Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PRG
Title	:	LIGAND BINDING DOMAIN OF THE HUMAN PEROXISOME PROLIF-ERATOR ACTIVATED RECEPTOR GAMMA
Authors	:	Nolte, R.T.; Wisely, G.B.; Milburn, M.V.
Deposited on	:	1998-07-02
Resolution	:	2.20 Å(reported)

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

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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
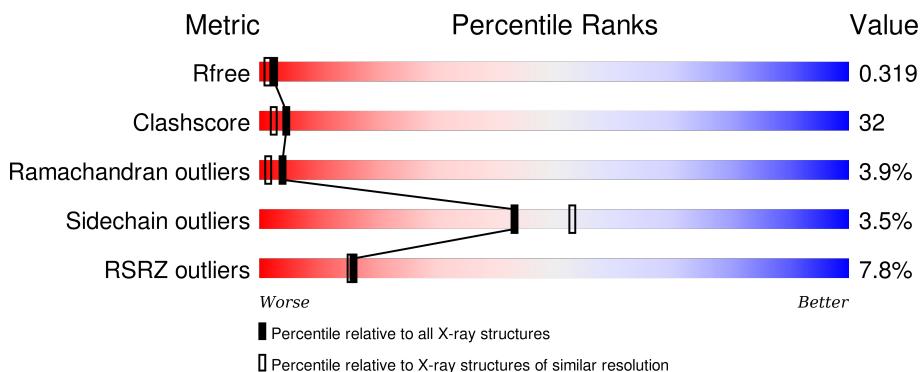
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	270	
1	B	270	
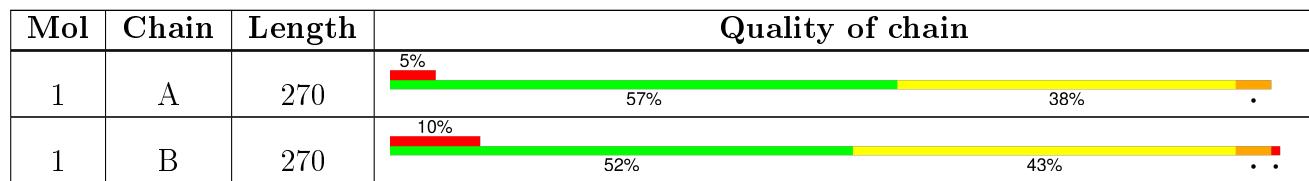
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4897 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 PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA).

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total 2166	C 1397	N 354	O 405	S 10	0	0	0
1	B	270	Total 2166	C 1397	N 354	O 405	S 10	0	0	0

- Molecule 2 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	288	Total 288	O 288	0	0
2	B	277	Total 277	O 277	0	0

3 Residue-property plots (i)

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: PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA)
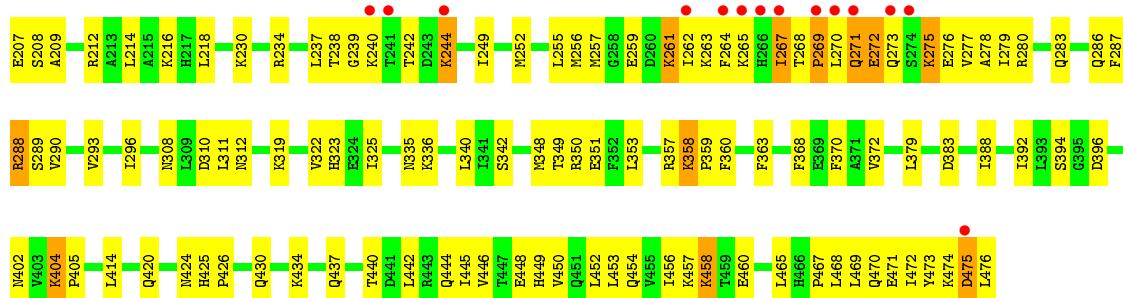
• Molecule 1: PROTEIN (PEROXISOME PROLIFERATOR ACTIVATED RECEPTOR GAMMA)
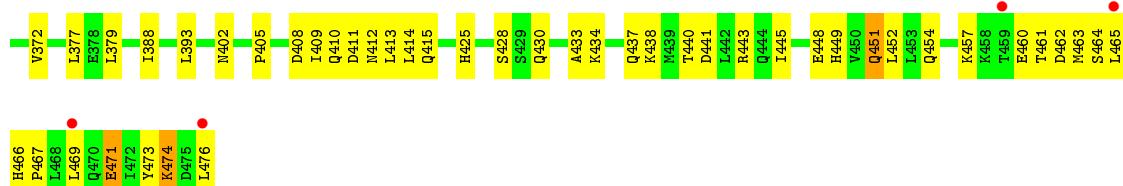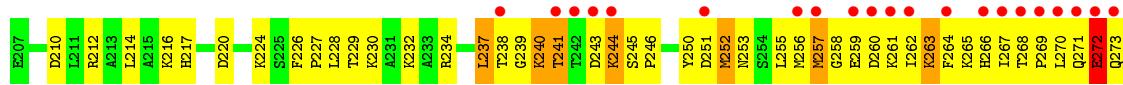
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	91.87Å　　62.00Å　　118.34Å 90.00°　　102.66°　　90.00°	Depositor
Resolution (Å)	60.00　–　2.20 50.99　–　2.00	Depositor EDS
% Data completeness (in resolution range)	83.8 (60.00-2.20) 76.1 (50.99-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.00Å)	Xtriage
Refinement program	CNS 0.0.3	Depositor
R, R_{free}	0.246　,　0.318 0.245　,　0.319	Depositor DCC
R_{free} test set	1122 reflections (4.03%)	DCC
Wilson B-factor (Å^2)	34.1	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 74.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 33487 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4897	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.34	0/2203	0.62	0/2967
1	B	0.34	0/2203	0.61	0/2967
