1	1.71	0.55
1:B:341:ILE:HG22	1:B:342:SER:H	1.70	0.55
1:B:444:GLN:O	1:B:448:GLU:HG3	2.07	0.55
1:A:401:LEU:C	1:A:402:ASN:ND2	2.56	0.55
1:A:417:LEU:O	1:A:421:LEU:HG	2.07	0.55
1:B:265:LYS:O	1:B:266:HIS:CG	2.59	0.54
1:A:272:GLU:HA	1:A:276:GLU:CB	2.37	0.54
1:A:262:ILE:HD13	1:A:346:GLY:HA3	1.90	0.54
1:B:282:PHE:HE1	1:B:363:PHE:HZ	1.52	0.54
1:A:288:ARG:O	1:A:288:ARG:HD3	2.08	0.54
1:A:410:GLN:C	1:A:412:ASN:H	2.12	0.54
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.88	0.54
1:B:404:LYS:HB3	1:B:405:PRO:CD	2.38	0.54
1:B:267:ILE:HG13	1:B:268:THR:N	2.24	0.53
1:A:435:LEU:O	1:A:438:LYS:HB2	2.09	0.53
1:B:266:HIS:CD2	1:B:267:ILE:H	2.27	0.53
1:B:262:ILE:CG2	1:B:264:PHE:CE1	2.89	0.53
1:A:393:LEU:O	1:A:410:GLN:HB2	2.08	0.53
1:B:460:GLU:O	1:B:461:THR:HB	2.08	0.53
1:A:334:MET:HG2	1:A:339:VAL:HB	1.91	0.52
1:B:232:LYS:HD2	3:B:534:HOH:O	2.08	0.52
1:A:271:GLN:NE2	1:A:276:GLU:HB2	2.25	0.52
1:A:290:VAL:HG11	1:A:466:HIS:CG	2.45	0.52
1:B:214:LEU:CD1	1:B:304:PRO:HG2	2.39	0.52
1:B:270:LEU:O	1:B:280:ARG:NH1	2.43	0.52
1:B:330:LEU:HD22	1:B:334:MET:SD	2.50	0.51
1:A:440:THR:HG23	1:A:441:ASP:N	2.24	0.51
1:B:279:ILE:O	1:B:283:GLN:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LYS:HB3	1:B:336:LYS:NZ	2.26	0.51
1:A:300:ALA:HA	1:A:303:ILE:HD12	1.92	0.51
1:A:263:LYS:O	1:A:263:LYS:HD3	2.11	0.51
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.92	0.51
1:B:341:ILE:CG2	1:B:342:SER:N	2.73	0.51
1:A:271:GLN:CG	1:A:272:GLU:H	2.23	0.50
1:A:301:LYS:HA	1:A:307:VAL:CG1	2.41	0.50
1:A:430:GLN:O	1:A:434:LYS:HG3	2.11	0.50
1:A:349:THR:HG22	1:A:351:GLU:N	2.27	0.50
1:B:271:GLN:HA	1:B:271:GLN:NE2	2.27	0.50
1:B:329:MET:O	1:B:332:SER:HB2	2.12	0.50
1:B:362:ASP:O	1:B:366:PRO:HD2	2.11	0.50
1:A:335:ASN:O	1:A:337:ASP:N	2.45	0.50
1:B:310:ASP:OD2	1:B:312:ASN:HB2	2.11	0.50
1:B:402:ASN:O	1:B:405:PRO:HG2	2.12	0.50
1:A:417:LEU:HD21	1:A:435:LEU:HD23	1.93	0.50
1:A:428:SER:OG	1:A:431:LEU:HB2	2.12	0.50
1:B:237:LEU:O	1:B:238:THR:C	2.50	0.50
1:B:228:LEU:HD23	1:B:232:LYS:CD	2.41	0.50
1:A:325:ILE:HG23	1:A:388:ILE:CD1	2.40	0.50
1:A:288:ARG:HG3	2:A:501:STL:C2	2.42	0.50
1:B:240:LYS:O	1:B:241:THR:C	2.50	0.50
1:B:403:VAL:O	1:B:404:LYS:C	2.50	0.49
1:B:266:HIS:CG	1:B:267:ILE:N	2.80	0.49
1:B:325:ILE:HD11	1:B:391:ILE:HB	1.94	0.49
1:B:409:ILE:O	1:B:413:LEU:HG	2.12	0.49
1:A:256:MET:HE3	1:A:269:PRO:HA	1.94	0.49
1:A:363:PHE:HE2	1:A:456:ILE:CD1	2.24	0.49
1:A:363:PHE:CE2	1:A:452:LEU:HD22	2.47	0.49
1:A:271:GLN:CD	1:A:272:GLU:N	2.66	0.49
