Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:06 AM GMT

PDB ID	:	2ZK1
Title	:	Human peroxisome proliferator-activated receptor gamma ligand binding domain complexed with 15-deoxy-delta12,14-prostaglandin J2
Authors	:	Waku, T.; Shiraki, T.; Oyama, T.; Fujimoto, Y.; Morikawa, K.
Deposited on	:	2008-03-12
Resolution	:	2.61 Å(reported)

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

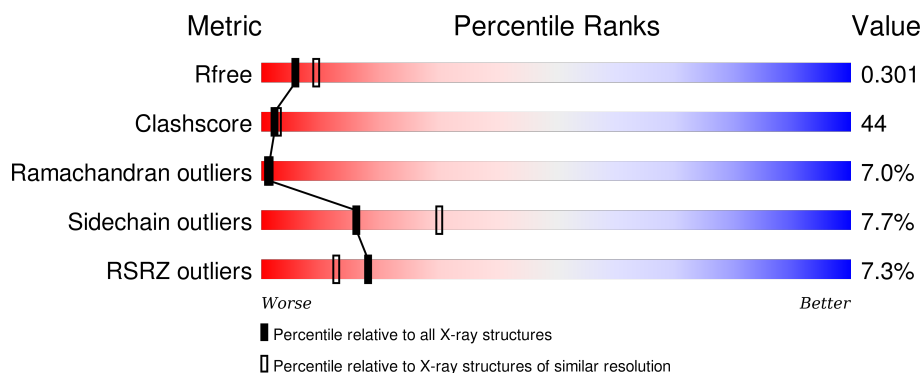|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.301
Clashscore		44
Ramachandran outliers		7.0%
Sidechain outliers		7.7%
RSRZ outliers		7.3%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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 <=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	6% — 50% / 37% / 9% · ·
1	B	286	8% — 34% / 48% / 9% · 8%

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	PTG	A	1	-	-	-	X
2	PTG	B	2	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4404 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,14E)-11-OXOPROSTA-5,9,12,14-TETRAEN-1-OIC ACID (three-letter code: PTG) (formula: $C_{20}H_{28}O_3$).
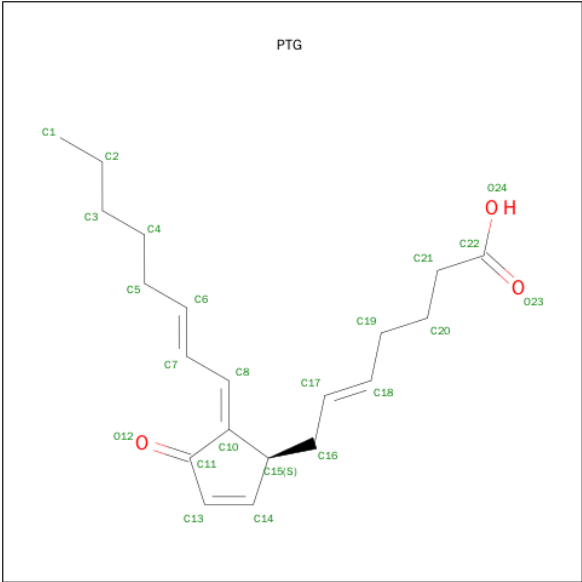
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 23	C 20	O 3	0	0
2	B	1	Total 23	C 20	O 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	27	Total 27	O 27	0	0

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
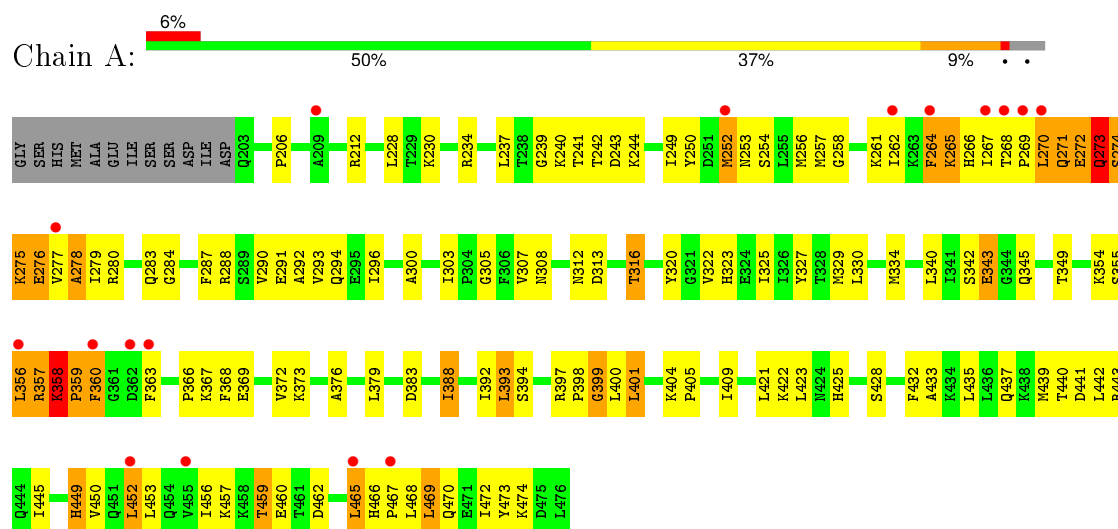
- Molecule 1: Peroxisome proliferator-activated receptor gamma
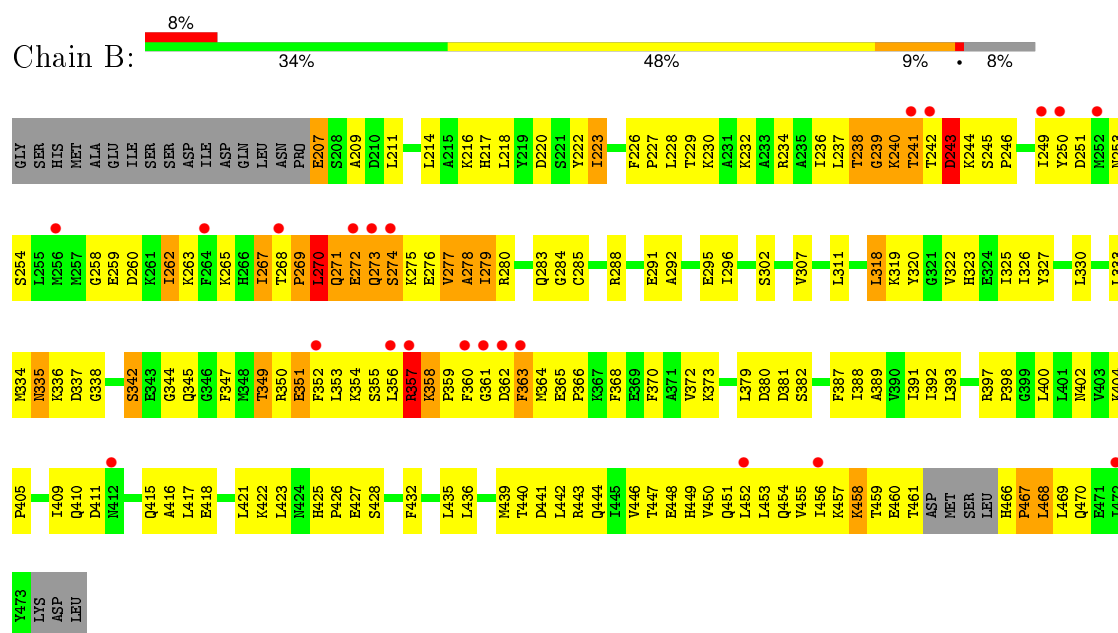
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.50Å 60.81Å 118.20Å 90.00° 103.02° 90.00°	Depositor
Resolution (Å)	35.84 – 2.61 48.60 – 2.61	Depositor EDS
% Data completeness (in resolution range)	92.7 (35.84-2.61) 92.8 (48.60-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.62 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.307 0.241 , 0.301	Depositor DCC
R_{free} test set	896 reflections (4.87%)	DCC
Wilson B-factor (Å^2)	54.0	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.33$	Xtriage
Outliers	0 of 19185 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4404	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: PTG

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	0.70	1/2995 (0.0%)
1	B	0.51	0/2146	0.71	0/2891
All	All	0.49	0/4369	0.70	1/5886 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	206	PRO	N-CA-CB	5.38	109.76	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	157	0
1	B	2110	0	2173	240	0
2	A	23	0	27	8	0
2	B	23	0	26	6	0
3	A	35	0	0	1	0
3	B	27	0	0	1	0
All	All	4404	0	4464	390	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 44.

All (390) 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:278:ALA:HB3	1:B:357:ARG:HH21	1.05	1.15
1:A:241:THR:HG21	1:A:244:LYS:HD2	1.23	1.09
1:A:267:ILE:HD12	1:A:284:GLY:HA3	1.31	1.08
1:B:274:SER:HB2	1:B:280:ARG:HE	1.03	1.07