All	All	0.34	0/4406	0.61	0/5934

There are no bond length outliers.

There are no bond angle outliers.

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	146	0
1	B	2166	0	2232	144	0
2	A	288	0	0	17	0
2	B	277	0	0	18	0
All	All	4897	0	4464	284	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 32.

All (284) 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:259:GLU:HG2	1:A:264:PHE:HB2	1.44	1.00

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HD12	1:B:388:ILE:HG23	1.47	0.97
1:A:293:VAL:HG22	1:A:322:VAL:HG21	1.54	0.89
1:A:357:ARG:HG2	1:A:359:PRO:HD2	1.55	0.89
1:A:349:THR:HG22	1:A:351:GLU:H	1.38	0.87
1:B:466:HIS:N	1:B:467:PRO:HD2	1.90	0.87
1:A:293:VAL:HG11	1:A:468:LEU:HD11	1.57	0.87
1:B:268:THR:HB	1:B:269:PRO:HD2	1.56	0.86
1:B:293:VAL:HG22	1:B:322:VAL:HG21	1.59	0.84
1:B:263:LYS:HE3	1:B:263:LYS:HA	1.60	0.83
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.62	0.82
1:B:267:ILE:HD13	1:B:280:ARG:HG2	1.62	0.81
1:B:275:LYS:HE3	1:B:275:LYS:HA	1.62	0.81
1:B:286:GLN:HG3	2:B:644:HOH:O	1.80	0.81
1:B:451:GLN:O	1:B:454:GLN:HG2	1.79	0.81
1:A:261:LYS:HD2	1:A:261:LYS:H	1.44	0.80
1:A:212:ARG:O	1:A:216:LYS:HD3	1.82	0.80
1:B:284:GLY:O	1:B:288:ARG:HG2	1.82	0.79
1:B:430:GLN:HE21	1:B:433:ALA:HB2	1.47	0.79
1:B:476:LEU:H	1:B:476:LEU:HD23	1.50	0.77
1:A:430:GLN:O	1:A:434:LYS:HG2	1.84	0.76
1:A:249:ILE:HD12	1:A:255:LEU:HA	1.67	0.76
1:A:440:THR:HB	1:B:440:THR:HG22	1.67	0.73
1:A:348:MET:SD	1:A:353:LEU:HD21	2.28	0.73
1:B:269:PRO:HA	1:B:280:ARG:NH2	2.03	0.73
1:B:258:GLY:O	1:B:262:ILE:HG22	1.89	0.72
1:B:340:LEU:O	1:B:341:ILE:HD12	1.89	0.72
1:A:458:LYS:HB3	1:A:458:LYS:NZ	2.05	0.72
1:B:463:MET:HB2	1:B:466:HIS:HD2	1.53	0.72
1:A:349:THR:HG22	1:A:351:GLU:N	2.04	0.71
1:A:238:THR:O	1:A:240:LYS:N	2.23	0.71
1:A:270:LEU:HD13	1:A:271:GLN:N	2.06	0.70
1:B:252:MET:O	1:B:256:MET:HG2	1.92	0.70
1:A:287:PHE:O	1:A:290:VAL:HG12	1.91	0.70
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.75	0.69
1:A:244:LYS:HA	2:A:694:HOH:O	1.92	0.68
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.22	0.68
1:B:430:GLN:HG3	1:B:433:ALA:HB3	1.76	0.68
1:A:271:GLN:HE21	1:A:276:GLU:HA	1.59	0.67
1:B:270:LEU:HD22	2:B:708:HOH:O	1.94	0.67
