WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:40 AM GMT

PDB ID : 2I4P

Title : Crystal structure of the complex between PPARgamma and the partial agonist LT127 (ureidofibrate derivative). Structure obtained from crystals of the apo-form soaked for 30 days.

Authors : Pochetti, G.; Mazza, F.

Deposited on : 2006-08-22

Resolution : 2.10 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 2.10 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		0.283
Clashscore		21
Ramachandran outliers		3.2%
Sidechain outliers		7.2%
RSRZ outliers		21.4%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
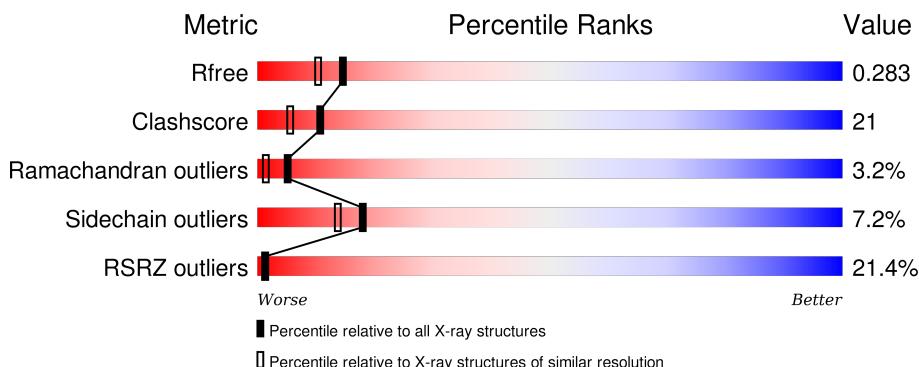
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	14% 58% 33% •• 6%
1	B	286	25% 58% 30% 5% • 6%
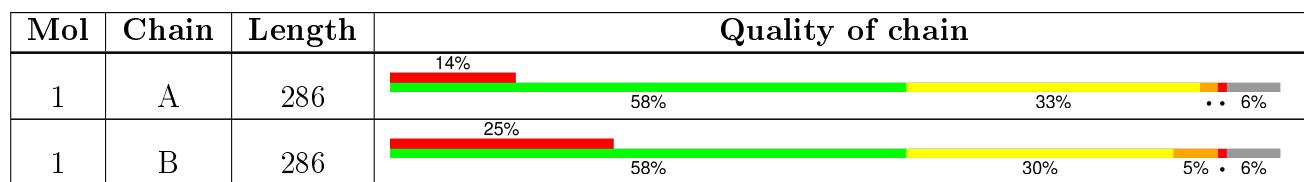
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DRH	A	999	X	-	X	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4478 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	270	Total	C	N	O	S	78	0	0
			2166	1397	354	405	10			
1	B	270	Total	C	N	O	S	107	0	0
			2166	1397	354	405	10			

There are 8 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is (2S)-2-(4-{2-[1,3-BENZOXAZOL-2-YL(HEPTYL)AMINO]ETHYL}PHENO XY)-2-METHYLBUTANOIC ACID (three-letter code: DRH) (formula: $C_{27}H_{36}N_2O_4$).
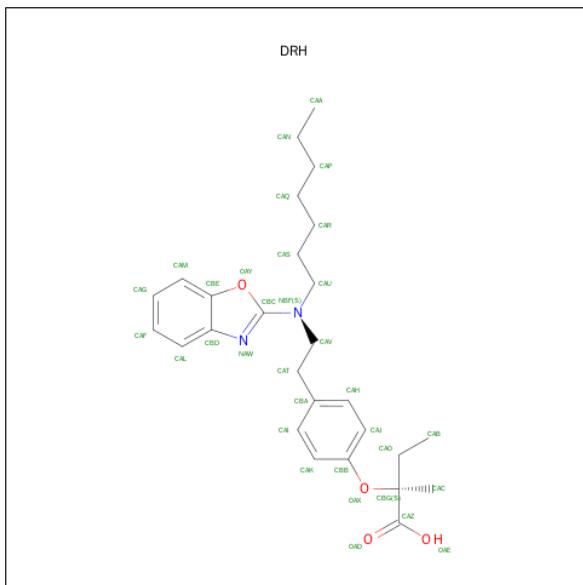
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	33	27	2	4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	67	67	67	0	0
3	B	46	46	46	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