1:B:277:VAL:HG13	1:B:278:ALA:H	1.20	1.06
1:B:274:SER:HB2	1:B:280:ARG:NE	1.77	0.99
1:B:466:HIS:HA	1:B:469:LEU:HD12	1.43	0.98
1:B:278:ALA:HB3	1:B:357:ARG:NH2	1.79	0.98
1:B:263:LYS:HG3	1:B:265:LYS:HG3	1.46	0.97
1:B:358:LYS:HB3	1:B:359:PRO:HD3	1.45	0.95
1:B:349:THR:HG22	1:B:352:PHE:H	1.30	0.95
1:B:242:THR:HG21	1:B:244:LYS:HE3	1.47	0.95
1:A:240:LYS:O	1:A:241:THR:HG23	1.68	0.94
1:B:335:ASN:ND2	1:B:338:GLY:H	1.69	0.89
1:A:241:THR:HG21	1:A:244:LYS:CD	2.04	0.88
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.55	0.88
1:A:359:PRO:HB2	1:A:456:ILE:HD11	1.56	0.87
1:B:358:LYS:HB3	1:B:359:PRO:CD	2.03	0.87
1:A:465:LEU:HD12	1:A:470:GLN:HG2	1.54	0.86
1:A:394:SER:HB2	1:A:397:ARG:HG2	1.56	0.85
1:B:357:ARG:HD3	1:B:357:ARG:H	1.42	0.84
1:A:250:TYR:HB3	1:A:349:THR:HG21	1.61	0.82
1:A:267:ILE:HG13	1:A:268:THR:H	1.43	0.82
1:A:358:LYS:CB	1:A:359:PRO:HD3	2.11	0.81
1:A:271:GLN:OE1	1:A:274:SER:HB3	1.80	0.81
1:A:274:SER:O	1:A:276:GLU:N	2.13	0.81
1:B:357:ARG:HH11	1:B:357:ARG:CG	1.94	0.80
1:B:358:LYS:CB	1:B:359:PRO:HD3	2.11	0.80
1:A:368:PHE:O	1:A:372:VAL:HG23	1.82	0.79
1:A:440:THR:HA	1:B:440:THR:HG23	1.64	0.79
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.47	0.79
1:B:267:ILE:HD13	1:B:268:THR:HG23	1.62	0.78
1:A:356:LEU:O	1:A:357:ARG:HB2	1.84	0.78
1:B:451:GLN:O	1:B:454:GLN:HB3	1.83	0.78
1:A:456:ILE:HA	1:A:459:THR:CG2	2.14	0.78
1:B:273:GLN:HG3	1:B:274:SER:H	1.48	0.77
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:PHE:O	1:B:355:SER:HB3	1.84	0.77
1:A:373:LYS:O	1:A:376:ALA:HB3	1.84	0.76
1:A:397:ARG:HB2	1:A:400:LEU:HD11	1.67	0.76
1:B:222:TYR:CE1	1:B:381:ASP:HB3	2.20	0.76
1:B:330:LEU:HD13	2:B:2:PTG:H19A	1.65	0.76
1:A:357:ARG:HG2	1:A:358:LYS:HD2	1.68	0.76
1:A:443:ARG:HD2	1:B:444:GLN:HE22	1.48	0.76
1:B:325:ILE:HG23	1:B:388:ILE:HD12	1.67	0.76
1:B:458:LYS:HG2	1:B:458:LYS:O	1.86	0.75
1:B:277:VAL:HG13	1:B:278:ALA:N	2.01	0.75
1:B:354:LYS:HA	1:B:361:GLY:O	1.86	0.74
1:A:358:LYS:HE2	1:A:358:LYS:H	1.49	0.74
1:B:330:LEU:HG	1:B:334:MET:CE	2.18	0.73
1:A:358:LYS:HB3	1:A:359:PRO:HD3	1.69	0.73
1:A:267:ILE:HG13	1:A:268:THR:N	2.02	0.73
1:B:274:SER:CB	1:B:280:ARG:HE	1.93	0.72
1:B:288:ARG:HD2	1:B:288:ARG:O	1.90	0.72
1:A:313:ASP:HA	1:A:316:THR:CG2	2.20	0.72
1:A:291:GLU:HA	1:A:294:GLN:OE1	1.89	0.72
1:B:350:ARG:HA	1:B:353:LEU:HD12	1.71	0.72
1:B:335:ASN:ND2	1:B:338:GLY:N	2.37	0.70
1:A:257:MET:O	1:A:261:LYS:HG2	1.91	0.70
1:A:456:ILE:HA	1:A:459:THR:HG22	1.73	0.69
1:B:335:ASN:HD22	1:B:335:ASN:C	1.96	0.69
1:B:349:THR:CG2	1:B:352:PHE:H	2.05	0.68
1:B:265:LYS:HA	1:B:268:THR:OG1	1.93	0.68
1:A:278:ALA:HA	1:A:356:LEU:HD22	1.76	0.68
1:A:397:ARG:HB2	1:A:400:LEU:CD1	2.24	0.67
1:A:357:ARG:HG2	1:A:358:LYS:N	2.09	0.67
1:B:455:VAL:O	1:B:458:LYS:HB3	1.94	0.66
1:B:364:MET:HE1	2:B:2:PTG:O12	1.94	0.66
1:B:239:GLY:C	1:B:241:THR:H	1.99	0.66
1:B:241:THR:O	1:B:242:THR:HB	1.94	0.66
1:B:365:GLU:OE1	1:B:365:GLU:HA	1.95	0.66
1:B:258:GLY:O	1:B:262:ILE:HG13	1.95	0.66
1:A:267:ILE:O	1:A:269:PRO:HD3	1.96	0.66