1:B:276:GLU:CB	1:B:357:ARG:HH22	2.07	0.67
1:B:323:HIS:HE1	1:B:476:LEU:HB2	1.61	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:LYS:HE2	1:A:472:ILE:HA	1.77	0.66
1:A:296:ILE:HB	2:A:605:HOH:O	1.94	0.66
1:A:267:ILE:HB	1:A:280:ARG:CZ	2.25	0.66
1:B:267:ILE:HG12	1:B:268:THR:H	1.60	0.66
1:B:469:LEU:O	1:B:469:LEU:HD13	1.96	0.65
1:A:268:THR:N	1:A:269:PRO:HD2	2.11	0.65
1:A:265:LYS:NZ	1:A:265:LYS:HB3	2.11	0.65
1:B:270:LEU:H	1:B:280:ARG:CZ	2.09	0.65
1:A:402:ASN:HB3	2:A:675:HOH:O	1.95	0.65
1:A:293:VAL:HG22	1:A:322:VAL:CG2	2.27	0.65
1:A:437:GLN:O	1:A:440:THR:HG22	1.96	0.64
1:B:271:GLN:NE2	1:B:277:VAL:HG23	2.13	0.64
1:A:475:ASP:HB3	2:A:565:HOH:O	1.98	0.64
1:B:214:LEU:HD21	1:B:413:LEU:HD23	1.80	0.64
1:A:271:GLN:O	1:A:276:GLU:HA	1.97	0.63
1:A:475:ASP:O	1:A:476:LEU:HB3	1.99	0.63
1:A:279:ILE:HG22	1:A:283:GLN:HE21	1.63	0.62
1:A:363:PHE:CE2	1:A:456:ILE:HD11	2.34	0.62
1:B:358:LYS:N	1:B:358:LYS:HE3	2.14	0.62
1:A:336:LYS:HD3	1:A:350:ARG:NH1	2.16	0.61
1:B:430:GLN:HE21	1:B:433:ALA:CB	2.14	0.60
1:A:244:LYS:HB2	1:A:244:LYS:NZ	2.16	0.60
1:B:275:LYS:CE	1:B:275:LYS:HA	2.31	0.59
1:A:276:GLU:OE2	1:A:278:ALA:HB3	2.03	0.59
1:B:270:LEU:H	1:B:280:ARG:NH2	1.99	0.59
1:A:256:MET:O	1:A:268:THR:HG23	2.02	0.59
1:A:261:LYS:HB2	2:A:710:HOH:O	2.02	0.59
1:B:358:LYS:HB2	1:B:359:PRO:HD3	1.85	0.59
1:A:230:LYS:HE2	1:A:379:LEU:O	2.02	0.59
1:A:271:GLN:HA	1:A:280:ARG:HH12	1.68	0.59
1:B:272:GLU:O	1:B:272:GLU:HG2	2.03	0.59
1:A:359:PRO:HG2	1:A:360:PHE:CD1	2.37	0.59
1:A:259:GLU:OE2	1:A:268:THR:HA	2.03	0.58
1:A:271:GLN:NE2	1:A:277:VAL:H	2.02	0.58
1:A:336:LYS:HD3	1:A:350:ARG:HH12	1.67	0.58
1:B:279:ILE:O	1:B:283:GLN:HG3	2.02	0.58
1:B:260:ASP:HB2	1:B:269:PRO:HG3	1.85	0.58
1:B:263:LYS:CE	1:B:263:LYS:HA	2.33	0.58
1:B:454:GLN:O	1:B:457:LYS:HB3	2.03	0.57
1:A:310:ASP:OD2	1:A:312:ASN:HB2	2.03	0.57
1:B:269:PRO:HA	1:B:280:ARG:HH22	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:GLU:O	1:A:452:LEU:HG	2.05	0.57
1:B:216:LYS:O	1:B:216:LYS:HD3	2.05	0.57
1:B:471:GLU:O	1:B:474:LYS:HG3	2.05	0.57
1:A:286:GLN:NE2	1:A:465:LEU:HD12	2.19	0.56
1:A:288:ARG:HD3	1:A:289:SER:N	2.19	0.56
1:A:276:GLU:CG	1:A:279:ILE:HG12	2.36	0.56
1:A:454:GLN:O	1:A:457:LYS:HB3	2.05	0.56