Chain A:

• Molecule 1: Peroxisome proliferator-activated receptor gamma

Chain B:
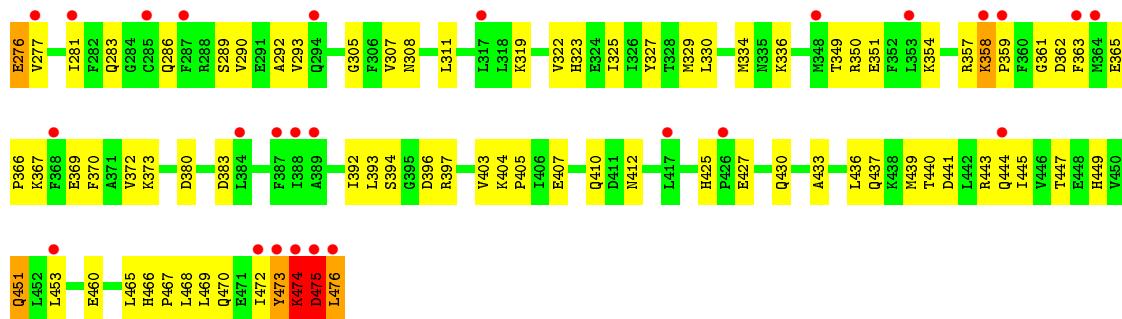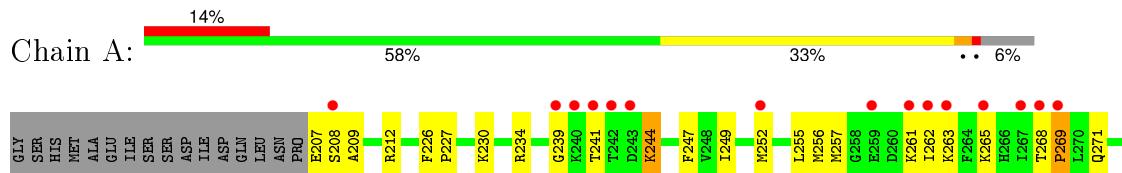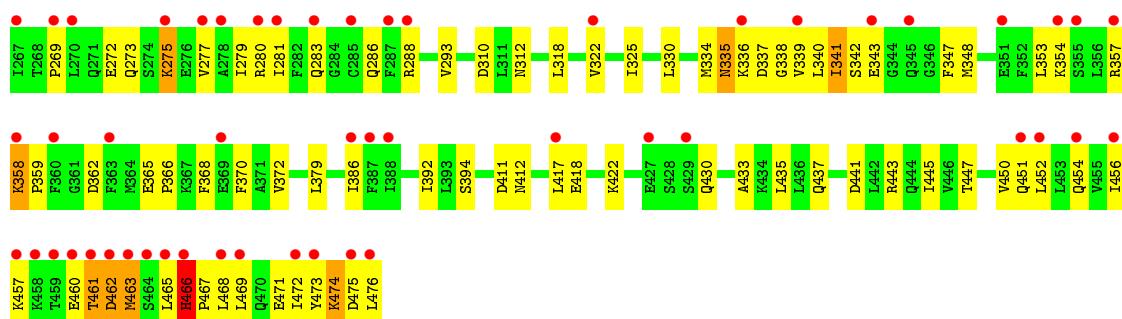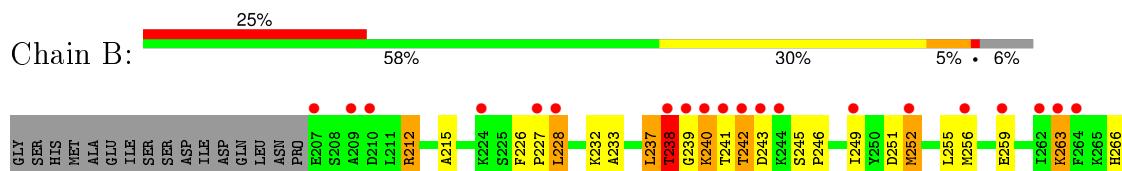
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	93.54Å 60.91Å 118.35Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	8.00 – 2.10 20.02 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (8.00-2.10) 85.4 (20.02-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.09Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.272 , 0.295 0.288 , 0.283	Depositor DCC
R_{free} test set	1576 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.539	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 32491 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4478	wwPDB-VP
Average B, all atoms (Å^2)	49.0	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.*