1:B:263:LYS:C	1:B:265:LYS:H	2.00	0.65
1:B:459:THR:HG22	1:B:460:GLU:H	1.61	0.65
1:B:265:LYS:O	1:B:269:PRO:HG3	1.95	0.65
1:A:241:THR:CG2	1:A:244:LYS:HD2	2.14	0.65
1:B:239:GLY:O	1:B:241:THR:N	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:GLN:HG3	1:B:274:SER:N	2.12	0.65
1:B:279:ILE:HD12	1:B:360:PHE:CZ	2.31	0.65
1:A:293:VAL:HG22	1:A:322:VAL:CG1	2.27	0.64
1:B:466:HIS:O	1:B:468:LEU:N	2.27	0.64
1:A:363:PHE:HZ	1:A:456:ILE:HG13	1.63	0.64
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.79	0.64
1:B:330:LEU:HG	1:B:334:MET:HE3	1.80	0.64
1:B:228:LEU:HD23	1:B:333:LEU:HD21	1.80	0.64
1:B:241:THR:C	1:B:243:ASP:H	2.01	0.64
1:A:441:ASP:O	1:A:445:ILE:HG12	1.98	0.64
1:B:335:ASN:HD21	1:B:338:GLY:N	1.94	0.64
1:B:222:TYR:HE1	1:B:381:ASP:HB3	1.62	0.64
1:B:402:ASN:O	1:B:405:PRO:HD2	1.98	0.63
1:B:267:ILE:HG13	1:B:284:GLY:HA2	1.81	0.62
1:B:359:PRO:HD2	1:B:360:PHE:CD2	2.33	0.62
1:B:357:ARG:H	1:B:357:ARG:CD	2.11	0.62
1:A:358:LYS:HE2	1:A:358:LYS:N	2.14	0.62
1:A:357:ARG:CG	1:A:358:LYS:HD2	2.28	0.62
1:B:450:VAL:HG12	1:B:451:GLN:NE2	2.15	0.62
1:B:263:LYS:NZ	1:B:263:LYS:HB2	2.15	0.62
1:B:263:LYS:HG3	1:B:265:LYS:CG	2.26	0.62
1:B:262:ILE:HG22	1:B:345:GLN:HB3	1.81	0.62
1:B:357:ARG:HH11	1:B:357:ARG:HG3	1.65	0.61
1:A:249:ILE:O	1:A:349:THR:HG23	2.00	0.61
1:A:443:ARG:HH11	1:A:443:ARG:HG3	1.65	0.61
1:A:356:LEU:O	1:A:357:ARG:CB	2.48	0.61
1:A:342:SER:O	1:A:343:GLU:HB2	1.99	0.61
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.81	0.61
1:A:359:PRO:CB	1:A:456:ILE:HD11	2.30	0.61
1:B:272:GLU:O	1:B:272:GLU:HG3	2.00	0.61
1:A:367:LYS:NZ	1:A:449:HIS:NE2	2.40	0.61
1:A:277:VAL:HG13	1:A:278:ALA:N	2.16	0.60
1:B:279:ILE:O	1:B:283:GLN:HG3	2.01	0.60
1:A:240:LYS:HG3	1:A:240:LYS:O	2.00	0.60
1:A:291:GLU:O	1:A:294:GLN:HB2	2.01	0.60
1:A:276:GLU:OE2	1:A:357:ARG:HD3	2.00	0.60
1:B:234:ARG:O	1:B:238:THR:HG23	2.01	0.60
1:B:358:LYS:CG	1:B:359:PRO:HD3	2.31	0.60
1:A:313:ASP:HA	1:A:316:THR:HG22	1.84	0.59
1:B:357:ARG:HG2	1:B:358:LYS:H	1.67	0.59
1:A:450:VAL:HG22	1:A:473:TYR:CD1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:TYR:CE2	1:B:254:SER:HB3	2.37	0.59
1:B:450:VAL:HG12	1:B:451:GLN:HE22	1.68	0.59
1:B:265:LYS:O	1:B:269:PRO:CG	2.51	0.59
1:A:453:LEU:HD13	2:A:1:PTG:O24	2.02	0.59
1:A:273:GLN:CD	1:A:273:GLN:O	2.42	0.59
1:B:365:GLU:N	1:B:366:PRO:CD	2.67	0.58
1:B:292:ALA:O	1:B:296:ILE:HG12	2.03	0.58
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.38	0.58
1:B:311:LEU:H	1:B:311:LEU:HD22	1.68	0.58
1:B:330:LEU:HG	1:B:334:MET:HE2	1.85	0.58
1:B:335:ASN:HD22	1:B:338:GLY:H	1.48	0.58
1:B:357:ARG:HD3	1:B:357:ARG:N	2.17	0.57
1:B:411:ASP:O	1:B:415:GLN:HG3	2.03	0.57
1:B:240:LYS:O	1:B:240:LYS:HG3	2.05	0.57
1:B:335:ASN:ND2	1:B:337:ASP:H	2.02	0.57
1:A:292:ALA:O	1:A:296:ILE:HG13	2.04	0.57
1:B:402:ASN:OD1	1:B:405:PRO:HD3	2.04	0.57
1:B:358:LYS:CB	1:B:359:PRO:CD	2.77	0.57
1:B:459:THR:HG22	1:B:460:GLU:N	2.20	0.56
1:B:325:ILE:HD13	1:B:388:ILE:HG23	1.87	0.56