1:B:271:GLN:O	1:B:272:GLU:HB3	2.06	0.56
1:A:388:ILE:HG13	2:A:693:HOH:O	2.06	0.56
1:B:358:LYS:CA	1:B:358:LYS:HE3	2.36	0.56
1:B:368:PHE:O	1:B:372:VAL:HG23	2.06	0.56
1:A:368:PHE:O	1:A:372:VAL:HG23	2.06	0.55
1:B:212:ARG:NH1	1:B:212:ARG:HB3	2.21	0.55
1:A:242:THR:O	1:A:242:THR:HG22	2.07	0.55
1:B:466:HIS:N	1:B:467:PRO:CD	2.67	0.55
1:A:357:ARG:HH12	1:A:460:GLU:CD	2.10	0.55
1:A:268:THR:HB	1:A:269:PRO:CD	2.37	0.55
1:B:473:TYR:O	1:B:474:LYS:C	2.45	0.55
1:B:271:GLN:HG3	1:B:271:GLN:O	2.07	0.55
1:A:404:LYS:HE3	2:A:567:HOH:O	2.07	0.55
1:A:275:LYS:O	1:A:280:ARG:HD3	2.07	0.54
1:A:276:GLU:HG2	1:A:279:ILE:HG12	1.88	0.54
1:B:282:PHE:O	1:B:286:GLN:HG2	2.07	0.54
1:A:440:THR:O	1:A:444:GLN:HG2	2.08	0.54
1:A:467:PRO:HB2	2:A:704:HOH:O	2.07	0.54
1:A:359:PRO:HG2	1:A:360:PHE:HD1	1.73	0.54
1:A:268:THR:H	1:A:269:PRO:HD2	1.72	0.54
1:B:267:ILE:HG12	1:B:268:THR:N	2.23	0.54
1:B:260:ASP:O	1:B:260:ASP:OD1	2.26	0.54
1:A:449:HIS:O	1:A:453:LEU:HB2	2.07	0.54
1:A:267:ILE:HD12	1:A:280:ARG:HD2	1.90	0.53
1:B:269:PRO:O	1:B:270:LEU:HD23	2.08	0.53
1:B:276:GLU:HB2	1:B:357:ARG:NH2	2.23	0.53
1:A:212:ARG:HH12	1:A:420:GLN:HA	1.74	0.53
1:A:263:LYS:HZ3	1:A:265:LYS:HG3	1.72	0.53
1:A:474:LYS:O	1:A:475:ASP:O	2.25	0.53
1:A:476:LEU:C	1:A:476:LEU:HD23	2.28	0.53
1:B:358:LYS:HE3	1:B:358:LYS:HA	1.91	0.53
1:B:273:GLN:OE1	1:B:273:GLN:N	2.42	0.53
1:B:276:GLU:HB2	1:B:357:ARG:HH22	1.72	0.53
1:A:471:GLU:C	1:A:473:TYR:H	2.11	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ILE:HG22	2:B:686:HOH:O	2.09	0.53
1:B:451:GLN:OE1	1:B:451:GLN:C	2.48	0.53
1:A:319:LYS:CE	1:A:472:ILE:HA	2.39	0.53
1:A:370:PHE:CZ	1:A:442:LEU:HD21	2.43	0.52
1:B:259:GLU:HG2	1:B:268:THR:HA	1.91	0.52
1:B:266:HIS:HE1	2:B:602:HOH:O	1.91	0.52
1:A:265:LYS:HZ2	1:A:265:LYS:HB3	1.73	0.52
1:B:273:GLN:HB2	2:B:548:HOH:O	2.09	0.52
1:A:267:ILE:HD12	1:A:275:LYS:HB3	1.92	0.52
1:A:335:ASN:HA	2:A:515:HOH:O	2.10	0.52
1:B:237:LEU:HD21	1:B:340:LEU:HG	1.91	0.52
1:B:408:ASP:HB3	2:B:558:HOH:O	2.08	0.52
1:B:256:MET:C	1:B:258:GLY:H	2.12	0.52
1:A:349:THR:HG23	2:A:691:HOH:O	2.09	0.52
1:B:275:LYS:O	1:B:280:ARG:HD2	2.09	0.52
1:B:441:ASP:O	1:B:445:ILE:HG12	2.10	0.52
1:A:230:LYS:O	1:A:234:ARG:HG2	2.10	0.52