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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: DRH

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	0.43	1/2203 (0.0%)	0.70	9/2967 (0.3%)
1	B	0.36	0/2203	0.57	0/2967
All	All	0.40	1/4406 (0.0%)	0.64	9/5934 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	LEU	C-OXT	6.60	1.35	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	LEU	CA-C-O	8.82	138.63	120.10
1	A	474	LYS	C-N-CA	8.14	142.04	121.70
1	A	475	ASP	N-CA-C	7.69	131.76	111.00
1	A	474	LYS	CA-C-N	-5.87	104.29	117.20
1	A	475	ASP	N-CA-CB	-5.76	100.22	110.60
1	A	475	ASP	C-N-CA	-5.40	108.20	121.70
1	A	474	LYS	N-CA-C	-5.34	96.57	111.00
1	A	475	ASP	CB-CA-C	-5.16	100.08	110.40
1	A	473	TYR	CB-CG-CD1	-5.02	117.99	121.00

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	2166	0	2232	90	0
1	B	2166	0	2232	82	0
2	A	33	0	35	22	0
3	A	67	0	0	11	0
3	B	46	0	0	7	0
All	All	4478	0	4499	180	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 21.

All (180) 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:A:475:ASP:O	1:A:476:LEU:CB	1.66	1.36
1:A:330:LEU:HD22	2:A:999:DRH:HAT1	1.36	1.06
1:A:473:TYR:O	1:A:474:LYS:HG3	1.59	1.01
2:A:999:DRH:OAD	2:A:999:DRH:HAK	1.59	1.00
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.53	0.91
1:B:293:VAL:HG21	1:B:476:LEU:HD11	1.51	0.89
1:A:247:PHE:HB2	1:A:261:LYS:HD3	1.54	0.89
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.57	0.86
1:A:244:LYS:HE2	3:A:8:HOH:O	1.76	0.83
1:A:449:HIS:NE2	2:A:999:DRH:HAC1	1.93	0.83
1:A:329:MET:SD	2:A:999:DRH:HAA3	2.20	0.82
1:A:475:ASP:O	1:A:476:LEU:HB2	0.93	0.81
1:B:212:ARG:HH11	1:B:212:ARG:HB3	1.47	0.80
1:A:330:LEU:HD13	2:A:999:DRH:HAV2	1.63	0.80
1:B:335:ASN:ND2	1:B:337:ASP:H	1.79	0.79
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.65	0.79
1:B:341:ILE:HD13	1:B:342:SER:H	1.47	0.78
1:B:335:ASN:HD22	1:B:335:ASN:C	1.86	0.77
1:B:358:LYS:N	1:B:358:LYS:HE3	2.00	0.76
1:A:261:LYS:HE2	1:A:262:ILE:HG13	1.66	0.76
1:A:475:ASP:O	1:A:476:LEU:CG	2.34	0.75
1:A:241:THR:HB	3:A:15:HOH:O	1.85	0.74
2:A:999:DRH:CAZ	2:A:999:DRH:HAK	2.19	0.72
1:A:473:TYR:O	1:A:474:LYS:CG	2.37	0.71
1:B:341:ILE:HD13	3:B:6:HOH:O	1.88	0.71
1:A:330:LEU:HD13	2:A:999:DRH:CAV	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:GLN:O	1:B:454:GLN:HG2	1.91	0.70