1:A:453:LEU:HD22	2:A:1:PTG:O24	2.04	0.56
1:B:357:ARG:HG2	1:B:357:ARG:NH1	2.19	0.56
1:B:272:GLU:O	1:B:273:GLN:HB3	2.06	0.56
1:B:307:VAL:HG23	3:B:1044:HOH:O	2.05	0.56
1:B:368:PHE:O	1:B:372:VAL:HG23	2.05	0.56
1:B:265:LYS:C	1:B:269:PRO:HD3	2.26	0.56
1:B:278:ALA:HB2	1:B:356:LEU:HD22	1.86	0.56
1:A:443:ARG:NH1	1:A:443:ARG:HG3	2.19	0.56
1:B:443:ARG:O	1:B:447:THR:HG23	2.05	0.56
1:A:288:ARG:O	1:A:288:ARG:HD2	2.05	0.56
1:B:357:ARG:HH11	1:B:357:ARG:HG2	1.67	0.55
1:B:259:GLU:HG2	1:B:268:THR:HG21	1.87	0.55
1:B:357:ARG:CG	1:B:357:ARG:NH1	2.61	0.55
1:A:404:LYS:N	1:A:405:PRO:HD2	2.20	0.55
1:A:443:ARG:HD2	1:B:444:GLN:NE2	2.20	0.55
1:B:228:LEU:HD23	1:B:333:LEU:CD2	2.37	0.55
1:B:240:LYS:C	1:B:242:THR:H	2.10	0.55
1:B:280:ARG:HA	1:B:283:GLN:NE2	2.21	0.54
1:A:307:VAL:HG22	3:A:1004:HOH:O	2.06	0.54
1:A:243:ASP:OD2	1:A:244:LYS:HG3	2.07	0.54
1:A:421:LEU:HD12	1:A:432:PHE:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD22	1:B:273:GLN:NE2	2.22	0.54
1:B:323:HIS:NE2	2:B:2:PTG:H2A	2.23	0.54
1:A:443:ARG:HG3	1:B:440:THR:CG2	2.38	0.54
1:A:264:PHE:C	1:A:266:HIS:H	2.10	0.54
1:A:465:LEU:HB2	1:A:470:GLN:OE1	2.08	0.54
1:A:425:HIS:HB3	1:A:428:SER:HB2	1.90	0.54
1:B:242:THR:O	1:B:243:ASP:HB3	2.07	0.54
1:B:239:GLY:C	1:B:241:THR:N	2.61	0.54
1:B:275:LYS:NZ	1:B:275:LYS:HB2	2.23	0.53
1:B:405:PRO:O	1:B:409:ILE:HG12	2.08	0.53
1:A:357:ARG:HH21	1:A:360:PHE:HE1	1.54	0.53
1:A:469:LEU:O	1:A:473:TYR:CD2	2.61	0.53
1:B:461:THR:O	1:B:470:GLN:NE2	2.41	0.53
1:A:468:LEU:C	1:A:468:LEU:HD13	2.29	0.53
1:B:276:GLU:HG2	1:B:279:ILE:HB	1.91	0.53
1:B:453:LEU:HD11	2:B:2:PTG:H1A	1.90	0.53
1:A:273:GLN:O	1:A:275:LYS:N	2.42	0.53
1:B:330:LEU:O	1:B:334:MET:HG2	2.09	0.53
1:B:354:LYS:HD3	1:B:365:GLU:OE2	2.08	0.53
1:B:269:PRO:O	1:B:270:LEU:C	2.47	0.53
1:A:240:LYS:O	1:A:241:THR:CG2	2.51	0.52
1:B:452:LEU:N	1:B:452:LEU:HD12	2.25	0.52
1:A:358:LYS:HE2	1:A:358:LYS:CA	2.40	0.52
1:B:263:LYS:C	1:B:265:LYS:N	2.62	0.52
1:A:300:ALA:HA	1:A:303:ILE:CD1	2.40	0.52
1:A:237:LEU:CD2	1:A:340:LEU:HD21	2.40	0.52
1:A:264:PHE:O	1:A:266:HIS:N	2.31	0.52
1:B:211:LEU:HD12	1:B:416:ALA:HB2	1.91	0.52
1:A:268:THR:HG21	1:A:280:ARG:HD3	1.91	0.52
1:B:238:THR:OG1	1:B:239:GLY:N	2.41	0.52
1:B:466:HIS:HA	1:B:469:LEU:CD1	2.29	0.52
1:A:271:GLN:OE1	1:A:274:SER:CB	2.53	0.52
1:A:277:VAL:HG13	1:A:278:ALA:H	1.74	0.51
1:B:466:HIS:N	1:B:467:PRO:CD	2.74	0.51
1:A:459:THR:HG23	1:A:460:GLU:HG2	1.92	0.51
1:B:320:TYR:HB3	1:B:397:ARG:HD2	1.93	0.51
1:A:358:LYS:CB	1:A:359:PRO:CD	2.81	0.51
1:A:312:ASN:O	1:A:316:THR:HG22	2.10	0.51
1:A:258:GLY:O	1:A:262:ILE:HG12	2.11	0.51
1:A:443:ARG:HG3	1:B:440:THR:HG22	1.93	0.51
1:B:291:GLU:O	1:B:295:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:VAL:CG1	1:B:278:ALA:H	2.03	0.51
1:A:393:LEU:HD12	1:A:409:ILE:HB	1.93	0.50
1:A:230:LYS:O	1:A:234:ARG:HG2	2.12	0.50
1:A:443:ARG:NH1	1:B:440:THR:HG22	2.27	0.50
1:B:230:LYS:NZ	1:B:379:LEU:O	2.40	0.50
1:A:272:GLU:O	1:A:274:SER:N	2.44	0.50