1:A:279:ILE:HD13	1:A:360:PHE:CZ	2.46	0.51
1:B:393:LEU:O	1:B:410:GLN:HB2	2.10	0.51
1:A:370:PHE:HB2	1:A:445:ILE:HD11	1.92	0.51
1:A:383:ASP:OD2	1:A:425:HIS:HE1	1.93	0.51
1:B:230:LYS:O	1:B:234:ARG:HG2	2.10	0.51
1:B:294:GLN:HG2	2:B:611:HOH:O	2.10	0.51
1:A:270:LEU:C	1:A:270:LEU:HD13	2.31	0.50
1:A:467:PRO:HA	1:A:470:GLN:HB3	1.93	0.50
1:A:336:LYS:HE2	1:A:372:VAL:HG21	1.92	0.50
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.92	0.50
1:A:388:ILE:HG21	2:A:693:HOH:O	2.10	0.50
1:A:252:MET:HB2	2:A:666:HOH:O	2.10	0.50
1:A:262:ILE:HD12	2:A:660:HOH:O	2.10	0.50
1:B:325:ILE:CD1	1:B:388:ILE:HG23	2.30	0.50
1:A:271:GLN:NE2	1:A:272:GLU:N	2.60	0.50
1:A:288:ARG:HB2	2:A:551:HOH:O	2.11	0.50
1:A:261:LYS:N	1:A:261:LYS:HD2	2.21	0.50
1:B:271:GLN:HA	1:B:271:GLN:HE21	1.76	0.50
1:A:207:GLU:HG3	1:A:209:ALA:HB3	1.94	0.50
1:B:460:GLU:HB2	2:B:590:HOH:O	2.11	0.49
1:B:339:VAL:HG13	1:B:341:ILE:CD1	2.41	0.49
1:B:367:LYS:HZ1	1:B:449:HIS:HB2	1.78	0.49
1:B:265:LYS:HG3	1:B:265:LYS:O	2.10	0.49
1:B:465:LEU:C	1:B:467:PRO:HD2	2.33	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:C	1:A:288:ARG:HD3	2.33	0.49
1:B:411:ASP:O	1:B:415:GLN:HG3	2.12	0.49
1:B:318:LEU:HG	2:B:686:HOH:O	2.12	0.49
1:B:425:HIS:HB3	1:B:428:SER:HB3	1.95	0.49
1:B:216:LYS:HE3	1:B:220:ASP:OD2	2.13	0.49
1:A:286:GLN:NE2	1:A:465:LEU:HA	2.28	0.49
1:B:408:ASP:HA	2:B:643:HOH:O	2.13	0.49
1:A:424:ASN:C	1:A:426:PRO:HD3	2.33	0.49
1:B:448:GLU:O	1:B:451:GLN:HB3	2.13	0.48
1:A:259:GLU:HA	1:A:262:ILE:O	2.13	0.48
1:B:264:PHE:HE2	1:B:267:ILE:HG22	1.76	0.48
1:A:430:GLN:HG2	1:B:414:LEU:HD13	1.94	0.48
1:B:294:GLN:HE21	1:B:294:GLN:HA	1.78	0.48
1:B:363:PHE:HE1	1:B:449:HIS:NE2	2.12	0.48
1:A:261:LYS:HG2	1:A:262:ILE:HG13	1.93	0.48
1:A:267:ILE:CD1	1:A:275:LYS:HB3	2.44	0.48
1:A:311:LEU:HD23	1:A:311:LEU:C	2.34	0.48
1:B:463:MET:HB2	1:B:466:HIS:CD2	2.42	0.48
1:A:319:LYS:CD	1:A:472:ILE:HA	2.45	0.47
1:A:257:MET:C	1:A:259:GLU:H	2.16	0.47
1:A:275:LYS:HB2	2:A:548:HOH:O	2.13	0.47
1:A:214:LEU:O	1:A:218:LEU:HG	2.15	0.47
1:A:359:PRO:HG2	1:A:360:PHE:H	1.79	0.47
1:B:341:ILE:HG23	1:B:342:SER:N	2.30	0.47
1:B:369:GLU:HG2	2:B:727:HOH:O	2.15	0.47
1:B:243:ASP:HB3	2:B:704:HOH:O	2.14	0.47