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.72	0.69
2:A:999:DRH:OAD	2:A:999:DRH:CAK	2.39	0.69
1:B:358:LYS:HE3	1:B:358:LYS:H	1.58	0.68
1:B:336:LYS:HG2	1:B:372:VAL:HG22	1.74	0.68
1:A:440:THR:O	1:A:444:GLN:HG2	1.94	0.68
1:A:349:THR:HG22	1:A:351:GLU:H	1.60	0.66
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.78	0.66
1:B:240:LYS:HG3	1:B:241:THR:H	1.63	0.64
1:A:440:THR:HB	3:B:39:HOH:O	1.97	0.63
1:B:341:ILE:CD1	1:B:342:SER:H	2.12	0.63
1:B:466:HIS:N	1:B:467:PRO:CD	2.62	0.62
1:A:474:LYS:H	1:A:475:ASP:HB2	1.64	0.62
2:A:999:DRH:OAY	2:A:999:DRH:HAT2	2.00	0.61
1:A:329:MET:SD	2:A:999:DRH:CAA	2.88	0.60
1:B:441:ASP:O	1:B:445:ILE:HG12	2.01	0.60
1:B:411:ASP:HB2	3:B:22:HOH:O	2.02	0.60
1:A:430:GLN:HG3	1:A:433:ALA:HB3	1.82	0.59
1:A:268:THR:N	1:A:269:PRO:HD2	2.17	0.59
1:A:268:THR:H	1:A:269:PRO:HD2	1.67	0.59
1:B:228:LEU:HD23	1:B:232:LYS:HB3	1.85	0.58
1:A:311:LEU:HD23	1:A:311:LEU:C	2.24	0.58
1:B:335:ASN:C	1:B:335:ASN:ND2	2.56	0.58
1:B:228:LEU:CD2	1:B:232:LYS:HB3	2.34	0.58
1:A:466:HIS:ND1	1:A:467:PRO:HD2	2.20	0.57
1:B:467:PRO:C	1:B:469:LEU:H	2.07	0.57
1:B:447:THR:O	1:B:450:VAL:HG22	2.04	0.56
1:A:441:ASP:O	1:A:445:ILE:HG12	2.06	0.56
1:B:335:ASN:ND2	1:B:338:GLY:H	2.04	0.56
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.36	0.55
1:A:292:ALA:CB	2:A:999:DRH:HAQ1	2.36	0.55
1:B:251:ASP:HB2	3:B:23:HOH:O	2.05	0.55
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.87	0.55
1:B:335:ASN:HD21	1:B:338:GLY:N	2.05	0.55
1:A:336:LYS:HE2	1:A:372:VAL:HG11	1.89	0.54
1:A:208:SER:O	1:A:212:ARG:HG2	2.07	0.54
1:B:433:ALA:O	1:B:437:GLN:HG2	2.07	0.54
1:B:325:ILE:HD11	1:B:392:ILE:HG13	1.90	0.54
2:A:999:DRH:HAL	3:A:116:HOH:O	2.07	0.53
1:A:370:PHE:HA	1:A:373:LYS:HE2	1.89	0.53
1:B:237:LEU:O	1:B:239:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LEU:CD2	1:B:281:ILE:HD11	2.39	0.53
1:B:252:MET:O	1:B:256:MET:HG2	2.09	0.53
1:B:365:GLU:N	1:B:366:PRO:HD2	2.24	0.53
1:B:466:HIS:N	1:B:467:PRO:HD2	2.23	0.52
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.40	0.52
1:A:475:ASP:O	1:A:476:LEU:HG	2.08	0.51
1:B:335:ASN:ND2	1:B:338:GLY:N	2.58	0.51
1:A:349:THR:HG21	3:A:91:HOH:O	2.09	0.51
1:A:286:GLN:N	2:A:999:DRH:HAB1	2.26	0.51
1:B:473:TYR:O	1:B:474:LYS:HB2	2.11	0.51
1:A:230:LYS:O	1:A:234:ARG:HG2	2.10	0.51
1:B:343:GLU:HG3	1:B:343:GLU:O	2.11	0.51
1:A:289:SER:O	1:A:293:VAL:HG23	2.12	0.50