1:B:466:HIS:CE1	1:B:469:LEU:HB2	2.47	0.49
1:A:290:VAL:HG23	1:A:469:LEU:CD2	2.42	0.49
1:B:326:ILE:HG22	2:B:2:PTG:H14	1.93	0.49
1:A:327:TYR:CE2	1:A:367:LYS:HE2	2.47	0.49
1:B:229:THR:OG1	1:B:232:LYS:HG3	2.11	0.49
1:A:443:ARG:NH1	1:B:440:THR:CG2	2.75	0.49
1:B:274:SER:HB2	1:B:280:ARG:CD	2.40	0.49
1:B:363:PHE:HD2	1:B:364:MET:HE2	1.78	0.49
1:A:399:GLY:O	1:A:401:LEU:HD23	2.13	0.49
1:A:269:PRO:O	1:A:270:LEU:C	2.51	0.49
1:A:320:TYR:CE1	1:A:398:PRO:HD2	2.48	0.49
1:A:465:LEU:CD1	1:A:470:GLN:HG2	2.34	0.49
1:A:323:HIS:CD2	1:A:472:ILE:HG21	2.46	0.49
1:A:253:ASN:O	1:A:256:MET:HB2	2.13	0.49
1:A:358:LYS:HB3	1:A:359:PRO:CD	2.40	0.49
1:B:427:GLU:HG3	1:B:428:SER:H	1.78	0.49
1:B:262:ILE:HG22	1:B:345:GLN:CB	2.42	0.48
1:B:353:LEU:HD13	1:B:368:PHE:HE2	1.77	0.48
1:A:268:THR:CG2	1:A:280:ARG:HH11	2.26	0.48
1:A:363:PHE:CZ	1:A:456:ILE:HG13	2.46	0.48
1:B:240:LYS:CG	1:B:240:LYS:O	2.61	0.48
1:B:230:LYS:HB3	1:B:381:ASP:OD2	2.13	0.48
1:B:351:GLU:OE1	1:B:354:LYS:HE3	2.13	0.48
1:A:433:ALA:O	1:A:437:GLN:HG3	2.13	0.48
1:A:437:GLN:O	1:A:440:THR:HG23	2.13	0.48
1:B:273:GLN:O	1:B:275:LYS:N	2.47	0.48
1:A:270:LEU:O	1:A:271:GLN:HB2	2.14	0.48
1:B:320:TYR:CZ	1:B:398:PRO:HG2	2.48	0.48
1:B:349:THR:HG22	1:B:352:PHE:N	2.13	0.48
1:B:350:ARG:NE	1:B:365:GLU:OE1	2.43	0.48
1:B:234:ARG:O	1:B:238:THR:CG2	2.62	0.48
1:A:450:VAL:HG22	1:A:473:TYR:CE1	2.48	0.47
1:B:466:HIS:ND1	1:B:469:LEU:HB2	2.29	0.47
1:A:250:TYR:CD2	1:A:250:TYR:N	2.81	0.47
1:B:418:GLU:O	1:B:422:LYS:HG2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ARG:O	1:B:400:LEU:HG	2.15	0.47
1:B:259:GLU:O	1:B:263:LYS:HA	2.13	0.47
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.44	0.47
1:A:279:ILE:O	1:A:283:GLN:HG2	2.15	0.47
1:B:271:GLN:O	1:B:273:GLN:N	2.48	0.47
1:B:363:PHE:CD1	1:B:452:LEU:HD23	2.49	0.47
1:B:267:ILE:C	1:B:269:PRO:HD2	2.34	0.47
1:A:252:MET:HE1	1:A:277:VAL:HG11	1.95	0.47
1:A:465:LEU:HD12	1:A:470:GLN:CG	2.37	0.47
1:A:250:TYR:HB3	1:A:349:THR:CG2	2.39	0.47
1:A:313:ASP:O	1:A:316:THR:HG23	2.15	0.47
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.98	0.47
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.96	0.47
1:B:359:PRO:HD2	1:B:360:PHE:HD2	1.80	0.47
1:B:241:THR:O	1:B:242:THR:CB	2.61	0.47
1:B:214:LEU:O	1:B:218:LEU:HG	2.15	0.47
1:A:366:PRO:O	1:A:369:GLU:HB2	2.15	0.47
1:B:251:ASP:H	1:B:254:SER:HG	1.58	0.47
1:B:358:LYS:NZ	1:B:459:THR:HG23	2.30	0.47
1:A:456:ILE:HD13	1:A:459:THR:HG21	1.97	0.47
1:B:458:LYS:CG	1:B:458:LYS:O	2.59	0.47
1:B:455:VAL:C	1:B:457:LYS:N	2.68	0.46
1:B:365:GLU:N	1:B:366:PRO:HD3	2.29	0.46
1:B:466:HIS:CG	1:B:469:LEU:HD12	2.50	0.46
1:A:394:SER:HB2	1:A:397:ARG:CG	2.37	0.46
1:A:401:LEU:N	1:A:401:LEU:HD23	2.31	0.46
1:A:357:ARG:NH2	1:A:360:PHE:HE1	2.14	0.46
1:A:254:SER:HA	1:A:257:MET:HB2	1.97	0.46
1:B:273:GLN:CG	1:B:274:SER:H	2.25	0.46
1:B:237:LEU:HD22	1:B:335:ASN:OD1	2.16	0.46
1:A:469:LEU:O	1:A:473:TYR:HD2	1.99	0.46
1:B:207:GLU:C	1:B:209:ALA:H	2.19	0.46