1:A:276:GLU:HG2	1:A:279:ILE:CG1	2.41	0.49
1:A:238:THR:O	1:A:240:LYS:N	2.45	0.49
1:A:252:MET:HE2	1:A:271:GLN:HG2	1.94	0.49
1:B:256:MET:C	1:B:258:GLY:N	2.67	0.48
1:B:325:ILE:O	1:B:329:MET:HG3	2.14	0.48
1:B:377:LEU:HD22	1:B:431:LEU:HD11	1.94	0.48
1:A:412:ASN:HA	1:A:415:GLN:HG3	1.95	0.48
1:A:268:THR:H	1:A:269:PRO:HD2	1.79	0.48
1:B:341:ILE:CG2	1:B:342:SER:H	2.27	0.48
1:B:377:LEU:HD22	1:B:431:LEU:CD1	2.44	0.48
1:A:370:PHE:HA	1:A:373:LYS:CE	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:LEU:HD11	1:A:409:ILE:HD12	1.94	0.48
1:A:448:GLU:O	1:A:452:LEU:HB2	2.12	0.48
1:B:319:LYS:HD2	3:B:532:HOH:O	2.12	0.48
1:B:327:TYR:HE1	3:B:525:HOH:O	1.97	0.48
1:A:259:GLU:HA	1:A:264:PHE:HB2	1.95	0.48
1:A:287:PHE:O	1:A:290:VAL:HG22	2.13	0.48
1:A:309:LEU:HD13	1:A:406:ILE:HG12	1.96	0.48
1:B:438:LYS:HB2	1:B:438:LYS:HZ3	1.77	0.48
1:B:459:THR:HG22	3:B:566:HOH:O	2.14	0.48
1:A:277:VAL:HG13	1:A:278:ALA:N	2.28	0.48
1:A:207:GLU:HG3	1:A:209:ALA:HB3	1.95	0.47
1:B:417:LEU:O	1:B:421:LEU:HG	2.14	0.47
1:A:220:ASP:OD2	1:A:224:LYS:HE3	2.15	0.47
1:B:330:LEU:O	1:B:334:MET:HG3	2.15	0.47
1:B:461:THR:HA	3:B:552:HOH:O	2.15	0.47
1:B:425:HIS:N	1:B:426:PRO:CD	2.77	0.47
1:A:252:MET:HE1	1:A:271:GLN:HG2	1.97	0.47
1:A:267:ILE:O	1:A:280:ARG:CZ	2.63	0.47
1:A:465:LEU:HD23	1:A:470:GLN:CG	2.45	0.46
1:B:343:GLU:HB2	3:B:519:HOH:O	2.15	0.46
1:B:402:ASN:OD1	1:B:405:PRO:HD2	2.15	0.46
1:A:245:SER:OG	1:A:246:PRO:HD2	2.15	0.46
1:B:246:PRO:HB2	1:B:346:GLY:O	2.16	0.46
1:B:248:VAL:HG12	1:B:249:ILE:N	2.31	0.46
1:A:373:LYS:O	1:A:376:ALA:HB3	2.16	0.46
1:B:323:HIS:HD2	1:B:327:TYR:HE2	1.64	0.46
1:A:220:ASP:O	1:A:224:LYS:HG3	2.16	0.46
1:A:340:LEU:HD23	1:A:347:PHE:HD1	1.80	0.46
1:A:348:MET:SD	1:A:353:LEU:HD21	2.56	0.46
1:A:363:PHE:CE2	1:A:456:ILE:HD11	2.39	0.45
1:A:268:THR:HB	3:A:627:HOH:O	2.16	0.45
1:B:336:LYS:NZ	1:B:336:LYS:CB	2.80	0.45
1:A:383:ASP:OD2	1:A:424:ASN:ND2	2.49	0.45
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.98	0.45
2:A:501:STL:H8	3:A:616:HOH:O	2.17	0.45
1:B:256:MET:HE2	1:B:271:GLN:HB3	1.94	0.45
1:B:288:ARG:O	1:B:291:GLU:HB2	2.15	0.45
1:B:253:ASN:CA	1:B:256:MET:HB2	2.45	0.45
1:A:419:LEU:HD13	1:A:422:LYS:HZ3	1.82	0.45
1:A:408:ASP:HB3	3:A:622:HOH:O	2.17	0.45
1:B:237:LEU:O	1:B:239:GLY:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HD23	1:B:384:LEU:HD23	1.99	0.44
1:A:263:LYS:C	1:A:264:PHE:HD1	2.21	0.44
1:B:336:LYS:HB3	1:B:336:LYS:HZ3	1.82	0.44
1:A:321:GLY:O	1:A:325:ILE:HG13	2.17	0.44
1:B:242:THR:O	1:B:242:THR:HG23	2.16	0.44