2:A:999:DRH:CBC	3:A:18:HOH:O	2.59	0.50
1:A:277:VAL:O	1:A:281:ILE:HG13	2.12	0.50
1:A:262:ILE:HG22	1:A:263:LYS:N	2.27	0.49
1:B:358:LYS:CE	1:B:358:LYS:H	2.22	0.49
1:A:404:LYS:N	1:A:405:PRO:HD2	2.28	0.49
1:A:207:GLU:HG3	1:A:209:ALA:HB3	1.93	0.49
1:A:255:LEU:HD21	1:A:277:VAL:HG23	1.95	0.49
1:B:228:LEU:HD22	1:B:233:ALA:HB2	1.95	0.49
1:A:453:LEU:HD21	3:A:1:HOH:O	2.12	0.48
1:A:256:MET:O	1:A:268:THR:HG23	2.13	0.48
1:B:336:LYS:HE3	1:B:372:VAL:HG11	1.96	0.48
1:B:242:THR:HA	3:B:61:HOH:O	2.13	0.48
1:A:286:GLN:CA	2:A:999:DRH:HAB1	2.44	0.48
1:A:263:LYS:HB3	3:A:86:HOH:O	2.14	0.48
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.96	0.48
1:A:433:ALA:O	1:A:437:GLN:HG3	2.13	0.48
1:A:380:ASP:HB2	3:A:32:HOH:O	2.13	0.48
1:A:330:LEU:HD22	2:A:999:DRH:CAT	2.26	0.47
1:A:292:ALA:HB1	2:A:999:DRH:HAQ1	1.96	0.47
1:B:335:ASN:ND2	1:B:337:ASP:N	2.56	0.47
1:A:437:GLN:O	1:A:440:THR:HG22	2.15	0.47
1:B:310:ASP:OD2	1:B:312:ASN:HB2	2.14	0.47
1:A:349:THR:HG22	1:A:351:GLU:N	2.28	0.47
1:B:288:ARG:HB3	3:B:13:HOH:O	2.13	0.47
1:B:457:LYS:O	1:B:461:THR:HG23	2.15	0.47
1:A:330:LEU:HD13	2:A:999:DRH:CAT	2.44	0.47
1:B:334:MET:HG2	1:B:339:VAL:HB	1.95	0.47
1:A:403:VAL:O	1:A:407:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:HG2	1:A:268:THR:O	2.15	0.46
1:B:418:GLU:O	1:B:422:LYS:HG3	2.14	0.46
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.45	0.46
1:B:452:LEU:O	1:B:456:ILE:HG13	2.16	0.46
1:B:463:MET:HG3	1:B:465:LEU:H	1.80	0.46
1:A:436:LEU:O	1:A:439:MET:HB2	2.16	0.46
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.31	0.46
1:A:307:VAL:HG22	3:A:10:HOH:O	2.15	0.46
1:B:275:LYS:HA	1:B:275:LYS:HE3	1.99	0.45
1:B:465:LEU:O	1:B:466:HIS:HB2	2.16	0.45
1:A:292:ALA:HB2	2:A:999:DRH:HAQ1	1.99	0.45
1:B:465:LEU:O	1:B:466:HIS:CB	2.64	0.45
2:A:999:DRH:HAC2	3:A:1:HOH:O	2.17	0.45
1:A:262:ILE:HG22	1:A:263:LYS:H	1.81	0.45
1:B:342:SER:O	1:B:343:GLU:HB3	2.16	0.45
1:B:215:ALA:HA	1:B:386:ILE:CD1	2.47	0.45
1:B:468:LEU:O	1:B:472:ILE:HG13	2.17	0.45
1:A:330:LEU:O	1:A:334:MET:HG3	2.18	0.44
1:B:325:ILE:HD11	1:B:392:ILE:CG1	2.46	0.44
1:B:430:GLN:NE2	1:B:433:ALA:HB2	2.31	0.44
1:A:383:ASP:OD2	1:A:425:HIS:HE1	2.00	0.44
1:A:305:GLY:HA2	1:A:308:ASN:HD22	1.81	0.44
1:B:255:LEU:HD23	1:B:277:VAL:HG13	2.00	0.44
2:A:999:DRH:OAY	2:A:999:DRH:CAT	2.65	0.44
1:B:259:GLU:OE1	1:B:280:ARG:NH2	2.47	0.44