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.46	0.46
1:B:379:LEU:HD11	1:B:435:LEU:HD13	1.97	0.46
1:B:260:ASP:O	1:B:263:LYS:NZ	2.49	0.45
1:B:279:ILE:HG13	1:B:461:THR:HG21	1.98	0.45
1:B:358:LYS:HG2	1:B:359:PRO:HD3	1.97	0.45
1:B:387:PHE:O	1:B:391:ILE:HG12	2.16	0.45
1:B:275:LYS:HB2	1:B:275:LYS:HZ1	1.81	0.45
1:A:473:TYR:OH	2:A:1:PTG:C21	2.65	0.45
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LYS:NZ	1:B:275:LYS:CB	2.79	0.45
1:B:335:ASN:C	1:B:335:ASN:ND2	2.68	0.45
1:B:446:VAL:O	1:B:450:VAL:HG23	2.16	0.45
1:A:272:GLU:OE1	1:A:273:GLN:HG3	2.17	0.45
1:B:417:LEU:HD21	1:B:435:LEU:HD23	1.99	0.45
1:B:288:ARG:HG3	2:B:2:PTG:H18	1.99	0.45
1:B:356:LEU:O	1:B:361:GLY:HA2	2.17	0.45
1:A:320:TYR:CZ	1:A:398:PRO:HD2	2.52	0.45
1:A:330:LEU:HD22	2:A:1:PTG:O12	2.16	0.45
1:B:211:LEU:HD22	1:B:211:LEU:N	2.31	0.45
1:A:473:TYR:OH	2:A:1:PTG:H21	2.16	0.45
1:B:236:ILE:CG2	1:B:246:PRO:HG2	2.47	0.45
1:B:421:LEU:HD12	1:B:432:PHE:HA	1.99	0.45
1:B:273:GLN:NE2	1:B:283:GLN:OE1	2.50	0.44
1:B:336:LYS:HG3	1:B:337:ASP:OD2	2.18	0.44
1:A:462:ASP:N	1:A:462:ASP:OD1	2.49	0.44
1:B:322:VAL:O	1:B:326:ILE:HG13	2.18	0.44
1:A:300:ALA:O	1:A:303:ILE:HG13	2.16	0.44
1:B:277:VAL:HG22	1:B:278:ALA:N	2.31	0.44
1:B:249:ILE:HD11	1:B:262:ILE:HD11	2.00	0.44
1:B:262:ILE:O	1:B:263:LYS:C	2.54	0.44
1:B:242:THR:O	1:B:243:ASP:CB	2.65	0.44
1:B:325:ILE:CD1	1:B:388:ILE:HG23	2.48	0.44
1:B:245:SER:HA	1:B:246:PRO:HD3	1.78	0.44
1:A:443:ARG:HH11	1:B:440:THR:HG22	1.82	0.44
1:B:307:VAL:O	1:B:307:VAL:HG12	2.18	0.43
1:B:268:THR:N	1:B:269:PRO:CD	2.81	0.43
1:A:457:LYS:HG2	1:A:457:LYS:O	2.19	0.43
1:B:279:ILE:HG22	1:B:280:ARG:N	2.32	0.43
1:A:320:TYR:HB2	1:A:397:ARG:HD2	2.01	0.43
1:B:402:ASN:OD1	1:B:405:PRO:CD	2.65	0.43
1:B:342:SER:C	1:B:344:GLY:H	2.22	0.43
1:B:319:LYS:HE3	1:B:319:LYS:HB2	1.75	0.43
1:B:277:VAL:O	1:B:280:ARG:N	2.52	0.43
1:B:234:ARG:CZ	1:B:237:LEU:HD12	2.48	0.43
1:A:325:ILE:HG23	1:A:388:ILE:HG12	2.00	0.43
1:B:279:ILE:CD1	1:B:360:PHE:CZ	3.01	0.43
1:A:257:MET:CE	1:A:261:LYS:HE2	2.48	0.43
1:B:353:LEU:HD22	1:B:364:MET:HG3	2.00	0.43
1:A:273:GLN:N	1:A:280:ARG:HH21	2.16	0.43
1:A:355:SER:O	1:A:356:LEU:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:HIS:O	1:A:467:PRO:C	2.57	0.43
1:B:360:PHE:O	1:B:361:GLY:C	2.57	0.43
1:A:264:PHE:C	1:A:266:HIS:N	2.71	0.43
1:B:327:TYR:OH	1:B:449:HIS:CG	2.72	0.43
1:B:466:HIS:CA	1:B:469:LEU:HD12	2.32	0.42
1:A:234:ARG:HH11	1:A:234:ARG:HG3	1.84	0.42
1:B:269:PRO:O	1:B:270:LEU:O	2.37	0.42
1:A:252:MET:CE	1:A:277:VAL:HG11	2.49	0.42
1:B:350:ARG:HE	1:B:365:GLU:CD	2.22	0.42
1:B:452:LEU:CD1	1:B:452:LEU:N	2.82	0.42
1:A:290:VAL:HG23	1:A:469:LEU:HD21	2.00	0.42
1:B:454:GLN:C	1:B:454:GLN:CD	2.78	0.42
1:A:288:ARG:HG2	2:A:1:PTG:H2	2.00	0.42
1:B:311:LEU:H	1:B:311:LEU:CD2	2.31	0.42
1:B:423:LEU:O	1:B:426:PRO:HD3	2.20	0.42
1:A:466:HIS:O	1:A:470:GLN:HG3	2.19	0.42
1:A:277:VAL:CG1	1:A:278:ALA:N	2.82	0.42
1:A:358:LYS:HE2	1:A:358:LYS:HA	2.00	0.42
1:B:211:LEU:HD22	1:B:211:LEU:H	1.84	0.42