1:B:293:VAL:HG22	1:B:322:VAL:CG2	2.47	0.44
1:B:288:ARG:NH1	1:B:292:ALA:HB2	2.31	0.44
1:A:419:LEU:O	1:A:419:LEU:HD12	2.17	0.44
1:A:427:GLU:O	1:A:429:SER:N	2.50	0.44
1:B:370:PHE:CZ	1:B:442:LEU:HD21	2.52	0.44
1:B:265:LYS:H	1:B:265:LYS:HD2	1.83	0.44
1:B:274:SER:O	1:B:275:LYS:O	2.36	0.44
1:B:330:LEU:O	1:B:330:LEU:CD2	2.65	0.44
1:B:463:MET:HB2	1:B:466:HIS:HD2	1.81	0.43
1:A:255:LEU:O	1:A:259:GLU:OE2	2.36	0.43
1:A:360:PHE:O	1:A:361:GLY:C	2.57	0.43
1:A:410:GLN:HE21	1:A:414:LEU:HD11	1.83	0.43
1:B:238:THR:O	1:B:239:GLY:C	2.57	0.43
1:B:268:THR:HB	1:B:269:PRO:CD	2.36	0.43
1:B:379:LEU:HD23	1:B:384:LEU:CD2	2.48	0.43
1:B:451:GLN:O	1:B:455:VAL:HG23	2.19	0.43
1:A:270:LEU:HD12	1:A:273:GLN:HB2	2.00	0.43
1:B:267:ILE:CG1	1:B:268:THR:N	2.80	0.43
1:B:453:LEU:O	1:B:456:ILE:HB	2.18	0.43
1:B:456:ILE:C	1:B:458:LYS:N	2.71	0.43
1:A:207:GLU:HG3	1:A:209:ALA:H	1.83	0.43
1:A:404:LYS:N	1:A:405:PRO:HD2	2.34	0.43
1:A:271:GLN:CD	1:A:272:GLU:HG2	2.39	0.43
1:A:281:ILE:HA	2:A:501:STL:C10	2.48	0.43
1:A:330:LEU:O	1:A:334:MET:HG3	2.18	0.43
1:B:234:ARG:NH2	1:B:334:MET:O	2.44	0.43
1:B:235:ALA:HB1	1:B:241:THR:OG1	2.19	0.43
1:B:285:CYS:HB2	3:B:518:HOH:O	2.18	0.43
1:B:341:ILE:HG23	3:B:554:HOH:O	2.18	0.43
1:A:358:LYS:HB2	1:A:359:PRO:HD3	2.02	0.42
1:B:365:GLU:N	1:B:366:PRO:CD	2.83	0.42
1:A:388:ILE:HD13	1:A:388:ILE:HA	1.74	0.42
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.55	0.42
1:A:441:ASP:O	1:A:445:ILE:HG13	2.19	0.42
1:A:286:GLN:HE21	1:A:465:LEU:HD12	1.76	0.42
1:A:267:ILE:O	1:A:280:ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:LYS:N	1:B:405:PRO:HD2	2.35	0.42
1:A:470:GLN:C	1:A:472:ILE:H	2.22	0.42
1:A:353:LEU:C	1:A:355:SER:H	2.24	0.41
1:B:214:LEU:HD13	1:B:304:PRO:HG2	2.01	0.41
1:B:324:GLU:HG2	1:B:442:LEU:HB3	2.01	0.41
1:A:249:ILE:HG21	1:A:255:LEU:HD13	2.02	0.41
1:B:241:THR:O	1:B:241:THR:HG22	2.19	0.41
1:B:309:LEU:O	1:B:314:GLN:NE2	2.53	0.41
1:B:444:GLN:NE2	1:B:448:GLU:OE2	2.54	0.41
1:B:456:ILE:C	1:B:458:LYS:H	2.24	0.41
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.56	0.41
1:B:341:ILE:CD1	1:B:348:MET:HB2	2.47	0.41
1:A:207:GLU:C	1:A:209:ALA:H	2.24	0.41
1:A:237:LEU:HD22	1:A:335:ASN:HD22	1.84	0.41
1:A:256:MET:O	1:A:259:GLU:HG2	2.20	0.41
1:A:272:GLU:N	1:A:276:GLU:HA	2.34	0.41
1:A:288:ARG:HD3	1:A:288:ARG:C	2.41	0.41
1:B:317:LEU:HD22	1:B:392:ILE:O	2.20	0.41
1:B:343:GLU:HG3	1:B:343:GLU:O	2.21	0.41
1:A:237:LEU:O	1:A:239:GLY:N	2.54	0.41
1:A:433:ALA:O	1:A:437:GLN:HG3	2.21	0.41
1:B:327:TYR:OH	1:B:449:HIS:CD2	2.74	0.41