1:A:357:ARG:O	1:A:358:LYS:C	2.53	0.47
1:A:468:LEU:C	1:A:468:LEU:HD13	2.35	0.47
1:B:434:LYS:O	1:B:437:GLN:HG2	2.15	0.46
1:B:438:LYS:O	1:B:441:ASP:HB2	2.16	0.46
1:B:457:LYS:HD2	1:B:457:LYS:O	2.15	0.46
1:A:430:GLN:HG2	1:B:414:LEU:CD1	2.45	0.46
1:B:348:MET:SD	1:B:353:LEU:HD21	2.56	0.46
1:A:264:PHE:HE1	1:A:342:SER:HB3	1.81	0.46
1:B:267:ILE:CD1	1:B:280:ARG:HG2	2.40	0.45
1:B:341:ILE:CG2	1:B:342:SER:N	2.78	0.45
1:A:458:LYS:HB3	1:A:458:LYS:HZ3	1.77	0.45
1:B:268:THR:O	1:B:270:LEU:HG	2.17	0.45
1:A:468:LEU:HD12	1:A:469:LEU:HD12	1.99	0.45
1:B:268:THR:HB	1:B:269:PRO:CD	2.36	0.45
1:B:268:THR:HG21	2:B:600:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ASN:OD1	1:B:405:PRO:HD2	2.17	0.45
1:A:276:GLU:HG3	1:A:279:ILE:H	1.81	0.45
1:B:262:ILE:HD11	1:B:345:GLN:HB2	1.98	0.45
1:A:276:GLU:OE2	1:A:357:ARG:CZ	2.65	0.45
1:A:458:LYS:HB3	1:A:458:LYS:HZ2	1.79	0.45
1:B:276:GLU:CB	1:B:357:ARG:NH2	2.78	0.45
1:B:212:ARG:HA	1:B:212:ARG:HH11	1.81	0.45
1:A:425:HIS:N	1:A:426:PRO:HD3	2.31	0.45
1:B:463:MET:CB	1:B:466:HIS:HD2	2.25	0.44
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.53	0.44
1:A:311:LEU:O	1:A:311:LEU:HD23	2.17	0.44
1:A:208:SER:O	1:A:212:ARG:HG2	2.17	0.44
1:B:319:LYS:HG3	1:B:476:LEU:HD11	1.98	0.44
1:B:277:VAL:HA	1:B:280:ARG:HD3	1.98	0.44
1:A:212:ARG:NH1	1:A:420:GLN:HA	2.32	0.44
1:B:430:GLN:NE2	1:B:433:ALA:HB2	2.24	0.44
1:B:234:ARG:HD3	2:B:554:HOH:O	2.17	0.44
1:A:453:LEU:CD2	1:A:473:TYR:CE2	3.00	0.44
1:A:336:LYS:HE2	1:A:372:VAL:HG11	1.99	0.44
1:A:238:THR:C	1:A:240:LYS:H	2.21	0.44
1:A:277:VAL:HG13	1:A:278:ALA:N	2.32	0.44
1:A:325:ILE:HD11	1:A:392:ILE:CG1	2.48	0.44
1:A:308:ASN:ND2	2:A:696:HOH:O	2.51	0.43
1:A:276:GLU:OE2	1:A:357:ARG:NE	2.51	0.43
1:A:383:ASP:OD2	1:A:425:HIS:CE1	2.71	0.43
1:A:237:LEU:HD21	1:A:340:LEU:HG	2.01	0.43
1:B:245:SER:HA	1:B:246:PRO:HD3	1.80	0.43
1:B:257:MET:O	1:B:261:LYS:HD2	2.19	0.43
1:B:217:HIS:HE1	1:B:302:SER:O	2.01	0.43
1:A:273:GLN:OE1	1:A:273:GLN:HA	2.18	0.43
1:B:340:LEU:C	1:B:341:ILE:HD12	2.39	0.42
1:A:286:GLN:HE21	1:A:465:LEU:CD1	2.32	0.42
1:B:255:LEU:CD2	1:B:277:VAL:HG13	2.49	0.42
1:B:220:ASP:O	1:B:224:LYS:HG2	2.18	0.42
1:B:237:LEU:O	1:B:239:GLY:N	2.52	0.42