1:A:252:MET:O	1:A:253:ASN:C	2.58	0.42
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.35	0.42
1:B:442:LEU:O	1:B:446:VAL:HG23	2.20	0.42
1:B:230:LYS:HB3	1:B:381:ASP:CG	2.39	0.42
1:A:212:ARG:NH1	1:A:423:LEU:HD12	2.34	0.42
1:B:263:LYS:HB2	1:B:263:LYS:HZ2	1.85	0.42
1:B:388:ILE:O	1:B:392:ILE:HG13	2.20	0.42
1:B:358:LYS:HZ1	1:B:459:THR:HG23	1.83	0.41
1:A:373:LYS:HE2	1:A:373:LYS:HB3	1.85	0.41
1:B:456:ILE:C	1:B:458:LYS:H	2.24	0.41
1:A:228:LEU:HD22	1:A:343:GLU:HA	2.02	0.41
1:B:263:LYS:CG	1:B:265:LYS:HG3	2.33	0.41
1:A:329:MET:HG3	1:A:388:ILE:HD11	2.02	0.41
1:B:236:ILE:HG23	1:B:246:PRO:HG2	2.01	0.41
1:B:360:PHE:H	1:B:360:PHE:HD2	1.67	0.41
2:A:1:PTG:H19A	2:A:1:PTG:H16A	1.89	0.41
1:B:223:ILE:HD13	1:B:229:THR:HG21	2.03	0.41
1:B:425:HIS:O	1:B:426:PRO:C	2.58	0.41
1:B:389:ALA:O	1:B:393:LEU:HD23	2.19	0.41
1:B:318:LEU:HD12	1:B:318:LEU:HA	1.88	0.41
1:B:448:GLU:O	1:B:452:LEU:HD13	2.20	0.41
1:B:455:VAL:O	1:B:456:ILE:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:LEU:O	2:A:1:PTG:H3	2.20	0.41
1:B:436:LEU:O	1:B:439:MET:HE2	2.20	0.41
1:B:240:LYS:C	1:B:242:THR:N	2.74	0.41
1:A:439:MET:HA	1:A:442:LEU:HD12	2.03	0.41
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.51	0.41
1:B:249:ILE:HA	1:B:254:SER:HB2	2.03	0.41
1:B:273:GLN:CG	1:B:274:SER:N	2.83	0.41
1:B:279:ILE:CG1	1:B:461:THR:HG21	2.50	0.41
1:B:335:ASN:HD22	1:B:337:ASP:H	1.67	0.41
1:B:370:PHE:CZ	1:B:442:LEU:HD21	2.55	0.41
1:B:320:TYR:CE1	1:B:398:PRO:HG2	2.55	0.41
1:B:360:PHE:CD2	1:B:360:PHE:N	2.89	0.41
1:B:258:GLY:O	1:B:262:ILE:CG1	2.67	0.41
1:B:373:LYS:HE2	1:B:373:LYS:HB3	1.72	0.41
1:B:217:HIS:HE1	1:B:302:SER:O	2.04	0.41
1:B:350:ARG:HH21	1:B:365:GLU:CD	2.25	0.40
1:A:277:VAL:O	1:A:279:ILE:N	2.54	0.40
1:B:393:LEU:O	1:B:410:GLN:HB2	2.21	0.40
1:A:342:SER:HB2	1:A:345:GLN:HB2	2.04	0.40
1:B:216:LYS:HE3	1:B:220:ASP:OD1	2.22	0.40
1:B:404:LYS:HB3	1:B:405:PRO:HD3	2.04	0.40
1:B:267:ILE:C	1:B:269:PRO:CD	2.89	0.40
1:B:270:LEU:HD22	1:B:273:GLN:CD	2.42	0.40
1:A:330:LEU:O	1:A:334:MET:HG3	2.22	0.40
1:B:311:LEU:N	1:B:311:LEU:HD22	2.35	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%)	232 (85%)	21 (8%)	19 (7%)	1	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	259/286 (91%)	216 (83%)	25 (10%)	18 (7%)	1	1
All	All	531/572 (93%)	448 (84%)	46 (9%)	37 (7%)	1	1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	GLN
1	A	274	SER
1	A	275	LYS
1	A	357	ARG
1	A	358	LYS
1	B	271	GLN
1	B	272	GLU
1	B	273	GLN
1	B	274	SER
1	B	277	VAL
1	B	342	SER
1	B	358	LYS
1	A	239	GLY
1	A	343	GLU
1	A	356	LEU
1	A	474	LYS
1	B	241	THR
1	B	243	ASP
1	B	269	PRO
1	B	270	LEU
1	B	468	LEU
1	A	265	LYS
1	A	270	LEU
1	A	271	GLN
1	A	278	ALA
1	A	360	PHE
1	A	401	LEU
1	A	465	LEU
1	B	239	GLY
1	B	278	ALA
1	B	363	PHE
1	B	467	PRO
1	A	359	PRO
1	A	399	GLY
1	A	354	LYS
1	B	357	ARG

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Mol	Chain	Res	Type
1	B	240	LYS

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	243/257 (95%)	226 (93%)	17 (7%)	19	36