1:A:228:LEU:HD12	1:A:232:LYS:HD3	2.01	0.41
1:A:242:THR:O	1:A:242:THR:CG2	2.67	0.41
1:A:286:GLN:HG2	1:A:469:LEU:HD12	2.02	0.41
1:A:365:GLU:N	1:A:366:PRO:CD	2.84	0.41
1:A:425:HIS:N	1:A:426:PRO:CD	2.84	0.41
1:B:237:LEU:HG	1:B:340:LEU:CD2	2.50	0.41
1:B:251:ASP:H	1:B:254:SER:CB	2.34	0.41
1:B:425:HIS:O	1:B:427:GLU:N	2.53	0.41
1:A:241:THR:O	1:A:241:THR:OG1	2.38	0.41
1:A:271:GLN:O	1:A:276:GLU:CA	2.67	0.41
1:A:297:THR:O	1:A:301:LYS:HG3	2.21	0.41
1:A:417:LEU:HD21	1:A:435:LEU:CD2	2.51	0.41
1:B:323:HIS:CD2	1:B:446:VAL:HG13	2.56	0.41
1:A:290:VAL:HG11	1:A:466:HIS:CD2	2.56	0.40
1:A:411:ASP:OD1	1:B:434:LYS:HD2	2.22	0.40
1:B:221:SER:HB3	1:B:302:SER:OG	2.20	0.40
1:B:245:SER:HA	1:B:246:PRO:HD3	1.93	0.40
1:B:228:LEU:HD22	1:B:233:ALA:HB2	2.02	0.40
1:A:208:SER:HB2	1:A:419:LEU:HD21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:438:LYS:HD3	1:A:438:LYS:HA	1.89	0.40
1:A:264:PHE:C	1:A:266:HIS:N	2.73	0.40
1:A:335:ASN:C	1:A:335:ASN:OD1	2.60	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	266/287 (93%)	218 (82%)	30 (11%)	18 (7%)	1 2
1	B	265/287 (92%)	218 (82%)	27 (10%)	20 (8%)	1 2
All	All	531/574 (92%)	436 (82%)	57 (11%)	38 (7%)	1 2

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	242	THR
1	A	269	PRO
1	A	363	PHE
1	B	245	SER
1	B	260	ASP
1	B	262	ILE
1	B	266	HIS
1	B	347	PHE
1	B	357	ARG
1	B	461	THR
1	B	462	ASP
1	B	467	PRO
1	A	336	LYS
1	A	428	SER

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Mol	Chain	Res	Type
1	B	227	PRO
1	B	240	LYS
1	B	259	GLU
1	B	272	GLU
1	B	275	LYS
1	A	275	LYS
1	B	238	THR
1	B	243	ASP
1	B	426	PRO
1	A	265	LYS
1	A	354	LYS
1	A	411	ASP
1	A	268	THR
1	A	272	GLU
1	A	276	GLU
1	A	358	LYS
1	B	232	LYS
1	B	394	SER
1	A	322	VAL
1	A	361	GLY
1	A	359	PRO
1	A	472	ILE
1	B	466	HIS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	241/258 (93%)	229 (95%)	12 (5%)	24	53
1	B	240/258 (93%)	220 (92%)	20 (8%)	11	29
All	All	481/516 (93%)	449 (93%)	32 (7%)	16	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	THR
1	A	245	SER
1	A	246	PRO
1	A	270	LEU
1	A	271	GLN
1	A	288	ARG
1	A	362	ASP
1	A	363	PHE
1	A	396	ASP
1	A	402	ASN
1	A	415	GLN
1	A	460	GLU
1	B	210	ASP
1	B	212	ARG
1	B	228	LEU
1	B	245	SER
1	B	252	MET
1	B	256	MET
1	B	257	MET
1	B	262	ILE
1	B	265	LYS
1	B	267	ILE
1	B	272	GLU
1	B	318	LEU
1	B	323	HIS
1	B	332	SER
1	B	336	LYS
1	B	412	ASN
1	B	438	LYS
1	B	443	ARG
1	B	444	GLN
1	B	469	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	A	286	GLN
1	A	402	ASN
1	A	410	GLN
1	A	424	ASN