1:B:296:ILE:HD12	1:B:322:VAL:HG23	2.01	0.42
1:B:476:LEU:H	1:B:476:LEU:CD2	2.26	0.42
1:B:240:LYS:O	1:B:241:THR:C	2.57	0.42
1:B:440:THR:HB	2:B:636:HOH:O	2.19	0.42
1:A:257:MET:C	1:A:259:GLU:N	2.73	0.42
1:A:471:GLU:C	1:A:473:TYR:N	2.72	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:C	1:A:276:GLU:HA	2.40	0.42
1:B:460:GLU:OE2	1:B:466:HIS:NE2	2.53	0.42
1:A:434:LYS:NZ	1:B:410:GLN:HE21	2.18	0.42
1:B:451:GLN:OE1	1:B:452:LEU:N	2.53	0.42
1:B:212:ARG:CA	1:B:212:ARG:HH11	2.32	0.42
1:B:244:LYS:HG3	1:B:244:LYS:O	2.19	0.42
1:A:434:LYS:HZ1	1:B:410:GLN:HE21	1.66	0.42
1:B:343:GLU:HG3	1:B:343:GLU:O	2.20	0.42
1:B:226:PHE:HA	1:B:227:PRO:HD3	1.92	0.42
1:B:457:LYS:O	1:B:461:THR:CG2	2.68	0.41
1:A:271:GLN:HB2	1:A:277:VAL:N	2.35	0.41
1:A:458:LYS:CB	1:A:458:LYS:NZ	2.81	0.41
1:B:437:GLN:HB2	2:B:593:HOH:O	2.21	0.41
1:B:259:GLU:OE2	1:B:267:ILE:HG23	2.21	0.41
2:A:749:HOH:O	1:B:438:LYS:HE2	2.20	0.41
1:B:240:LYS:HE3	2:B:515:HOH:O	2.21	0.41
1:A:268:THR:N	1:A:269:PRO:CD	2.81	0.41
1:A:319:LYS:HD3	1:A:472:ILE:HA	2.01	0.41
1:B:434:LYS:HA	1:B:437:GLN:NE2	2.35	0.41
1:B:253:ASN:O	1:B:257:MET:HG3	2.21	0.41
1:A:446:VAL:O	1:A:450:VAL:HG23	2.20	0.41
1:B:377:LEU:HB2	1:B:379:LEU:HD13	2.01	0.41
1:A:404:LYS:N	1:A:405:PRO:HD2	2.35	0.41
1:B:267:ILE:HD11	1:B:270:LEU:HD12	2.02	0.41
1:B:335:ASN:ND2	1:B:337:ASP:HB2	2.36	0.41
1:B:250:TYR:HD1	1:B:251:ASP:OD2	2.04	0.41
1:B:256:MET:HE3	1:B:271:GLN:HB3	2.03	0.41
1:A:349:THR:CG2	1:A:351:GLU:H	2.20	0.41
1:A:268:THR:HB	1:A:269:PRO:HD3	2.01	0.41
1:A:271:GLN:HA	1:A:280:ARG:NH1	2.35	0.41
1:A:414:LEU:CB	1:B:430:GLN:HG2	2.51	0.41
1:B:227:PRO:HG2	2:B:589:HOH:O	2.21	0.41
1:A:286:GLN:NE2	1:A:465:LEU:CD1	2.83	0.40
1:A:325:ILE:HD11	1:A:392:ILE:HG13	2.03	0.40
1:A:323:HIS:NE2	1:A:472:ILE:HD11	2.36	0.40
1:B:405:PRO:O	1:B:409:ILE:HG13	2.22	0.40
1:B:229:THR:OG1	1:B:232:LYS:HB2	2.22	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	268/270 (99%)	242 (90%)	17 (6%)	9 (3%)	5	2
1	B	268/270 (99%)	236 (88%)	20 (8%)	12 (4%)	3	1
All	All	536/540 (99%)	478 (89%)	37 (7%)	21 (4%)	4	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	GLY
1	A	272	GLU
1	A	475	ASP
1	B	237	LEU
1	B	240	LYS
1	B	272	GLU