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.33	0.44
1:A:323:HIS:CE1	1:A:473:TYR:CE2	3.06	0.44
1:A:207:GLU:HG3	1:A:209:ALA:H	1.82	0.43
1:B:469:LEU:O	1:B:469:LEU:HD13	2.17	0.43
1:A:469:LEU:O	1:A:473:TYR:CD1	2.71	0.43
1:A:325:ILE:HD11	1:A:392:ILE:HG13	2.00	0.43
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.87	0.43
1:A:394:SER:O	1:A:397:ARG:HG2	2.19	0.43
1:B:379:LEU:HD21	1:B:435:LEU:HD22	1.99	0.43
1:B:215:ALA:HA	1:B:386:ILE:HD11	2.01	0.43
1:B:237:LEU:HD21	1:B:340:LEU:HG	2.01	0.43
1:B:379:LEU:HD12	3:B:84:HOH:O	2.17	0.43
1:B:237:LEU:HB3	1:B:238:THR:H	1.64	0.42
1:A:263:LYS:HZ1	1:A:265:LYS:HE2	1.84	0.42
1:A:290:VAL:HG13	1:A:468:LEU:HD23	2.01	0.42
1:B:370:PHE:HE1	1:B:441:ASP:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PRO:HA	1:B:280:ARG:NH2	2.34	0.42
1:B:368:PHE:O	1:B:372:VAL:HG23	2.20	0.42
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.84	0.42
1:B:354:LYS:HD3	1:B:365:GLU:CG	2.49	0.42
1:A:447:THR:O	1:A:451:GLN:HG3	2.19	0.42
1:A:252:MET:O	1:A:256:MET:HG3	2.20	0.42
1:B:245:SER:HA	1:B:246:PRO:HD3	1.91	0.42
1:B:475:ASP:O	1:B:476:LEU:HB3	2.20	0.42
1:A:369:GLU:O	1:A:373:LYS:HG3	2.20	0.42
1:A:276:GLU:OE2	1:A:357:ARG:CZ	2.68	0.41
1:B:249:ILE:HD12	1:B:255:LEU:HA	2.01	0.41
1:B:286:GLN:HB3	1:B:473:TYR:CE2	2.55	0.41
1:B:348:MET:SD	1:B:353:LEU:HD21	2.60	0.41
1:A:319:LYS:O	1:A:472:ILE:HG23	2.19	0.41
1:A:393:LEU:CD2	1:A:393:LEU:N	2.82	0.41
1:A:370:PHE:HA	1:A:373:LYS:CE	2.50	0.41
1:B:279:ILE:O	1:B:283:GLN:HG3	2.20	0.41
1:B:467:PRO:C	1:B:469:LEU:N	2.73	0.41
1:A:330:LEU:CD2	2:A:999:DRH:HAT1	2.26	0.41
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.55	0.41
1:A:207:GLU:HA	3:A:90:HOH:O	2.19	0.41
1:B:457:LYS:NZ	1:B:461:THR:HG21	2.36	0.41
1:A:239:GLY:C	1:A:241:THR:N	2.72	0.41
1:B:467:PRO:O	1:B:468:LEU:HB3	2.20	0.41
1:A:365:GLU:N	1:A:366:PRO:HD2	2.36	0.41
1:B:255:LEU:HD22	1:B:281:ILE:HD11	2.02	0.40
1:B:386:ILE:HB	1:B:417:LEU:HD13	2.03	0.40
1:A:354:LYS:HA	1:A:361:GLY:O	2.21	0.40
1:A:327:TYR:CD1	1:A:367:LYS:HD2	2.57	0.40
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.87	0.40
1:A:397:ARG:HH11	1:A:443:ARG:NH2	2.19	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	268/286 (94%)	254 (95%)	10 (4%)	4 (2%)	13	7
1	B	268/286 (94%)	235 (88%)	20 (8%)	13 (5%)	3	0
All	All	536/572 (94%)	489 (91%)	30 (6%)	17 (3%)	5	1