1	B	236/257 (92%)	216 (92%)	20 (8%)	13	25
All	All	479/514 (93%)	442 (92%)	37 (8%)	16	30

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	THR
1	A	252	MET
1	A	264	PHE
1	A	265	LYS
1	A	272	GLU
1	A	273	GLN
1	A	276	GLU
1	A	287	PHE
1	A	316	THR
1	A	358	LYS
1	A	388	ILE
1	A	393	LEU
1	A	422	LYS
1	A	449	HIS
1	A	452	LEU
1	A	459	THR
1	A	469	LEU
1	B	207	GLU
1	B	223	ILE
1	B	238	THR
1	B	243	ASP
1	B	253	ASN

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Mol	Chain	Res	Type
1	B	262	ILE
1	B	267	ILE
1	B	270	LEU
1	B	279	ILE
1	B	285	CYS
1	B	318	LEU
1	B	335	ASN
1	B	349	THR
1	B	351	GLU
1	B	357	ARG
1	B	362	ASP
1	B	380	ASP
1	B	382	SER
1	B	441	ASP
1	B	458	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	ASN
1	A	312	ASN
1	A	323	HIS
1	A	425	HIS
1	A	430	GLN
1	A	437	GLN
1	B	217	HIS
1	B	273	GLN
1	B	283	GLN
1	B	308	ASN
1	B	335	ASN
1	B	424	ASN
1	B	430	GLN
1	B	444	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	PTG	A	1	1	18,23,23	5.19	2 (11%)	17,27,27	2.27	2 (11%)
2	PTG	B	2	1	18,23,23	5.40	2 (11%)	17,27,27	1.91	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	PTG	A	1	1	-	1/15/30/30	0/1/1/1
2	PTG	B	2	1	-	1/15/30/30	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	PTG	C7-C8	4.12	1.56	1.43
2	A	1	PTG	C7-C8	4.42	1.57	1.43
2	A	1	PTG	C8-C10	21.37	1.56	1.34
2	B	2	PTG	C8-C10	22.33	1.57	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	PTG	C15-C10-C11	-8.34	96.43	107.09
2	B	2	PTG	C15-C10-C11	-7.28	97.78	107.09
2	A	1	PTG	C14-C15-C10	-2.67	96.67	100.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	PTG	C7-C8-C10-C11
2	B	2	PTG	C7-C8-C10-C11

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PTG	8	0
2	B	2	PTG	6	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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.39	17 (6%)	24	18	30, 51, 78, 92	0
1	B	263/286 (91%)	0.52	22 (8%)	14	9	32, 52, 82, 94	0
All	All	537/572 (93%)	0.45	39 (7%)	18	13	30, 51, 82, 94	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	270	LEU	5.5
1	A	277	VAL	4.8
1	A	267	ILE	4.8
1	B	360	PHE	4.7
1	B	363	PHE	4.4
1	B	272	GLU	4.3
1	B	274	SER	4.0
1	B	242	THR	3.9
1	B	456	ILE	3.9
1	A	360	PHE	3.5
1	B	452	LEU	3.5
1	B	357	ARG	3.2
1	A	269	PRO	3.2
1	A	209	ALA	3.2
1	A	264	PHE	2.9
1	B	273	GLN	2.7
1	A	362	ASP	2.7
1	B	362	ASP	2.6
1	B	268	THR	2.6
1	B	356	LEU	2.5
1	B	361	GLY	2.5
1	B	250	TYR	2.4
1	B	249	ILE	2.4
1	B	412	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	241	THR	2.3
1	B	352	PHE	2.3
1	A	252	MET	2.3
1	B	252	MET	2.3
1	A	363	PHE	2.3
1	A	268	THR	2.2
1	A	262	ILE	2.2
1	A	455	VAL	2.2
1	B	264	PHE	2.2
1	A	356	LEU	2.1
1	B	472	ILE	2.1
1	A	452	LEU	2.1
1	A	465	LEU	2.1
1	B	256	MET	2.0
1	A	467	PRO	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	PTG	A	1	23/23	0.75	0.44	4.42	62,78,84,86	0
2	PTG	B	2	23/23	0.66	0.38	2.27	76,82,84,86	0

6.5 Other polymers (i)

There are no such residues in this entry.