1	B	474	LYS
1	A	267	ILE
1	A	394	SER
1	B	244	LYS
1	B	257	MET
1	B	464	SER
1	A	269	PRO
1	B	238	THR
1	B	241	THR
1	B	275	LYS
1	B	462	ASP
1	A	244	LYS
1	A	358	LYS
1	A	275	LYS
1	B	358	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	243/243 (100%)	237 (98%)	6 (2%)	55	67
1	B	243/243 (100%)	232 (96%)	11 (4%)	34	41
All	All	486/486 (100%)	469 (96%)	17 (4%)	43	53

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	LYS
1	A	271	GLN
1	A	288	ARG
1	A	396	ASP
1	A	404	LYS
1	A	458	LYS
1	B	210	ASP
1	B	228	LEU
1	B	252	MET
1	B	263	LYS
1	B	272	GLU
1	B	330	LEU
1	B	358	LYS
1	B	412	ASN
1	B	443	ARG
1	B	451	GLN
1	B	471	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	A	271	GLN
1	A	283	GLN
1	A	286	GLN
1	A	308	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	314	GLN
1	A	345	GLN
1	A	402	ASN
1	A	410	GLN
1	A	425	HIS
1	A	449	HIS
1	A	451	GLN
1	A	454	GLN
1	A	470	GLN
1	B	217	HIS
1	B	253	ASN
1	B	266	HIS
1	B	271	GLN
1	B	294	GLN
1	B	308	ASN
1	B	323	HIS
1	B	410	GLN
1	B	412	ASN
1	B	430	GLN
1	B	437	GLN
1	B	444	GLN
1	B	449	HIS
1	B	466	HIS
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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	270/270 (100%)	0.08	14 (5%)	31	30	27, 43, 82, 90	0
1	B	270/270 (100%)	0.39	28 (10%)	8	8	26, 45, 83, 93	0
All	All	540/540 (100%)	0.24	42 (7%)	16	15	26, 44, 83, 93	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	268	THR	11.9
1	B	270	LEU	11.5
1	B	269	PRO	10.5
1	B	242	THR	8.0
1	A	274	SER	7.4
1	B	271	GLN	7.1
1	B	267	ILE	7.0
1	B	274	SER	7.0
1	B	238	THR	6.2
1	A	266	HIS	5.3
1	A	269	PRO	5.2
1	B	257	MET	4.9
1	A	267	ILE	4.8
1	B	262	ILE	4.8
1	B	264	PHE	4.3
1	A	270	LEU	4.3
1	B	259	GLU	3.8
1	B	273	GLN	3.6
1	B	256	MET	3.3
1	A	264	PHE	3.3
1	A	265	LYS	3.3
1	B	465	LEU	3.2
1	B	261	LYS	3.1
1	A	273	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	475	ASP	2.9
1	B	476	LEU	2.8
1	A	271	GLN	2.8
1	B	243	ASP	2.7
1	A	240	LYS	2.5
1	B	266	HIS	2.4
1	A	244	LYS	2.3
1	B	459	THR	2.3
1	B	272	GLU	2.3
1	B	469	LEU	2.3
1	B	251	ASP	2.2
1	B	244	LYS	2.1
1	B	358	LYS	2.1
1	B	276	GLU	2.1
1	B	260	ASP	2.1
1	B	241	THR	2.1
1	A	262	ILE	2.1
1	A	241	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.