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	269	PRO
1	A	474	LYS
1	B	237	LEU
1	B	357	ARG
1	B	394	SER
1	B	462	ASP
1	B	466	HIS
1	A	358	LYS
1	B	238	THR
1	B	240	LYS
1	B	242	THR
1	B	263	LYS
1	A	276	GLU
1	B	266	HIS
1	B	474	LYS
1	B	463	MET
1	B	243	ASP

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%)	229 (94%)	14 (6%)	25	21
1	B	243/257 (95%)	222 (91%)	21 (9%)	13	9
All	All	486/514 (95%)	451 (93%)	35 (7%)	18	14

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	244	LYS
1	A	257	MET
1	A	271	GLN
1	A	283	GLN
1	A	362	ASP
1	A	363	PHE
1	A	396	ASP
1	A	410	GLN
1	A	412	ASN
1	A	427	GLU
1	A	451	GLN
1	A	460	GLU
1	A	470	GLN
1	A	475	ASP
1	B	212	ARG
1	B	228	LEU
1	B	238	THR
1	B	252	MET
1	B	263	LYS
1	B	272	GLU
1	B	273	GLN
1	B	275	LYS
1	B	318	LEU
1	B	330	LEU
1	B	335	ASN
1	B	341	ILE
1	B	358	LYS
1	B	362	ASP
1	B	412	ASN
1	B	443	ARG
1	B	460	GLU
1	B	461	THR
1	B	462	ASP
1	B	466	HIS
1	B	471	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	283	GLN
1	A	286	GLN

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Mol	Chain	Res	Type
1	A	308	ASN
1	A	314	GLN
1	A	402	ASN
1	A	410	GLN
1	A	412	ASN
1	A	425	HIS
1	A	430	GLN
1	A	451	GLN
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	308	ASN
1	B	335	ASN
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN
1	B	444	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 carbohydrates 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	DRH	A	999	-	29,35,35	0.83	0	28,47,47	1.20	3 (10%)

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	DRH	A	999	-	1/1/3/3	1/22/30/30	0/2/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	999	DRH	CAU-NBF-CBC	-3.89	115.12	120.55
2	A	999	DRH	CAV-NBF-CBC	2.63	124.22	120.55
2	A	999	DRH	CBG-OAX-CBB	2.68	125.68	121.13

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	999	DRH	NBF

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	999	DRH	CAT-CAV-NBF-CBC

There are no ring outliers.