1	A	444	GLN
1	A	454	GLN

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Mol	Chain	Res	Type
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	271	GLN
1	B	286	GLN
1	B	308	ASN
1	B	323	HIS
1	B	412	ASN
1	B	437	GLN
1	B	444	GLN
1	B	449	HIS
1	B	451	GLN
1	B	470	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	STL	A	501	-	18,18,18	3.11	13 (72%)	24,24,24	2.10	4 (16%)

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	STL	A	501	-	-	0/5/5/5	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	STL	C4-C3	4.92	1.46	1.39
2	A	501	STL	C11-C10	4.65	1.47	1.38
2	A	501	STL	C2-C3	4.30	1.45	1.39
2	A	501	STL	C14-C13	3.93	1.45	1.38
2	A	501	STL	C13-C12	3.89	1.46	1.38
2	A	501	STL	C2-C1	3.78	1.44	1.39
2	A	501	STL	C10-C9	3.69	1.46	1.39
2	A	501	STL	C6-C1	3.62	1.44	1.39
2	A	501	STL	C4-C5	3.47	1.45	1.39
2	A	501	STL	C11-C12	2.88	1.44	1.38
2	A	501	STL	C6-C5	2.64	1.44	1.39
2	A	501	STL	C8-C7	2.25	1.42	1.31
2	A	501	STL	C14-C9	2.03	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	STL	O2-C3-C2	-5.91	104.47	119.84
2	A	501	STL	O2-C3-C4	5.62	134.46	119.84
2	A	501	STL	C14-C13-C12	-2.76	116.85	119.88
2	A	501	STL	O3-C1-C2	-2.35	113.73	119.84

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	501	STL	3	0

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	268/287 (93%)	-0.10	14 (5%) 27 22	27, 55, 114, 150	0
1	B	264/287 (91%)	0.06	22 (8%) 11 8	20, 56, 129, 144	1 (0%)
All	All	532/574 (92%)	-0.02	36 (6%) 17 13	20, 55, 127, 150	1 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	THR	9.7
1	B	465	LEU	8.0
1	A	269	PRO	7.7
1	B	271	GLN	7.1
1	B	274	SER	6.4
1	A	267	ILE	5.7
1	B	269	PRO	5.5
1	B	464	SER	5.0
1	B	461	THR	5.0
1	B	270	LEU	4.9
1	A	266	HIS	4.6
1	A	264	PHE	4.4
1	B	257	MET	4.3
1	B	273	GLN	4.2
1	A	240	LYS	4.0
1	B	241	THR	3.8
1	B	209	ALA	3.4
1	B	268	THR	3.4
1	B	272	GLU	3.3
1	A	273	GLN	3.1
1	A	270	LEU	3.0
1	B	207	GLU	3.0
1	A	241	THR	2.9
1	B	462	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	451	GLN	2.8
1	A	263	LYS	2.7
1	B	263	LYS	2.6
1	B	236	ILE	2.5
1	A	271	GLN	2.4
1	A	265	LYS	2.4
1	B	258	GLY	2.3
1	B	240	LYS	2.3
1	B	463	MET	2.3
1	A	252	MET	2.2
1	B	275	LYS	2.2
1	A	274	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (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. The B-factors column lists the minimum, median, 95^{th} 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
2	STL	A	501	17/17	0.65	0.53	60,65,83,83	17

6.5 Other polymers (i)

There are no such residues in this entry.