1 monomer is involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	999	DRH	22	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	262/286 (91%)	1.08	41 (15%)	3	4	29, 45, 66, 75	2 (0%)
1	B	261/286 (91%)	1.63	71 (27%)	1	1	27, 45, 79, 90	7 (2%)
All	All	523/572 (91%)	1.35	112 (21%)	1	1	27, 45, 74, 90	9 (1%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	ILE	25.8
1	B	242	THR	14.0
1	B	465	LEU	12.6
1	B	463	MET	12.1
1	B	270	LEU	11.7
1	A	268	THR	11.2
1	A	240	LYS	10.2
1	B	264	PHE	9.7
1	A	476	LEU	9.7
1	B	464	SER	9.0
1	B	461	THR	8.8
1	B	263	LYS	8.3
1	B	462	ASP	8.0
1	B	238	THR	7.9
1	A	263	LYS	7.6
1	B	285	CYS	6.8
1	B	262	ILE	6.5
1	A	269	PRO	6.4
1	B	240	LYS	6.0
1	B	269	PRO	5.9
1	A	265	LYS	5.7
1	B	358	LYS	5.1
1	A	473	TYR	5.1
1	B	241	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	267	ILE	4.9
1	B	460	GLU	4.6
1	B	244	LYS	4.6
1	A	262	ILE	4.3
1	B	427	GLU	4.2
1	B	475	ASP	4.1
1	B	476	LEU	4.0
1	B	259	GLU	4.0
1	B	275	LYS	3.9
1	B	243	ASP	3.7
1	A	363	PHE	3.7
1	B	459	THR	3.6
1	A	472	ILE	3.4
1	B	466	HIS	3.3
1	B	345	GLN	3.3
1	A	364	MET	3.3
1	B	228	LEU	3.2
1	B	288	ARG	3.2
1	A	287	PHE	3.1
1	B	351	GLU	3.1
1	A	239	GLY	3.1
1	B	369	GLU	3.1
1	B	454	GLN	3.0
1	B	468	LEU	2.9
1	A	475	ASP	2.9
1	B	458	LYS	2.9
1	B	280	ARG	2.8
1	B	469	LEU	2.8
1	A	285	CYS	2.8
1	B	210	ASP	2.8
1	B	336	LYS	2.7
1	B	252	MET	2.7
1	A	259	GLU	2.7
1	A	241	THR	2.7
1	B	343	GLU	2.6
1	A	358	LYS	2.6
1	B	472	ILE	2.6
1	A	261	LYS	2.6
1	B	360	PHE	2.6
1	B	207	GLU	2.6
1	B	287	PHE	2.6
1	A	453	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	473	TYR	2.5
1	B	227	PRO	2.5
1	B	357	ARG	2.5
1	B	283	GLN	2.5
1	B	387	PHE	2.5
1	B	239	GLY	2.5
1	A	252	MET	2.4
1	B	256	MET	2.4
1	A	353	LEU	2.4
1	A	444	GLN	2.3
1	B	388	ILE	2.3
1	B	429	SER	2.3
1	B	277	VAL	2.3
1	B	386	ILE	2.3
1	B	209	ALA	2.3
1	B	224	LYS	2.3
1	B	339	VAL	2.3
1	B	249	ILE	2.3
1	B	452	LEU	2.3
1	A	368	PHE	2.3
1	B	363	PHE	2.3
1	B	355	SER	2.3
1	A	417	LEU	2.3
1	A	426	PRO	2.3
1	A	277	VAL	2.2
1	B	322	VAL	2.2
1	B	457	LYS	2.2
1	A	243	ASP	2.2
1	A	281	ILE	2.2
1	A	317	LEU	2.2
1	B	281	ILE	2.2
1	A	294	GLN	2.2
1	B	451	GLN	2.2
1	A	387	PHE	2.2
1	A	388	ILE	2.2
1	B	278	ALA	2.1
1	A	208	SER	2.1
1	A	389	ALA	2.1
1	A	474	LYS	2.1
1	B	354	LYS	2.1
1	A	242	THR	2.1
1	B	456	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	359	PRO	2.1
1	B	417	LEU	2.1
1	A	348	MET	2.1
1	A	384	LEU	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	DRH	A	999	33/33	0.60	0.36	3.14	63,71,72,72	0

6.5 Other polymers (i)

There are no such residues in this entry.